



IPA









Condensed Matter Physics

2024

8<sup>th</sup> to 11<sup>th</sup> December

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## **ABOUT AC2MP 2024**

On behalf of Association of Asia Pacific Physical Society and Indian Physics Association, department of physics at Indian Institute of Technology Patna (IITP) is pleased to invite you to attend the Asia-Pacific Condensed Matter Physics Conference 2024 (AC2MP 2024)

AC2MP 2024 is the fourth meeting of its series and aims to gather experts from field of condensed matter physics and related fields of physics from the Asia Oceanic region. Through the conference, we hope to foster international collaboration and contribute to the expansion of knowledge in the field.

The conference would be held offline at the venue of IITP located at Bihta. Bihta is a satellite town of Patna, capital city of state of Bihar. Nestled in the historical city of Patna in the State of Bihar, surrounded by cultural richness and academic excellence, it is anticipated that the active participation of attendees will enhance the conference experience and contribute significantly to the global discourse on condensed matter physics. We hope that AC2MP 2024 will provide an excellent opportunity for networking and engaging in fruitful discussions with professionals.

We sincerely welcome you to join us at the AC2MP 2024. We believe your presence and active participation will enrich the conference and contribute to the promotion of international exchange in condensed matter physics and related fields.

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Prof. T. N. Singh Director **निदेशक कार्यालय** भारतीय प्रौद्योगिकी संस्थान पटना बिहटा, पटना - 801106

**Office of the Director** Indian Institute of Technology Patna Bihta, Patna - 801106



#### Message

I am happy to know 4 days international conference on the topic "Asia-Pacific Conference on Condensed Matter Physics 2024" sponsored by DCMP, quantum design, DRDO, JEOL, NESERB, IOP Publishing, IR TECH, apctp, BARC and IPA is being organized by the Department of Physics, IIT Patna under the leadership of convenors Dr. Manoranjan Kar and Dr. Ajay D. Thakur & Secretary Dr. Soumya Jyoti Ray from 8th-11th December, 2024.

I am confident, experts, academician and researchers will deliberate upon the role of science in sustainable development in greater depth. We are happy that so many academicians and researchers are coming together to the IIT Patna campus, which will greatly improve our visibility.

I congratulate Dr. Manoranjan Kar, Dr. Ajay D. Thakur and his team and wish the conference a great success.

(Prof. T. N. Singh)

# **MESSAGE FROM PRESIDENT, AAPPS**

First, I would like to thank all members of the DCMP for the contributions to the AC2MP 2024 in Patna, India. Also, I would like to thank the leadership of IPA to organize the AC2MP 2024. I also thank the local organizers to make this event. The AC2MP conference is now becoming a chain of events rather than a single occasional event like an isolated particle. In a chain, there is history and there is a direction for the development of the condensed matter physics community of future. With more mass, the activity would accelerate its speed. I believe that AC2MP2024 will put large amount of energy for the activity of DCMP.

The DCMP now open the call for the DCMP young scientist award. As you may know, we have CN-Yang Award in AAPPS for young researchers. However, it is limited to three persons for each year. We sometime feel a frustration in the unbalance between the limited sheets and the number of excellent candidates. After more than one year of preparation, we decided to setup the DCMP young scientist award from this year. The specialty of the DCMP award is that it has two steps for selection. The review of the application documents and the presentation in AC2M P2024. We believe the judgement with direct hearing of your presentation will be very effective to select the worthy winners. Finally, I hope all participants enjoy the AC2MP2024 at Patna.

> Prof. Hiroyuki Nojiri Institute for Material Research, Tohoku University, Japan.



**Government of India** Bhabha Atomic Research Centre Trombay, Mumbai 400085, India



Dr. S. M. Yusuf, D.Sc(hc), FNA, FASc, FNASc, FTWAS(2025) Distinguished Scientist-DAE Director, Physics Group, BARC Senior Professor, Homi Bhabha National Institute President, AONSA Phone: +91 2225595608 Email: <u>smyusuf@barc.gov.in</u>

Dec 4, 2024

## MESSAGE

On behalf of the Indian Physics Association (IPA), it is my great pleasure to extend a warm welcome to all participants of the Asia-Pacific Condensed Matter Physics Conference 2024 (AC2MP 2024). The Division of Condensed Matter Physics (DCMP) was established on 1<sup>st</sup> January 2021 to promote the progress and disseminate condensed matter physics knowledge and its applications through research presentations, exchange of knowledge, and corporation among members and other academic societies in the Association of Asia Pacific Physical Society (AAPPS). Being a founding member of the DCMP, I feel proud that the AC2MP 2024, the fourth conference in the series, is being held in India. The IPA is committed to connecting the physics community of India with its global counterparts through associations with international societies. As a member of AAPPS, the IPA received communication from the Chair of the DCMP-AAPPS regarding the possibility of organizing AC2MP 2024 in India, under the IPA banner. I would like to express my gratitude to IIT Patna for accepting the bid and stepping forward as the host institution for this prestigious event.

The AC2MP 2024 aims to gather experts from the field of condensed matter physics and related communities across the Asian-Oceanic region. The topics to be covered during the conference include - 2D materials, Topological condensed matter & quantum materials, Soft condensed matter, Nano and Functional materials, Renewable Energy (Conversion & Storage), Magnetism & Superconductivity, Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators), Analytical tools in condensed matter, Artificial Intelligence and Machine learnings in Physics, Multiferroics & Heterostructures, etc. The invited talks, 71 in number, will give glimpses of recent advances in these areas. I am glad to know that there are around 200 participants from various institutes and universities for the AC2MP 2024.

AC2MP 2024 will serve as a vital platform for researchers, academics, and students to engage in meaningful exchanges of ideas, share recent advancements, and explore the latest developments in the discipline of condensed matter physics. We encourage all attendees of the AC2MP 2024 to engage in discussions, and establish meaningful collaborations.

(vii)

S M Yusuf President, Indian Physics Association & Founding member of the DCMP- AAPPS

#### MESSAGE FROM CONFERENCE ORGANISERS

#### Ladies and Gentlemen,

On behalf of the organizing committee, it is our great pleasure to welcome you to the Asia Pacific Conference on Condensed Matter Physics (AC2MP-2024) at the prestigious Indian Institute of Technology (IIT) Patna. We are delighted to host this significant event from December 8-11<sup>ch</sup>, 2024, and to have you join us for what promises to be an inspiring and productive gathering.

This conference held under the auspices of the Association of Asia-Pacific Physical Society (AAPPS)-Division of Condensed Matter Physics (DCMP) and supported by the Indian Physics Association (IPA) and the Asia-Pacific Center for Theoretical Physics (APCTP) brings together leading researchers, practitioners, and scholars from around the globe to discuss the latest advancements and innovations in the fields of Condensed Matter Physics. We are excited to provide a platform for the exchange of ideas, collaboration, and the fostering of new partnerships.

Dur program includes a diverse range of keynote speeches, technical sessions, and workshops, all designed to stimulate discussion and encourage the sharing of knowledge. We are honoured to have distinguished speakers who will share their insights and expertise, contributing to the rich academic and professional discourse. The conference will have 65 invited talks, 30 contributory oral talks, and 180 posters which will be arranged in three parallel sessions.

We are thankful to DCMP and the Association of Asia-Pacific Physics Society for giving us the opportunity to organize the prestigious event AC2MP-2024. We are grateful to SERB (ANRF), JEOL, Quantum Design, DRDO, BRNS, DCMP, NLABO, IDP Publishing, APCTP, IR TECH, Splendid Instruments, Fore Vision and IPA for the sponsorship. We would like to express our gratitude to the Hon'ble Director, Prof. T. N. Singh (IIT Patna), Head of the Department (Physics), National and International Advisory Board members, Chief guest, Guest of honour, Keynote speakers, Invited speakers and all the participants for their cooperation and support. The event won't have been possible without the constant help and hard work of the departmental members; students and research scholars, faculty colleagues and staff members, whom we can't thank enough. We are happy to see that the participants across the globe have responded to our call, and definitely, the conference will be beneficial for all of them.

We hope you will take this opportunity to engage with your peers, explore new concepts, and enjoy the vibrant atmosphere of 11T Patna. Thank you for being a part of AC2MP-2024. We look forward to a successful and memorable conference.

Warm regards,



Manoranjan Kar Convener AC2MP-2024, 11T Patna



Ajay D. Thakur Convener AC2MP-2024, IIT Patna



Soumya Tyoti Ray Secretary, AC2MP-2024, 11T Patna

# **HOD'S MESSAGE**

On behalf of the Department of Physics, it is my great pleasure to welcome you to the AC2MP 2024 Conference at the prestigious Indian Institute of Technology (IIT) Patna. We are delighted to host this significant event from December 8-11. This conference held under the



auspices of the Association of Asia-Pacific Physical Society (AAPPS)-Division of Condensed Matter Physics (DCMP), brings together leading researchers, practitioners, and scholars from around the globe to discuss the latest advancements and innovations in the fields of Condensed Matter Physics.

The Department of Physics was established and started its activity from the year 2008. The department has rich tradition of teaching and research. Currently, we offer a two-year M.Sc. program in physics, and a Ph.D. program in various fore-front research areas of experimental and theoretical physics. The department introduced a four-year B.Tech. program in Engineering Physics from 2021 and five-year dual degree B.Tech. in Engineering Physics, IIT Patna – MBA (IIM, Bodh Gaya) from academic year 2024-25 onwards. The salient features of the B.Teck. in Engineering Physics program include a solid grounding in core areas, a sound training in physics, a rich variety of electives, and an exposure to frontier technologies.

Esteemed faculty members of the department are actively involved in research and development in challenging areas of both theory and experiment. Currently, the main research emphasis of the department comprises Condensed Matter Physics, Energy Storage and Management, Quantum Physics, Quantum Technology, Optics & Photonics, Biophysics, Atomic & Molecular Physics, High-Energy Physics and Cosmology. The department has state of the art research facilities to support the academic programs and research related activities.

Warm regards,

Dr. Raghavan K. Easwaran HoD Physics

## Spin Quantum Entanglement and Quantum Technology

Prof. S M Yusuf Bhabha Atomic Research Centre, Mumbai smyusuf@barc.gov.in

Entanglement is a non-local property of quantum states, and plays a decisive role in quantum information, especially in quantum communication. We have made experimental realization of quantum entanglement of electronic spins in novel low dimensional spin systems. In my talk, I shall introduce the subject of quantum entanglement including the spin entanglement. I shall then present experimental as well as theoretical results of our several recent studies in this area. My talk will also outline the underlying physics that is responsible for the exotic spin entangled states. I will highlight the relevance of such entangled states in quantum technology. My talk will also include the current efforts on quantum technology in BARC in the backdrop of National Quantum Mission Program.

# Low dimensional Heusler alloys with phase purity and high crystalline order

A Srinivasan

Department of Physics, Indian Institute of Technology Guwahati, Guwahati – 791039 Central Institute of Technology, Kokarjhar, Balagaon, Kokrajhar – 783370

Ever since F. F. Heusler found ferromagnetism in bulk  $X_2YZ$  alloys, these alloys named after him have been prototype ternary ferromagnetic alloys with diverse applications. Discovery of ferromagnetic shape memory effect and half-metallic character in these alloys brought them more attention. Controlling the phase purity, elemental composition and atomic disorder in these alloys have always been a challenge to researchers. With increasing demand of nanomagnetic devices, there is a general interest in obtaining these alloys in low dimensional form. Thin films (2-dimensional materials) of Heusler alloys have been successfully obtained by physical vapour deposition methods. However, there has not been much success in obtaining high quality Heusler alloys in other 2-dimensional or 1dementionsal (nanowire) and 0-dimentaional (nanoparticle) forms. In this talk, Heusler alloys will be introduced and some recent advances made in the synthesis of nanoparticle, nanowire and thin film forms using facile and novel techniques would be presented with examples. For example, a facile template-less methodology developed by our group for the synthesis of highly ordered Heusler alloy nanoparticles, electrospinning based Heusler alloy nanowire synthesis and adoption of low cost electrodeposition technique for the synthesis of Heusler alloy films with some novel compositions will be discussed.

#### **Compact Pulsed Magnetic Field for Quantum Beam Experiments**

H. NOJIRI<sup>1</sup>

<sup>1</sup> Institute for Materials Research, Tohoku University, Japan \*Contact: nojiri@imr.tohoku.ac.jp

Category: Invited

Keywords: high magnetic field, X-ray, phase transition, X-FEL

Recently, the installation of a pulsed magnet has brought a new breakthrough in x-ray experiments in high magnetic fields. It expands the magnetic field range from 10-15 Tesla to\_30-50 Tesla. In such strong magnetic fields, the effect of a magnetic field is not a weak perturbation but is a cause of the intrinsic and significant phenomena in many cases. We report recent progresses in high magnetic field X-ray experiments with SR and XFEL sources.

X-ray diffraction for fundamental peaks is useful to determine the magnetic field dependence of lattice constants and volume in valence transitions in 4f-intermetallics, spin-crossover transitions in 3d-magnetic-complexes, and in charge density wave transitions. The information of x-ray diffraction is complementary with magnetostriction and sound velocity measurements. In frustrated magnets, a magnetic transition is, in many cases, accompanied with a symmetry change. Such lowering of symmetry can stabilize the related ground state by lifting the degeneracy originated from the frustration. The observation of the breaking of extinction rule by x-ray is the key to investigate such anomalies. A sizable lattice deformation is also observed in multi-ferroic, in which the local distortion of atoms generates ferroelectricity. With strong SR source, one can measure the field dependence of the Bragg peak position and intensity under a pulse field of msec- to several tens ms-pulsewidth by time-dependent measurement. This has an advantage in the capability of monitoring the field dependence continuously. However, the availability is limited by the short accumulation time for weak peaks appearing in small symmetry changes. Moreover, the observation of weak super-lattice peaks caused by electronic transitions such as CDW, Fermi surface nesting and others is very difficult in SR source. The breakthrough has been made by the combination of the high intense XFEL beam and the single shot pulsed field. A tiny CDW peaks in YBCO have been observed successfully in a single short diffraction. It will extend the application of pulsed field x-ray diffraction for systems with weak spin-charge-lattice couplings.

In this talk, the technical developments, recent examples of experiments, and the future development such as resonant scattering will be presented.

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

Rajeev Ahuja

Indian Institute of Technology Ropar, Rupnagar 140001 Punjab, India

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Department of Physics & Astronomy, Uppsala University, Uppsala, Sweden

Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modelled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent studies in the field of hydrogen storage materials & rechargeable battery research with the focus how computational material science can play an important role in search and design of new hydrogen storage materials & next generation battery materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates.

#### The initiation and evolution of research in physics in India since circa 1850:

#### A comprehension

Arun Kumar Grover\* Honorary Professor, Punjab Engineering College (Deemed to be University), Chandigarh-160012 arunkgrover@gmail.com

I shall present a personal account of research in physics in institutions all across India from the creation of three affiliating universities by the East India Company (EIC) in the mid-nineteenth century to the establishment of University Grants Commission (UGC) after independence in 1953. The first education policy to regulate school and college education in Indian sub-continent was enunciated via the Wood's dispatch (1854), after the complete annexation (1849) of Maharaja Ranjit Singh's empire spanning the North West of India by EIC. The British teachers appointed to teach science in the colleges forming the nuclei of first thee universities did not engage native students in any research activity until the enactment of common Indian Universities Act (1904) for the then five Universities of India. The said Act enjoined every university to appoint teachers and create faculties in different subjects, however, no additional support was provided to do so by the colonial government. Each university followed a different path, and it took nearly two decades to yield noticeable research output by the native teachers and their research students. Dr. J C Bose was the first native scientist to set up physics research laboratory in Presidency College Calcutta in 1894. The Indian Association of Cultivation of Science (IACS) had been set up by the medical doctor Dr. Mahendra Lal Sirkar in 1876, however, research activity in IACS was commenced by C V Raman only after 1908. The School of Physical Sciences in Calcutta got going with the innovative moves of the legendary Vice Chancellor Justice Asutosh Mukherjee.

The Indian Institute of Science (IISc.) at Bangalore had been established in 1909, however, its Department of Physics came into being after C V Raman became its Director in 1934. Meghnad Saha and S N Bose had commenced nurturing research students at Allahabad and Dacca, respectively from mid-1920s. Saha's students P K Kiichlu and D S Kothari were inducted as faculty members in the universities at Lahore and Delhi, respectively. The Physics Honours School of Panjab University Lahore got going in 1934, and the MSc. classes in Physics in Delhi University were commenced in 1942. BHU, AMU and Andhra University had also established research oriented Departments by 1940. CSIR came into being in 1942 with Shanti Swarup Bhatnagar as its first Director. Homi Bhabha's TIFR commenced operation in Bombay in December 1945, Saha's Institute of Nuclear Physics at Calcutta was eventually established by him in 1949, and Vikram Sarabhai's Physical Research Laboratory (PRL) at Ahmedabad had come into being in November, 1947, all the three institutions had received financial support from CSIR in their initial phases. UGC Chairman S S Bhatnagar and Lok sabha Member Meghnad Saha passed away in 1955 and 1956, respectively, and it donned on Bhabha as Chairman Atomic Energy Commission (AEC) and Kothari as Chairman UGC to expand and strengthen the research in Physics in institutions and universities of independent India.

## **Other Emerging Areas**

## The Nature of Eigenstates in Disordered Quantum Many-Body Systems and Some Special Random Matrix Models

Debojyoti Kundu, Amrita Ahuja, and <u>Subhra Sen Gupta</u>\* Shiv Nadar Institution of Eminence (SN IoE) - Delhi-NCR \*Contact: subhra.sengupta@snu.edu.in

#### **Category**: Invited **Keywords**: Quantum Spin Systems, Disorder, Quantum Chaos, Multifractality, Random Matrix Theory

We have studied Integrable-to-Chaotic transitions in some quantum spin models with intrinsic disorder and/or coupled to inhomogeneous random magnetic fields, as signalled by changes in both short-range and intermediate-range spectral (eigenvalue) correlations (Nearest Neighbour Spacings Distribution - NNSD, Ratio Distribution - RD, Next Nearest Neighbour Spacings Distribution - nNNSD etc.) within the Random Matrix Theory (RMT) framework [1-3]. We have also carried out a detailed analysis of corresponding eigenstates (wave functions) across the full spectral range, via a study of multifractal dimensions as well as singularity spectra in these systems [4]. Based on this study we are able to trace transitions between Ergodic and Many-body Localized (MBL) phases in these systems. It turns out that the multifractal behaviour in the quantum chaotic regime is quite complex and differs significantly from that seen in the standard RMT ensembles. A further study of certain special Random Matrix models sheds more light on the origin of this complex behaviour [5].

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[5] Amrita Ahuja and Subhra Sen Gupta\*, Non-uniform Eigenstate Multifractality in some Special Random Matrix models, (Manuscript in Preparation).

#### Rumi De

## Department of Physical Sciences, IISER Kolkata Mohanpur, Nadia 741246, West Bengal, India Email: rumi.de@iiserkol.ac.in

**Title:** The dynamics of evasion and pursuit in prey swarms and the emergence of various escape strategies during a predator attack.

Abstract: Cohesive group formation has been observed in diverse species, such as a flock of birds, a school of fishes, and a swarm of insects. In nature, swarming behavior has generally been found in search of food, for breeding, to avoid predators, etc. It is quite intriguing how a large number of individuals self-organize to form collective groups and generate complex organized patterns. In this talk, I will discuss how simple computational models, specifically self-propelled particle models, help get an insight into the underlying dynamics of a prey swarm under a predator attack. Our study shows that varying ranges of interaction strongly influence the trajectory of prey when chased by a predator. As seen in nature, diverse escape patterns emerge, such as circling, chasing, maneuvering into an arc, dividing into subgroups, and merging again into a single group to avoid the predator attack. We also find that inertia plays a pivotal role in the survival dynamics of the prey swarm. Our research reveals the existence of three distinct regimes based on the predator-to-prey mass ratio: (i) frequent chase and capture leading to the non-survival of the prey swarm, (ii) the survival regime without the capture of prey, and (iii) an intermediate regime where competition between pursuit and capture occurs, resembling an arms race as seen in natural ecosystems. Interestingly, our study demonstrates the existence of a favorable predator-prey mass ratio for efficient predation, which corroborates with the field studies.

### Luminescent Nanoparticles and Composites

#### Jitendra Sharma<sup>\*</sup>

School of Physics, Shri Mata Vaishno Devi University, Katra, UT of J&K, India

\*Contact: jitendra.sharma@gmail.com

#### Category: Invited

Keywords: Nanophosphor, polymers, nanocomposites, photoluminescence

Nanoparticles exhibiting luminescence such as photoluminescence (fluorescense and phosphorescence) and chemiluminescence etc are very commonly synthesized in the laboratory and have extensively been studied for their optical property attributes [1-3]. In order to get useful materials for different applications luminescent nanoparticles (LNs) such as gold, zinc oxide and rare-earth ions doped nanophosphors are often dispersed in suitable matrix (fluid or solid) forming bulk composites and films. Inorganic LN or nanophosphors (of oxides and nitrides etc) when doped in small fractions of activator ions of rare-earth elements could readily be synthesized by combustion. when such nanophosphors are dispersed in a suitable polymer matrix they give rise to luminescent phosphor-polymer nanocomposites (LPPNCs). Synthesis, structural characterization (XRD and TEM etc), optical (via photoluminescence and UV-Vis etc) and thermal (DSC, etc) property attributes of such LNs in general and LPPNCs in particular will be discussed.

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#### Tunning phases with pressure for strongly correlated systems

#### Rudra Sekhar Manna

#### Department of Physics, IIT Tirupati, Tirupati, Andhra Pradesh 517619, India

Phases of matter can be tuned with various parameters, viz., chemical pressure (doping), physical pressure, magnetic field etc. In this talk, I will focus mainly on the pressure driven metal-insulator transition for strongly correlated electron systems. The delicate balance between bandwidth (W) and electron correlation (U) can be tunned with pressure for a Mott metal-insulation transition. One of the prime examples is the organic charge transfer salts where such phase can be obtained with moderate pressure [1]. Another example where the metal-insulator transition is revealed is inorganic double perovskite oxide which we studied very recently. Upon applying hydrostatic pressure, the system shows a series of transitions: from antiferromagnetic insulator (AFM-I) to antiferromagnetic metal (AFM-M), and ultimately to itinerant nonmagnetic metal. The transition from AFM-I to AFM-M is concomitant with a spin-state (high-spin to low-spin) transition. Energy level diagram shows a significant modification in the crystal field splitting between Co- $t_{2g}$  and Co- $e_g$  levels, driven by the robust hybridization of Co-d and O-p orbitals [2].

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## Size Effects on Statics and Dynamics of Ferroelectric Domain Walls

Somnath Kale<sup>1</sup>, **Rohit Soni<sup>1</sup>** 

<sup>1</sup>Department of physical sciences, Indian institute of Science Education and Research Berhampur, Berhampur 760010, India

\*Presenter E-mail: rsoni@iiserbpr.ac.in

#### **ABSTRACT**

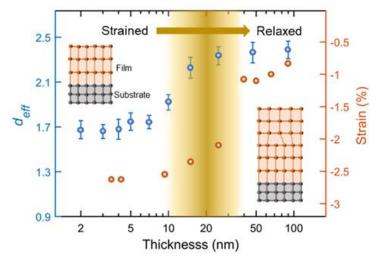
Domain walls, which separate differently oriented polarization regions in ferroelectric materials, profoundly impact nanoscale materials and device functionalities. While progress has been made in understanding the size effects on ferroelectric properties, the behavior of domain walls in ferroelectric nanostructures remains inadequately explored, limiting their potential applications. Therefore, comprehending the thickness scaling effects on ferroelectric domain wall behavior is pivotal for advancing miniaturized ferroelectric and domain wall-based devices. Here, we employ piezoresponse force microscopy to investigate the influence of epitaxial BaTiO<sub>3</sub> film thickness (from 2 to 90 nm) on the critical scaling universality of domain wall dynamical creep and static roughness exponents, including dimensionality. We independently estimate static roughness exponents within the range of 0.34-0.28, while the dynamical creep exponents transition from 0.54 to 0.22 elucidating a dimensionality transition from two- to quasi-one-dimension within the thickness range of 10 to 25 nm, which is further validated by evaluating effective and critical dimensionality inside the random-bond disorder. The observed interdimensional transition is plausibly mediated by compressive strain and long-range strain-dipolar interactions, as revealed by structural analyses and additional measurements incorporating modified substrate-induced strain. These results provide fresh insights into the understanding of size effects in nanoscale ferroelectricity, thereby paving the way for future nanodevices.

Keywords: Ferroelectric, Ultrathin, Domain Wall, Dimensionality.

Theme: Multiferroics & Heterostructures

Category: Poster/Oral

Figure/Scheme (if any, not more than one):



### Dipolar Interactions and Magnetic Anisotropy: Key Factors in Optimizing Self-Heating Efficiency for Magnetic Hyperthermia with Rare Earth-Substituted Ferrites J.P.Borah

Department of Physics, NIT Nagaland, Chumukedima-797103, India Email: jpborah@rediffmail.com

Hyperthermia is one of the cancer therapy which is considered to be an artificial way of increasing the body tissue temperature by delivering heat obtained from external sources to remotely destroy cancerous cells or prevent their further growth. The relevant physics in Ferrite-Based Magnetic nanoparticles and their response to the heat generation validates the efficacy for the approach. In single-domain superparamagnetic nanoparticles the magnetic anisotropy play an important role in modulating the energy barrier and hence heat dissipation by the magnetic nanoparticles. However, the role of magnetic anisotropy in controlling self-heating efficiency is a topic of debate. The debate surrounding the role of magnetic anisotropy in self-heating efficiency stems from the complex interplay of various factors involved in the heat generation process. Thus, understanding the physics of magnetic nanoparticles and controlling their magnetic properties represent hot topics not only for fundamental studies but also for technological applications. In this talk, I will first introduce the basic mechanism behind the magnetic hyperthermia and will discuss the effect of magnetic anisotropy to control self heating response in reference to the recent finding of rare earth substitute ferrite based magnetic nanoparticles. This lecture will combine insights into fundamental physics of magnetic nanostructures along with recent research advances in their application to magnetic hyperthermia.

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## **Exciton Dissociation by Topological Edge States**

Udo Schwingenschlögl

Physical Science and Engineering Division, King Abdullah University of Science and Technology

Contact: udo.schwingenschlogl@kaust.edu.sa

#### Category: Invited

Exciton dissociation by edge states can enhance the power conversion efficiency of solar cells. To evaluate the potential of this mechanism for carbon nanotubes as absorber material, we show that the topology of carbon nanotubes can be characterized by winding numbers related to the orbital angular momentum. The tight-binding Hamiltonian of any carbon nanotube with CN symmetry can be represented by N tight-binding Hamiltonians of decoupled molecular chains, for which a pseudospin formulation, characterized by specific paths in a two-dimensional auxiliary space, is developed. The quantum phases are given by the N winding numbers of these paths. The paths rotate in the auxiliary space when a magnetic field of varying strength is applied along the carbon nanotube, which gives rise to quantum phase transitions.

## **Two-Dimensional (2D) Materials**

## **Thermal Transport in 2D materials**

Nikhil Joseph Joy<sup>1</sup>, Ranjuna M K<sup>1</sup>, and Jayakumar Balakrishnan<sup>1</sup>

Indian Institute of Technology Palakkad \*Contact: jayakumar@iitpkd.ac.in

Category: Invited

Keywords: 2D Materials, edge thermal transport, Graphene, MoS2

The effect of phonon-boundary scattering on the thermal transport in 2D materials is less explored. Here, we explore experimentally the thermal transport near graphene edges -zig zag and arm chair [1]. The microscopic roughness at the boundaries lead to dominant diffuse reflections, there by significantly reducing the thermal conductivity- at least by 50% near the edges in our samples. The results are in good agreement with the recent theoretical predictions [2]. Finally, I will also briefly discuss our results on other 2D materials like MoS<sub>2</sub> [3].

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## Theme : Two-dimensional (2D) materials

## Utilizing Flexible MXene Composites for Photo- and Piezoelectric- Induced Surface Enhanced Raman Scattering

Monidipa Pramanik<sup>1</sup>; Mukta V. Limaye<sup>1</sup>; Parul Kumar Sharma<sup>1</sup>; Madhusudan Mishra<sup>2</sup>; Sukanta K. Tripathy<sup>2</sup>; Shashi B. Singh<sup>\*,1</sup>

- 1 Department of Physical Sciences, Indian Institute of Science Education and Research, Berhampur 760010 Odisha, India
- 2 Department of Physics, Berhampur University, Odisha 760007, India;

\*Contact: sbsingh@iiserbpr.ac.in

#### Category: Invited

*Keywords:* MXene, Surface Enhanced Raman Scattering, 2-dimansional materials, MXene Composites, Nanomaterials

Surface-enhanced Raman spectroscopy (SERS) is a powerful technique with application in biosensing, helth monitoring, food safty and environmental pollutant detection. This study introduce a synergistic approach to enhance the SERS signal of 2D Mxnene by combining photo-irradiation and electrifiled modulation. By interating Mxene with a piezoelectric polyvinylidene fluoride (PVDF) plymer, a flexible composite filem is created. This PVDF/Mxene film shows a ~10-fold increases in the SERS intensity compare to pure PVDF, with further enhancement of ~ 3.5-fold from photo-irradiation and ~ 4.5-fold from mechanical force. This approach holds promise for expanding the use of 2D Mxene in rapid, on-site sensing.

## Theme

## Title of the abstract

#### Simrandeep Kaur, Tanima Chanda, Kazi Rafsanjani Amin, Divya Sahani, Kenji Watanabe, Takashi Taniguchi, Unmesh Ghorai, Yuval Gefen, GJ Sreejith, Aveek Bid

\*Contact: aveek@iisc.ac.in

Category: Invited

Keywords: Fractional quantum Hall effect, phase transitions

Fractional quantum Hall (FQH) phases, emerging from strong electronic interactions, are characterized by anyonic quasiparticles with unique topological parameters, fractional charge, and statistics. In contrast, integer quantum Hall (IQH) effects arise from the band topology of non-interacting electrons. In this talk, I report a surprising superuniversality in the critical behavior across all FQH and IQH transitions, revealing identical critical scaling exponent  $k = 0.41 \pm 0.02$ , localization length exponent  $g = 2.4 \pm 0.2$  and the dynamical exponent  $z \approx 1$  for both. These results were obtained using ultra-high mobility trilayer graphene devices with a metallic screening layer close to the conduction channels. Previous studies on these global critical exponents were inconclusive due to significant sample-to-sample variations in measured values of k in conventional semiconductor heterostructures dominated by long-range correlated disorder. I will demonstrate that these robust scaling exponents are valid in the limit of short-range disorder correlations<sup>1</sup>.

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## **Theme: Artificial Intelligence and Machine learnings in Physics**

## Classification of Wetting States of the Droplet Placed on Rectangular Textured Surfaces Using Machine Learning

Ganesh Sahadeo Meshram<sup>1, \*</sup>, Suman Chakraborty<sup>1</sup> and Partha P Chakrabarti<sup>2</sup>

1 Department of Mechanical Engineering, IIT Kharagpur, Kharagpur, India 721302 2 Department of Computer Science & Engineering, IIT Kharagpur, Kharagpur, India 721302 \*Contact: ganeshmeshram.iitkgp@gmail.com

#### Category: Poster

Keywords: Machine learning, Classification, Wetting states, Contact angle

The accurate categorization and anticipation of wetting conditions on surfaces with texture play a crucial role in the advancement of specialty materials that possess customized characteristics suitable for various applications, such as self- cleaning surfaces, anti-fouling coatings, and fluid manipulation technologies [1]. The conventional approaches for assessing wetting states (Wenzel state, Cassie state, and Cassie-Baxter state), predominantly relying on contact angle measurements, encounter constraints in terms of operational efficiency, scalability, and responsiveness, especially when confronted with textured surfaces. The present study investigates the use of machine learning (ML) models [2] to address these obstacles, presenting an ML strategy for the automated categorization and predictive modeling of wetting phenomena on rectangular textured surfaces. The experimentation on ML models provide evidence of the accurate and effectives in properly classifying Wenzel state, Cassie state, and Cassie-Baxter state, resulting in a substantial reduction in the time and effort required compared to conventional estimation techniques. From this present study, it has been found that Random Forest and XGBoost models are found to be more accurate in classifying the surfaces based on droplet spreading.

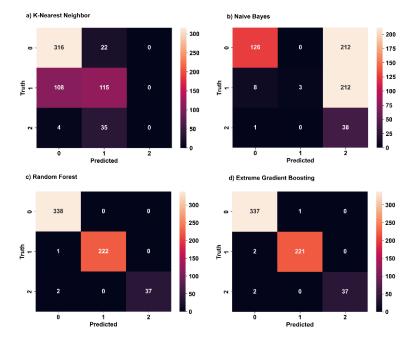


Figure 1 Confusion matrix comparison of the models. Here, 0, 1, and 2 denotes for Wenzel state, Cassie state, and Cassie-Baxter state, respectively.

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## Magnetism and Superconductivity

# Signatures of non-reciprocal supercurrent transport across Nb-Pt-Ni-Pt-Nb Josephson junctions.

Debashree Nayak, Anshuman Padhi, Tapas Senapati, and <u>Kartik Senapati</u> School of Physical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha, India-752050 \*Contact: kartik@niser.ac.in

#### Category: Invited

Keywords: (Josephson Junctions, Non-reciprocal supercurrent, superconducting spintronics)

Non-reciprocal current transport in semiconducting p-n junctions is at the heart of the present day electronics. In a similar spirit, non-reciprocal superconducting devices hold the potential of transforming the superconducting electronics and superconducting spintronics areas. Currently several routes are being explored and optimized to induce non-reciprocal supercurrent in multilayer superconducting tracks and also in superconducting Josephson devices. We will discuss a new approach based on a theoretical model proposed by Bergeret et al., which relies on asymmetric generation of spin-triplet supercurrent across a Josephson junction. We will describe our experimental attempt in this direction within the premise of the model proposed by Bergeret et al. We will present initial transport data on Nb-Pt-Ni-Pt-Nb Josephson nano-junctions fabricated via a combination of optical lithography and focused ion beam lithography. Our data shows signature of non-reciprocal transport across Josephson Junctions as a function of magnetic field.

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#### 2D Materials for Quantum and Neuromorphic Technologies

Department of Physics, Indian Institute of Science, Bangalore, Karnataka 560012 Email: aksy@iisc.ac.in

Abstract: Two-dimensional (2D) materials are relevant for optoelectronics, quantum technologies and neuromorphic computing. In this talk, I will first present a short overview of why 2D materials are interesting for both technologies and fundamental physics. I will then present our group's work on the creation of ultralow density of defects in monolayer MoS<sub>2</sub>, using ultralow energy electron irradiation, for hosting single photon emitters (SPEs) [1, 2]. We believe this is a disruptive technology for spatially deterministic creation of emitters, with potential spatial accuracy < 10 nm. I will discuss the potential defect origin, and optical properties of the SPEs. I will then discuss the concept of mixed optical-electrical signals in hBN-graphene heterostructures for next-generation defect-mediated neuromorphic computing [3].

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#### **Exploration of Spin Currents and Orbital Currents**

M. Venkata Kamalakar\*

Uppsala University, Box 516, SE-751 20 Uppsala, Sweden \*venkata.mutta@physics.uu.se

Spin-polarized currents or spin currents form the basis for present-day spintronic technologies. In recent decades, atomically thin two-dimensional (2D) materials have emerged as test beds for novel spintronic phenomena. Here, graphene is an ideal material with over tens of microns of spin transport at room temperature, up to hundreds of times longer than typical metals [1], serving as a promising platform for implementing 2D spintronic devices. Despite this potential, charge transfer and spin-orbit coupling at interfaces can induce spin relaxation, reducing spin diffusion length and spin lifetime in graphene. One obstacle to practical graphene spin circuits is the realization of large-scale fabrication with chemical vapor-deposited (CVD) graphene devices, which must withstand high current densities and provide a stable and efficient platform suitable for integrating 2D spintronic device concepts. In this talk, I will discuss our progress in addressing these challenges, in particular, our device engineering strategies to minimize contact-induced spin relaxation and obtain the highest spin parameters and extended spin communication lengths, reaching up to 45  $\mu$ m at room temperature [2], observing the highest current carrying capacity [3], and other critical effects of metal oxide layers on graphene [4], including surface passivation to enhance stability and performance [5]. I will discuss how these results contribute to flexible graphene spin devices with high diffusive spin transport [6] enabled with flexible ferromagnetic nanowires [7]. Following these developments, I will introduce direct-grown CVD van der Waals heterostructures that bring new opportunities for scalable opto-spintronic circuits and ultrafast devices [8]. Finally, I will discuss how, in addition to spin, the orbital angular momentum of electrons can also be harnessed to generate novel orbital currents, and our recent observation of nanoscale orbital accumulation [9].

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## Theme - Two-dimensional (2D) materials

## Defects-activated CDW and excitonic luminescence in 2D quantum materials

Pratap K. Sahoo\*

Ion Beam and Nanomaterials Laboratory(IBNL), School of Physical Sciences, National Institute of Science Education and Research (NISER), An OCC of Homi Bhabha National Institute, Jatni, Odisha - 752050, India.

\*Contact: pratap.sahoo@niser.ac.in

Category: Invited

Keywords: 2D materials, TiSe2, Defect, Luminescence, excitons

Understanding the excitonic properties by controlling defects in the 2D- nanomaterials is of great interest to the large community of advanced quantum materials and application groups. Depending on the doping parameters, various defects can be created and annihilated in the host matrix either by ion implantation or chemical doping that can modulate the optical, magnetic, and electronic properties of the materials. This talk emphasizes the excitonic properties of two-dimensional Titanium diselenide (TiSe2) that exhibit tunable charge density wave (CDW) order below a thermal transition scale (TCDW)  $\approx 200$  K and defect-induced ferromagnetism, as well as bandgap tunability in TiSe2 and Bi2Se3 2D materials. Low energy ion implantation was employed to introduce Au as a controlled disorder potential in TiSe2 and Bi2Se3 by the ion beam fluence. We demonstrate a notable effect of in-plane vibrational modes via excitons, where disorder enhances the temperature windows of short-range CDW correlations to 2.5 times the TCDW of the Au-free sample [1-3]. Along with that, the excitons are responsible for ferromagnetic order that is tuned with Au impurities. A qualitative model has been proposed for the experimentally observed magnetization as a function of the ion fluence, corroborated with high-resolution transmission electron microscopy. Depending on the Au nanoparticle size, magnetization saturates faster at a much lower applied magnetic field. The co-existence of CDW, excitons, and magnetism holds the potential to expand the range of 2D ferromagnetic materials for spintronic and magnetic-sensing device applications.

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#### Magnetic Properties of Fe-Pt-Co Ternary Alloys Thin Films

S. K. Srivastava\*

Department of Physics, Central Institute of Technology Kokrajhar, Kokrajhar, Assam \*Corresponding author's email address: sk.srivastava@cit.ac.in

#### Abstract

Recently FePt based films attracted the attention of the researchers due to its intriguing features such as magnetic anisotropy, high saturation magnetization, and other tunable properties, leading to their promising application in magnetic storage devices. It was further empahsized that adding a thrird transition metal elements in such materials will enhance its properties. In this work, we have deposited thin films of FePtCo ternary alloys using a DC sputtering technique. The magnetic properties of these films have been studied in a great details in a corelation to crystal structure, surface roughness and topography. Moreover, we have looked into the influence of in-situ annealing of the subtrate as well as post-annealing on its magnetic properties. These films were found to be crystallized in the face centered cubic structure and its was evident that surface roughness varies under different conditions. The in-plane and outplane magnetizationa versus field measurements indicate that these films exhibit in-plane magnetic anisotropy and the saturation magnetiz properties of these films prepared under three different conditions will be discussed.

**Keywords**: FePtCo Ternary Alloys; Thin Films; Magnetic Properties; Crystal Structure; Surface Roughness

## Mixed-Dimensional vdW Heterostructures for Integrated Analog and Digital Electronics

Bipul Karmakar<sup>1</sup>, Bikash Das<sup>1</sup>, Kapildeb Dolui<sup>2</sup>, Subhadeep Datta<sup>1,\*</sup>

<sup>1</sup> School of Physical Sciences, Indian Association for the Cultivation of Science, 2A & amp; B Raja S. C. Mullick Road, Jadavpur, Kolkata- 700032, India

<sup>2</sup> Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB30FS, United Kingdom

Email: sspsdd@iacs.res.in

## Abstract

Mixed-dimensional van der Waals (vdW) heterostructures, combining 1D and 2D materials, offer exceptional potential for unifying analog and digital electronics. These heterostructures enable precise control over electronic properties through tailored band alignments, interfacial coupling, and charge transport mechanisms. A key feature is the depletion region at heterointerfaces, which governs critical functionalities such as rectification, signal modulation, and switching. By leveraging the unique electronic, optical, and mechanical properties of 1D/2D materials, advanced components like diodes, transistors, and memory devices can be integrated seamlessly. This work highlights the pivotal role of mixed-dimensional vdW heterostructures in advancing multifunctional, next-generation electronic systems.

Reference:

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## **Theme: Quantum Materials**

## **Exploring the patterns of Entanglement within Quantum Matter**

Siddhartha Lal<sup>1,\*</sup>

1 Department of Physical Sciences, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, W.B. 741246, India

\*Contact: slal@iiserkol.ac.in

Category: Invited

Keywords: many-particle entanglement, quantum liquids

The many-particle entanglement encoded with the wavefunctions of strongly interacting states of quantum matter can offer insights that are complementary to those obtained from traditional many-body methods. I will present results obtained by us on the nature of long-range entanglement observed in various gapless (e.g., Fermi and non-Fermi liquids) as well as gapped (e.g., topologically ordered) quantum liquids that arise from strong electronic correlations. These results offer some understanding of the emergence of novel states of matter that lie beyond the Ginzburg-Landau-Wilson paradigm of broken symmetries and local order parameters.

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# **Soft Condensed Matter**

#### LOCAL RIGID CLUSTERS ENCODE MECHANICAL MEMORIES IN SHEAR-JAMMED DENSE SUSPENSIONS

Sachidananda Barik<sup>1</sup>, H A Vinutha<sup>2</sup>, and Sayantan Majumdar<sup>\*1</sup>

1 Raman Research Institute, Bangalore, India 2 Georgetown University, USA \*Contact: smajumdar@rri.res.in

#### Category: Invited

Keywords: Dense-suspensions, Rheology, Shear-jamming, memory, rigidity

Dense granular suspensions of frictional particles transform into a transient solid-like state under applied stress/strain perturbation, a phenomenon known as shear-induced jamming. Once the perturbation is removed, the system relaxes back to the liquid-like state usually within a few seconds [1]. Here we uncover a novel and unexpected memory formation in these systems, that helps the system to enhance the shear-thickening response under certain types of training. In our experiments, we report that if we repeatedly perturb the system in the same direction, the system gradually transforms to a much stronger solid-like jammed state. However, if the perturbation direction is alternatively reversed, the jammed state becomes weaker or, not reached at all. Remarkably, the same effect persists even when the time gap between the successive perturbations is much larger than the bulk stress relaxation time-scale of the system. This implies that the liquid-like state after the complete stress relaxation encodes a structural memory. Using in situ boundary imaging, we confirm that such direction-dependent enhancement/weakening of mechanical response also reflects in the shear-induced dilation behaviour of the sample. Numerical simulations suggest that such an effect originates from the gradual structural evolution of the system under repeated unidirectional perturbations. Such perturbations increase the number and size of the locally rigid-clusters and thereby enhance the strength of the solid-like jammed state. We observe that such local rigidity also plays a crucial role in stress-anisotropy and shear-reversal response of the system. Our results may open up the possibility of designing smart materials where the mechanical properties can be reversibly tuned by encoding structural memories in the system.

References:

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#### **Multiferroics & Heterostructures**

# Crystal field induced band gap tuning with enhanced energy storage in cobalt modified BiFeO<sub>3</sub>

Manoj K. Singh1, Bushra Khan<sup>1</sup>, Preeti Yadav<sup>1</sup>

<sup>a</sup>Centre of Material Sciences, University of Allahabad, Prayagraj,-211002, India \*Contact: mksingh100@allduniv.ac.in

#### Category: Invited

Keywords: Permittivity, Energy storage, Band gap, Optical electro-negativity, Magnetoelectric coupling.

Multiferroic bismuth ferrite (BiFeO<sub>3</sub>) doped with transition metal ions have been a hot topic for a few years because of their multiple functions in photovoltaic and energy storage device applications[1,2]. This study presents the intrinsic and physical characteristics of BiFeO<sub>3</sub> and BiFe<sub>0.9</sub>Co<sub>0.1</sub>O<sub>3</sub> for practical applications. The materials are synthesized by the sol-gel method. The crystal structure remains rhombohedral after doping, exhibiting variations in bond length and bond angle with iron octahedral ( $FO_6$ ) distortion. The SEM analysis revealed that the grains are similar and almost square/rectangular in shape. Compared to pure BiFeO<sub>3</sub>, the absorption peaks of the doped sample shifted towards the lower wavelength side, exhibiting an apparent blue shift along with a smaller direct optical band gap. The decrease in band gap might result from octahedral distortion of molecular orbitals of Fe-O and explained by crystal field splitting of the *d*-orbital for *Fe* and *Co* ions in BiFeO<sub>3</sub>. The incorporation of cobalt shows a 20% enhanced refractive index (n) value with two modified dominant spectral features in the visible region. A small change in optical electro-negativity was found in the doped sample. After Co doping,  $\varepsilon$  increases and *tan*  $\delta$  decreases as the frequency increases and shows high temperature dispersion due to phase transition. Cobalt-modified BiFeO<sub>3</sub> also shows relaxor-type ferroelectric behavior with enhanced the ferroelectric and ferromagnetic properties, which significantly gives high storage density  $(E_U)$  0.40 J/cm<sup>3</sup> at 30kV/cm and an efficiency of 89.21%. The high resistivity and small grain size of the cobalt modified BiFeO<sub>3</sub> exhibit high ME response which was revealed by magneto-impedance analysis; at the same time it exhibits good optical and multiferroic properties along with enhanced storage property that make it suitable for preparing flexible magnetoelectric coupling based microelectronics devices and opening up the possibility for the application in magnetophotovoltaic devices.

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### **Topological condensed matter & quantum**

# Discovery and Deep Investigation of Novel Quasiparticles in Various Quantum Systems

Junzhang Ma Department of Physics, City University of Hong Kong Contact: junzhama@cityu.edu.hk

Category: Invited / Prefer Online

Keywords: ARPES, Topological Physics, Quasiparticles, Quantum Materials

When atoms are orderly arranged into crystals, a plethora of rich and diverse quantum states emerge, such as topologically nontrivial states, superconductors, charge density waves, and various quasiparticle excitations. ARPES is an instrument that can directly probe the electronic structure of solids. It not only directly detects the single-electron spectral function in crystals but also reflects quasiparticle excitations, energy gaps and their symmetries, and the interactions between electrons and other degrees of freedom. Focusing on these scientific issues, we use the state-of-the-art ARPES to investigate the peculiar electronic structures formed by the interactions among charge, orbitals, spin, and lattice, aiming to explore novel states in condensed matter systems. In the talk, we will present our previous works of discovery and deep investigation of novel quasiparticles in various quantum systems including: The discovery and investigation of various quasiparticle fermions such as Weyl fermions in TaAs, hourglass fermions in KHgSb, three-component fermions and Fermi arcs in WC and MoP, fluctuating magnetic Weyl fermions, non-trivial magnetic Dirac fermions and axions in EuCd<sub>2</sub>As<sub>2</sub>, and unpaired singular Weyl Fermions in GaPt; Our research also extends to studying new quantum quasiparticles include investigating mobile excitons in quasi-1D metallic material TaSe<sub>3</sub>, Cooper pairs and polarons in Iron-based superconductor Ba<sub>2</sub>Ti<sub>2</sub>Fe<sub>2</sub>As<sub>4</sub>O, and different quantum novel states in Kagome metals.

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#### **Renewable Energy (Conversion & Storage)**

# Efficient Photocatalytic Green Hydrogen Production using Borophene based Nanostructures under Visible Light

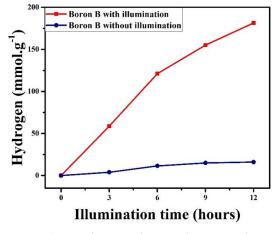
S.M. Abzal<sup>1</sup>, Kurapati Kalyan<sup>1</sup>, Sai Lakshmi Janga<sup>1</sup> and <u>Jatis Kumar Dash</u><sup>1,\*</sup> <sup>1</sup>Department of Physics, SRM University-AP, Andhra Pradesh, India-522240

\*Contact: Jatis.d@srmap.edu.in

#### **Category: Oral**

Keywords: Energy Materials, Green Hydrogen, Photo catalysis, Boron nanostructures, Hydrogen evolution

Borophene, the monolayer boron sheet, possesses a highly anisotropic surface structure, making it the lightest and thinnest elemental 2D material. Unlike graphene, borophene is predicted to exhibit a higher gravimetric hydrogen storage density. Boron demonstrates a high gravimetric hydrogen generation potential, estimated at 277 g H<sub>2</sub> per kg of B.<sup>1</sup> The application of particulate semiconductors in photocatalytic water splitting introduces a potentially scalable and economically viable technology for converting solar energy into hydrogen. Overcoming the challenge of efficiently transferring photoelectrons and photoholes for both reduction and oxidation on the same catalyst is a significant hurdle in photoca-



**Fig. 1**. Photocatalytic Hydrogen evolution comparison of dark and light conditions using Boron nanostructures.

talysis. In this context, we introduce highly efficient crystalline elemental boron nanostructures as photocatalysts, employing a straightforward and scalable synthesis method yield green hydrogen production without the need for additional co-catalysts or sacrificial agents.<sup>2</sup> The resulting photocatalyst demonstrates stability and high activity in H<sub>2</sub> production, achieving over 1% solar-to-hydrogen energy conversion efficiency (>15,000 µmol. g<sup>-1</sup>.h<sup>-1</sup>) during continuous 12-hour illumination (Fig.1). This efficiency is credited to broad optical absorption and the crystalline nature of boron nanostructures, paving the way for potential scale-up of reactors using crystalline boron photocatalysts.

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# Quasiperiodic potential induced corner states in a quadrupolar insulator

Srijata Lahiri and Saurabh Basu

Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India

The topological and localization properties of a quadrupolar insulator represented by the celebrated Benalcazar-Bernevig-Hughes model is studied in presence of a quasiperiodic disorder. While disorder is expected to disturb the existence of topological order in a system, we observe that a disorder driven topological phase emerges where the original (clean) system demonstrates trivial behavior. This phenomena is confirmed by the re-emergence of the zero energy states together with the non-trivial values of the quadrupole moment. Moreover, the distribution of the excess electronic charge shows a pattern that clearly corresponds to the bulk quadrupole topology. To elaborate upon the localization properties of the mid-band states, we compute the inverse participation and normalized participation ratios. It is observed that the in-gap states become critical (multifractal) at the point that discerns a transition from a topological localized to a trivial localized phase. Finally, we carry out a similar investigation to ascertain the effect of the quasiperiodic disorder on the quadrupolar insulator when the model exhibits topological properties in the absence of disorder. Again, we note a multifractal behavior of the eigenstates in the vicinity of the transition.

#### Reconfigurable Spin Logics and High-density Multistate Memory in a Single Spin-orbit Torque Device

#### Debangsu Roy Department of Physics IIT Ropar, Ropar, Punjab

The integration of modern artificial intelligence (AI) into various sectors has outpaced advancements in contemporary computing hardware which is based on Von Neumann architecture and leads to notable power consumption and latency issues. Analog computing, with its network of multistate memory elements, addresses these concerns by allowing parallel computing within the memory itself. Due to their non-volatility and low power consumption, spin-orbit Torque (SOT)-based memory devices are promising candidates for analogue computing[1,2]. In SOT based memory element current through a heavy metal layer can generate SOTs which can manipulate the magnetic orientation of adjacent ferromagnetic layer[3,4]. However, mechanisms for achieving multistate behaviour in SOT memory elements are often material or device-specific. Here, we explore the combined symmetry of SOT and a static DC field to stabilize multistate behaviour [5]. Further we, experimentally demonstrate reconfigurable logic operations within a single SOT device using W/Pt/Co/AlOx heterostructures [6]. Our results show that multistate tuning by SOT integration with out-ofplane magnetic field enables reconfigurable logic operations, including AND, OR, NOR, NAND, and Always ON, within a single device. Additionally, we found that careful selection of input logic operations allows multiple configurations to achieve the same logic function within a single memory device. To enhance multistate memory density, we proposed and experimentally verified a two-step writing process, achieving the highest reported multistate memory density in SOT-based memory devices. These findings highlight the potential of integrating SOT and magnetic field effects to realize high-density, multifunctional in-memory logic devices.

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# Novel high-performance differential magneto-spectroscopy techniques: results and challenges

#### Ashish Arora

Department of Physics, Indian Institute of Science Education and Research, Dr. Homi Bhabha Road, 411008 Pune, Maharashtra, India

#### Abstract.

Magneto-optical spectroscopy on 2D materials is traditionally performed by magnetophotoluminescence and magneto-reflectance spectroscopy methods. These techniques provide vital information on various aspects of 2D semiconductors and magnets such as spin-valley-layer-resolved band structure, circularly-polarized excitons and trions, magneto-valley polarization, valley coherence, and single-photon emission. However, one normally needs large magnetic fields such as B > 5 T for a reasonable signal-to-noise ratio. For measurements under low magnetic fields (B < 1 T), differential magneto-optical spectroscopy such as Faraday and Kerr effect spectroscopy is highly desirable. In this talk, I will discuss our recent developments on establishing some of these techniques (Faraday rotation, Faraday ellipticity, and spectroscopic ellipsometry). We overcome the bottleneck of long measurement times in these methods, and enhance the speed of data acquisition by two-to-three orders of magnitude using our innovations. I will describe our first results of Zeeman spectroscopy of intra- and interlayer excitons, and trions in 2D materials such as MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub>. For the first time, we are able to extract the complete dielectric tensor of these 2D materials. Many challenges are faced in the development of Kerr spectroscopy on micron scales, which will be discussed. Our work opens new paradigms to explore new spin-valley physics in 2D semiconductors and magnets using sensitive magneto-optical spectroscopy.

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#### Cation Substitution-Driven Polar Phase Engineering for High-Energy Storage and

#### **Actuator Application in Green Ferroelectrics**

Ranjan Kumar Sahu, Krishnarjun Banerjee and Saket Asthana

Advanced Functional Materials Laboratory, Department of Physics, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502284, Telangana, India

Corresponding author: asthanas@phy.iith.ac.in

#### ABSTRACT

In this invited talk, I will present a novel compositional design framework for enhancing the energy density, efficiency, and thermal stability of ceramic materials through the engineering of weakly coupled polar phases achieved by cation substitutions [1]. High-energy storage materials are essential for advancing green energy solutions, and relaxor ferroelectrics (RFEs) have emerged as promising candidates due to their exceptional dielectric properties and high-energy densities. Central to improving the performance of RFEs is citation engineering technique that allows fine-tuning of the local structure and phase transitions within the material. By adjusting the Eu-cation distribution, it is possible to enhance the formation of polar nanoregions (PNRs), which contribute significantly to the enhanced dielectric and energy storage capabilities of 1.7 J/cm<sup>3</sup> RFEs. Our approach focuses on leveraging perovskite and related structures, where precise cation substitutions induce weakly coupled polar regions, thus enabling high energy storage capabilities with minimized dielectric loss. By selectively tuning ionic radii, valency, and spatial distribution of substituted cations, we can finely control polarization dynamics and phase transitions. leading to optimized energy density and thermal resilience [2]. This weak coupling of polar domains is key to reducing energy dissipation, increasing efficiency, and providing enhanced stability under high thermal and cyclic loading conditions. An emerging focus is on ensuring biocompatibility within these materials, particularly for applications in biomedical devices and environmentally friendly energy systems. This design strategy represents a transformative pathway for next-generation capacitive materials, with implications for high-performance energy storage, advanced electronic applications, and environments demanding superior thermal endurance. I look forward to sharing these insights and discussing the potential impact of this approach on future energy-efficient ceramic technologies [3].

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# Multifunctional 2D Material-Based Sensors and Energy Harvesting Systems

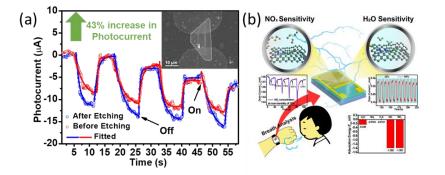
Prof. Kaushik Ghosh\*, Seema Rani, Subhabrata Das (\*kaushik@inst.ac.in)

Institute of Nano Science & Technology, Knowledge City, Sector-81, SAS Nagar, 140306, Mohali,

Punjab

Over 15 years after the first report of 2D material, Graphene and 2D material remain an active field of research considering their large surface area, excellent electrical and thermal conductivity, and abundance of catalytic sites in the field of electronic, photonic, sensing and energy harvesting. Although the layered structures demonstrate many beneficial attributes in this field, doping, functionalization, and patterning of these materials further open up a large area of research for enhancing sensitivity and active sites. Despite their potential, the challenge lies in fully harnessing these properties to develop multifunctional devices that can address complex real-world problems. One such challenge is the growing demand for advanced sensors for healthcare and environmental monitoring as well as efficient energy conversion systems towards sustainable energy solutions.

Our research has been centred on advancing the application of 2D materials and graphene-based systems, with a focus on creating integrated solutions for sensing, energy harvesting, and environmental monitoring. We explore how various stimuli influence their electrical properties, discovering that chemical vapor deposition-grown SnSe flakes exhibit negative photoconductivity. This phenomenon is attributed to the adsorption and desorption of water and oxygen molecules at the edge active sites of SnSe. By etching the flakes along their most active planes, further enhancing their photodetection capabilities (Figure 1a). Additionally, its sensitivity to humidity has been harnessed to create a highly responsive humidity sensor, which can be utilized for monitoring human respirationan important application in medical diagnostics.<sup>1</sup> To further enhance the utility of these materials, we have functionalized them with specific dopants, enabling their application in energy harvesting. SnSe, after functionalization, is used as an electrocatalyst in electrochemical hydrogen generation, showing improved catalytic performance with an overpotential decrease by several hundred millivolts. Furthermore, an on-chip microcell configuration facilitates the study of light and electric field effects on the catalytic properties and identifying the active catalytic sites. Parallelly, we developed self-powered ultrafast sensors using nitrogen-doped graphene anchored with cobalt nanoclusters (Co-N-Gr) which exhibits triboelectric nanogenerators (TENGs) not only provide exceptional sensitivity for detecting  $NO_x$  levels in human respiration but also offer the ability to differentiate respiratory conditions, such as acute exacerbations of chronic obstructive pulmonary disease (AECOPD) (Figure 1b).<sup>2</sup> This work laid the foundation for exploring the broader potential of Co-N-Gr towards energy harvesting. The hydrophilicity and enhanced charge transfer capabilities of the such doped carbonaceous system allowed us to achieve a significant increase in power generation by 108 times, particularly in environments with varying pH levels and the presence of acidic contaminants. This seamless transition from sensing to energy harvesting highlights the versatility of 2D materials as multifunctional materials capable of integrating environmental monitoring, healthcare with sustainable energy solutions.



**Figure 1.** (a) SnSe flakes show increased photocurrent after being etched along the most active plane directions; (b) Co-N-Gr template being used for detecting NO<sub>x</sub> levels and human respiration monitoring

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# Theme

## **Restarting can expedite target search**

Anupam Kundu ICTS-TIFR \*Contact: anupam.kundu@icts.res.in

#### Category: Invited

*Keywords:* Resetting, First passage, Steady State, Relaxation (maximum 5)

Stochastic resetting has recently become a subject of immense interest. Most of the theoretical studies so far focused on instantaneous resetting at a constant rate which can be a major impediment to practical realisation or experimental verification in the field. This is because in the real world, taking a particle from one place to another requires finite time and also the resetting rate would be time dependent. In this talkI will discuss possible generalisations of the existing theory by incorporating time dependent rate in the instantaneous resetting problem and also by considering non-instantaneous resetting. I will demonstrate how different features of a brownian particle, such as non-equilibrium stationary state, relaxation to it and search efficiency get affected by these generalisations.

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# Light-matter interaction driven enhanced photo-response in 2D-0D hybrid

### Atindra Nath Pal

Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Kolkata – 7000106

Two-dimensional (2D) layered materials (graphene, TMDs etc.) offer a new viable alternative to the conventional semiconductors used in 2D optoelectronics due to their promising electronic and optical properties. While graphene is considered as an outstanding channel material for a transistor due to its ultrahigh charge carrier mobility, it has limitations in the field of optoelectronics because of its gapless nature, low absorption cross-section etc. Among various possibilities, a popular strategy is to create a noble device structure by incorporating light absorbing nanomaterials like Si quantum dots, natostructured PbS, ZnO etc. into graphene. In this typical hybrid structure, graphene is used for carrier transport channel and interaction between the photosensitive material and graphene is the prime factor for the ultrasensitive photodetection. Being layered semiconductors, some members of the transition metal dichalcogenide (TMDC) family (MX2; M = Mo, W; X = S, Se) are natural partners of graphene for optically active heterostructures. In this talk, I will discuss our recent works on large area gate tunable hybrid 2D/2D or 2D/0D photo transistor devices based on graphene/TMD heterostructure. Firstly, I will discuss the effects of morphology and quantum confinement of the TMD nanostructure on the performance of the device. Then we will discuss how alloy engineering can improve the device characteristics by modifying the defect levels. Finally, I will describe how light-matter interaction mediated by exciton plasmon coupling enhances the light-absorption as well as the photo response of the large area devices. Additionally, the effect of mobile disorder, substrate and interfaces leading to low frequency noise will also be discussed.

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- 2. High performance Broadband Photodetection Based on Graphene MoS2xSe2(1-x) Alloy Engineered Phototransistors, Shubhrasish Mukherjee, Didhiti Bhattacharya, Samit Kumar Ray\* and Atindra Nath Pal\*, ACS Appl. Mater. Interfaces 2022, https://doi.org/10.1021/acsami.2c08933, arXiv:2206.15032
- 3. High-Responsivity Gate-Tunable Ultraviolet-Visible Broadband Phototransistor Based on Graphene-WS2 Mixed-Dimensional (2D-0D) Heterostructure, Shubhrasish Mukherjee, Didhiti Bhattacharya, Sumanti Patra, Sanjukta Paul, Rajib Kumar Mitra, Priya Mahadevan, Atindra Nath Pal\*, Samit Kumar Ray\*, ACS Appl. Mater. Interfaces 2022, 14, 5775-5784 (2022). https://doi.org/10.1021/acsami.1c18999; arXiv:2111.05159, 2021

# Effects of doping and nanostructuring on magnetic and thermoelectric properties of multicomponent alloys

Archana Tiwari

Department of Physics, Institute of Science, Banaras Hindu University, Varanasi 221005, India

#### **ABSTRACT:**

We explored thermoelectric properties of an aluminium-copper-iron quasicrystal (QC) nanocomposite with soft tin (Sn) phase reinforcement, revealing enhanced electrical and thermal transport properties upon annealing. The ratio of electrical and thermal conductivity for annealed QC (with 20% Sn) was found to be the highest ( $\sigma/\kappa \sim 4704$  S K/W). Owing to changes in the crystallite size, magnetic anisotropy and number of moments were also refined [1,2]. At low temperatures, these QC present weak ferromagnetic interactions. Further, research was conducted to understand how milling intensity affect the structure, morphology, magnetic, and thermoelectric properties of non-equiatomic nanostructured AlSiCrMnFeNiCu high entropy alloy (HEA) powders, which were produced by cryomilling. These powders, cryomilled at varying ball-topowder ratios (BPR), exhibited a dual-phase structure with a dominant B2-type phase and a minor  $Cr_5Si_3$ type phase. An increase in BPR resulted in more refined crystallite size, grain size, and particle size, along with reduction in the phase fraction of the minor Cr<sub>5</sub>Si<sub>3</sub>-type phase. Magnetic measurements at room temperature indicated that increase in BPR leads to a shift from multi-domain to single-domain behavior, thereby enhancing soft magnetic properties. Thermal variation of magnetization led to magnetic phase transitions, which also varied with increasing BPR. Additionally, a change in charge carrier type from p-type to n-type was observed as grain size decreased. The figure of merit decreased from 2 x 10<sup>-5</sup> for as-cast powders to the lowest value in the smallest grain-sized sample, primarily due to reduced electrical conductivity[3]. This work demonstrates the potential for developing non-equiatomic, low-density QCs and HEAs with customizable functional properties, providing flexibility in material design for magnetothermoelectric applications[4].

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#### NANO AND FUNCTIONAL MATERIALS

# Atomic Switch Networks of Ag-Ag<sub>2</sub>S Core-Shell Nanoparticles for Neuromorphic computing

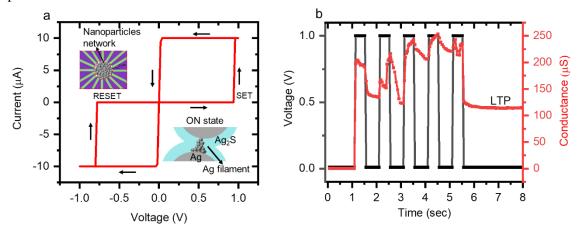
Samapika Mallik<sup>1,2</sup>, Thien Tan Dang<sup>1</sup>, Yusuke Nakaoka<sup>1</sup>, Yuki Usami<sup>1,2</sup>, Hirofumi Tanaka<sup>1,2</sup> <sup>1</sup> Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology (Kyutech), 2-4 Hibikino, Wakamatsu, Kitakyushu, 808-0196, Japan <sup>2</sup> Research Center for Neuromorphic AI Hardware, Kyutech, Kitakyushu, 808-0196, Japan \*Contact: mallik.samapika146@mail.kyutech.jp

#### Category: Invited

Keywords: Neuromorphic Computing, Atomic Switch Network, Core-Shell Nanoparticles, Synaptic Plasticity

Atomic switch networks (ASNs), made of interconnected switches, mimic synaptic plasticity and enable memory functions similar to the human brain, combining individual memristive properties with large-scale system features<sup>1</sup>. These networks play a vital role in neuromorphic computing by supporting dynamic adaptation, parallel processing, and energy-efficient computation. In this work, we demonstrate the synaptic behavior of an ASN using Ag-Ag<sub>2</sub>S core-shell nanoparticles.

Ag-Ag<sub>2</sub>S nanoparticles were synthesized using a modified Brust-Schiffrin method<sup>2</sup>. The device structure (inset, Figure 1a) features 16 electrodes with nanoparticles drop-cast into a circular gap. Figure 1a shows the typical current-voltage (I-V) characteristics of the network at room temperature. Under the sweeping of positive bias from 0 to 1 V with a voltage step of 20 mV, the device exhibited a SET process at 0.94 V from the OFF to the ON state (Inset of Figure 1a). When the voltage was swept back from 1 V to -1 V, the device RESET at -0.8 V, indicating bipolar resistive switching, which is the basis for non-volatile memories. Figure 1b shows that the increased conductance under applied voltage pulses persisted even after the pulses were removed, indicating long-term potentiation (LTP). Our results reveal stable switching behavior and quantized conductance states at integer multiples of  $2e^2/h$  (G<sub>0</sub>). Repeated voltage sweeps and pulse applications triggered a transition from volatile to non-volatile switching, analogous to the shift from short-term to long-term memory in biological synapses. By sweeping to higher voltages, we successfully achieved a longer retention time of 92 minutes, indicating the potential of the Ag-Ag<sub>2</sub>S nanoparticle network for long-term memory applications. These findings suggest that the nanoparticle network could be promising candidate for neuromorphic system development.



**Figure:** (a) I-V characteristics of the Ag-Ag<sub>2</sub>S nanoparticle network. Inset (upper left): schematic of the device structure (green: electrodes, gray: nanoparticles); lower right: schematic of the ON state. (b) Increased conductance under voltage pulses, maintained after pulse removal, demonstrating long-term potentiation (LTP).

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# Electronic Transport in two-dimensional single crystalline SnSe<sub>2</sub>

P. A. Bhobe

Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Simrol, 453 552 Indore, India Email ID- <u>pbhobe@iiti.ac.in</u>

Keywords: Two-dimensional (2D) material, Electronic transport, Metal-Insulator Transition, SnSe2

Since the discovery of graphene, interest in fundamental physics of low dimensional materials has led to development of many other layered compositions. Held together by the van der Waal's forces, these layered structures offer tuneability in band structure that shows amazing dependence on the number of layers at nanoscale. Also, the highly anisotropic character of charge and heat transport in these materials earns them the acronym as 2D materials. We have been studying one such low dimensional material that has the chemical composition as SnSe<sub>2</sub>, and belongs to the chalogenide family of compounds. It has a band gap of ~1 eV which matches with that of Si, making it a potential candidate to explore various advanced nanoelectronics device applications. We have synthesized single crystalline flakes of phase pure SnSe<sub>2</sub> and explored its electrical transport characteristics by assembling it as a FET device. Measurement of its transport characteristics bring to fore the influence of charged impurity defects on carrier density. Further, tuning the carrier density through the application of gate voltage leads to a smooth switching between insulating and metallic phases. Interestingly, we also observe metal-like characteritics in the single crystalline flakes with highly reduced thickness, and insulating behaviour in thicker flakes.

# Embracing disorder in quantum materials design

Srimanta Middey<sup>1</sup>,

1 Department of Physics, Indian Institute of Science, Bengaluru 560012

\*Contact: smiddey@iisc.ac.in

#### Category: Invited

Keywords: Compositionally complex quantum materials, local structure, magnetism, electronic transport

Many of the most exciting materials discoveries in fundamental condensed matter physics are made in systems hosting some degree of intrinsic disorder. While disorder has historically been regarded as something to be avoided in materials design, it is often of central importance to correlated and quantum materials. This is largely driven by the conceptual and theoretical ease to handle, predict, and understand highly uniform systems that exhibit complex interactions, symmetries, and band structures. In this talk, I will discuss how flipping this paradigm has enabled exciting possibilities in the emerging field of high entropy oxides (HEOs). These materials host high levels of cation or anion compositional disorder while maintaining unexpectedly uniform single crystal lattices. HEOs offer potentials for unique properties beyond traditional materials as their compositional complexity allows for the breaking of spin, charge, orbital, and magnetic exchange interaction symmetries across all length scales while maintaining a long-range crystalline order. While significant progress has been made in synthesizing HEOs with various crystal structures and exploring their potential applications, a key obstacle remains in understanding the complex interplay between their local structural distortions and physical properties. In this presentation, I will highlight our recent efforts to shed light on this aspect of HEOs using real-space and momentum space based methods.

#### Theme: Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)

#### Opportunities of ZnO@β-SiC based Memristor for Neuromorphic Computing

Bisweswar Santra<sup>1</sup>, and Aloke Kanjilal<sup>1,\*</sup>

1 Department of Physics, School of Natural Sciences, Shiv Nadar Institution of Eminence, Delhi-NCR, Gautam Buddha Nagar, UP-201314, India

\*Contact: aloke.kanjilal@snu.edu.in

#### Category: Invited

Keywords: Memristor, ZnO@β-SiC composite, thin film, Zn<sub>2</sub>SiO<sub>4</sub> nanocrystals, neuromorphic computing

The technological advancement of the memristor-based artificial synapse has attracted considerable interest for neuromorphic applications. The current memristive technology is however more promising for metal oxidebased memristors, though it requires precise structural and chemical engineering [1,2]. Here, we show a novel route for realizing electroforming free non-volatile memory devices in rf magnetron sputtering grown ZnO@ $\beta$ -SiC composite film. A switching from high resistance state to low resistance state is shown to be achieved at an extremely low voltage of ~0.1V with a set/reset switching speed of ~40/50 ns, where the device stability is found to be over 10<sup>4</sup> cycles with a retention of ~10<sup>4</sup> sec. This is shown to be associated with the formation of Zn<sub>2</sub>SiO<sub>4</sub> nanocrystals in an amorphous layer as conformed by detailed structural studies followed by chemical and microstructure analyses. This is interpreted in terms of the formation and dissolution of conductive filaments made of oxygen ions and/or zinc vacancies. Furthermore, excellent synaptic properties such as excitatory post-synaptic current, pair pulse facilitation, potentiation/depression, and long-term memory/short-term plasticity have also been established and discussed for sustainable development of the artificial intelligence with in-memory neuromorphic computing.

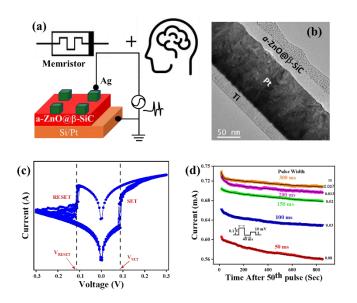


Fig. 1: (a) Schematic view of the Ag/a-ZnO@ $\beta$ -SiC/Pt memristor. (b) Cross sectional TEM image showing different layers including the ZnO@ $\beta$ -SiC composite film. (c) Typical I-V characteristic of the Ag/ZnO@ $\beta$ -SiC/Pt device in semi-logarithmic scale, where (d) shows the retention or plasticity measured after 50th number of pulse with varying pulse width.

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### **Topological condensed matter & quantum materials**

#### Field-induced strongly correlated state in BiSb

<u>Masashi Tokunaga<sup>1</sup></u>

1 The Institute for Solid State Physics, The University of Tokyo \*Contact: tokunaga@issp.u-tokyo.ac.jp

#### Category: Invited

Keywords: topological semimetal, quantum limit state, semimetal-semiconductor transition

Recent extensive research on topological semimetals has led to a paradigm shift in understanding the band electrons. Since charge carriers in these materials have small effective masses, we usually utilize the band theory, which ignores the effects of electron correlation, to describe their electronic states. We aim to introduce the electron correlation effects by applying high magnetic fields to these topological semimetals.

Applying a sufficiently high magnetic field realizes a quantum limit state where all carriers occupy only the lowest Landau subband. Further increasing the magnetic field in this state of three-dimensional materials continuously reduces the bandwidth toward zero. Therefore, a strongly correlated state is realized in a sufficiently high magnetic field in which the Coulomb interaction between carriers dominates the bandwidth. It has yet to be clarified what kind of quantum states are realized by electron correlation in the ultra-quantum limit state of three-dimensional systems [1].

We have investigated the high-field properties of  $Bi_{1-x}Sb_x$  alloys near the semimetal-semiconductor transition to realize this ultra-quantum limit state. For a topological insulator sample with  $x \sim 0.10$ , we applied a magnetic field along the trigonal axis of the crystal. The bulk band gap collapses to a semimetallic state in a magnetic field of about 11 T. We applied higher magnetic fields from this state to continuously increase the number of electrons and holes by increasing the band overlap. Then, the system exhibits an insulating behavior below  $\sim$ 4 K in a magnetic field of about 20 T (Fig. 1) [2]. This insulating behavior cannot be explained by the shift of Landau subbands, suggesting the importance of many-body effects. In this situation, the realization of an excitonic phase has long been expected [3]. Our estimation of exciton binding energy and the condensation temperatures suggests the possible emergence of the excitonic phase.

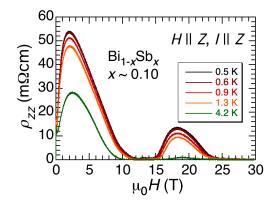


Fig. 1 Longitudinal magnetoresistace of  $Bi_{1-x}Sb_x$  with  $x \sim 0.10$ ,

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1.35

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#### Layered perovskite-type oxides for oxygen transport membrane application

Atul Kumar Agrawal, Shivendra Kumar Jaiswal\*

Department of Physics, National Institute of Technology Patna, Bihar 800-005, India.

\*Email: skj@nitp.ac.in (S. K. Jaiswal)

#### **ABSTRACT:**

Mixed ionic-electronic conductors (MIECs) have garnered a lot of consideration due to their applications in fuel cells, waste reduction, nitrous oxide storage and reduction to limit the greenhouse effect, improving fuel economic efficiency and recovery, gas sensors, oxygen pumps, capacitors, etc. [1-3]. Oxygen-deficient layered perovskites, characterized by their distinctive layered structure, are suitable for oxygen transport membrane applications due to substantial number of oxygen vacancies and improved ionic conductivity. An attempt has been made here to synthesize layered perovskite-type (YBa)(FeCu<sub>0.80</sub>M<sub>0.20</sub>)O<sub>6-δ</sub> (M = Cu, Zn, Cd, Al, Cr) oxides and characterize with regards to structural, Raman spectra, oxygen permeation properties, etc. X-ray diffraction patterns and Rietveld refinement indicate that say; (YBa)(FeCu)O<sub>6-δ</sub> exhibits tetragonal structure with space group P4/mmm. The Raman spectra also highlight some significant features. The oxygen permeability of membrane disc has been found maximum value as ~1.16 ml/cm<sup>2</sup>-min at 750 °C for (YBa)(FeCu<sub>0.80</sub>Cr<sub>0.20</sub>)O<sub>6-δ</sub> oxides (say). These findings suggest applications in oxygen separation technologies.

Keywords: Oxygen-deficient layered perovskites; X-ray diffraction; Raman spectra.

#### Acknowledgement

This work is supported by the Council of Scientific and Industrial Research (CSIR) New Delhi, India, under the grant (File number: 22 (0849)/20/EMR-II).

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# Probing Magnetic Ordering in intrinsic magnetic topological insulator, MnBi<sub>2</sub>Te<sub>4</sub> using ultrafast and THz Spectroscopy

#### N. Kamaraju

#### Department of Physical Sciences, Indian Institute of Science Education Research Kolkata Email: <u>nkamaraju@iiserkol.ac.in</u>

MnBi<sub>2</sub>Te<sub>4</sub>, an intrinsic antiferromagnetic topological insulator, has garnered significant attention due to its involvement with exotic quantum phenomena such as anomalous quantum hall effect and axion insulator state. The Fermi level of MnBi<sub>2</sub>Te<sub>4</sub> can be tuned across the bulk band gap via Sb-substitution, yielding phases with enhanced topological functionality and facilitating its implementation in device fabrication. In this study, THz time-domain spectroscopy was employed to investigate MnBi<sub>2</sub>Te<sub>4</sub> and Sbsubstituted MnBi<sub>2</sub>Te<sub>4</sub> thin films, which were grown using the pulsed laser deposition technique. THz conductivity spectra (in the 0.4-2 THz range) at various temperatures (from 7K to room temperature) were obtained from our measurements. The THz studies [1] indicate metallic behaviour for both samples, while the transport studies reveal a metallic nature for  $MnBi_2Te_4$  and a semiconducting nature for  $Mn_{1,7}Sb_{0,7}Te_4$ . The THz conductivity spectrum, fitted with a Drude-Fano-Lorentz model, reveals a strong IR active Eu phonon absorption peak and its significant changes around the Néel temperature of ~25K, indicating a coupling between magnetic ordering and electronic band structure. The frequency of the Eu phonon shows an anomalous blue-shift with increasing temperatures for both materials, more pronounced in the Sb-doped MnBi2Te4. This suggests that both anharmonicity and electron-phonon coupling contribute to the higher anomalous blue shift of phonons in Sb-doped MnBi2Te4. Additionally, pump-probe reflectivity measurements [2] reveal the presence of a Raman active A1g coherent phonon mode with normal temperature dependence.

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#### **Short Bio:**

N. Kamaraju received his PhD degree in March 2011 on ultrafast experimental condensed matter physics from Department of Physics, IISc Bangalore. After his Ph.D, he worked in the field of terahertz physics in Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin (for two years), and Department of Electrical and Computer Science Engineering, RPI, Troy, NY, USA (for one year). Later he did his final postdoctoral research in Los Alamos National labs, NM, USA on using THz to study two dimensional systems under high magnetic fields. He is now an assistant professor in Dept of Physical Sciences, IISER Kolkata, India from July 2016.

#### **RESEARCH INTERESTS:**

Ultrafast dynamics in condensed matter systems using femtosecond pump-probe spectroscopy, Nonlinear Spectroscopy, picosecond ultrasonics and time and frequency resolved terahertz (THz) spectroscopy. The pump and probe pulses range from UV, VIS, IR and THz wavelengths. Some examples of excellent candidates to use THz and femtosecond pulses are quantum materials like 2D layered materials, topological systems, strongly correlated systems and artificially created metamaterials along with energy harvesting materials. Another direction is to discover new techniques to investigate these quantum condensed matter systems.

# Theme: Analytical tools in condensed matter

# **Distribution of Charge Centers in Matter from Geometric Phases of Electrons**

Joyeta Saha, Sujith Nedungattil Subrahmanian, Joydeep Bhattacharjee\*

School of Physical Sciences National Institute of Science Education and Research (NISER) An Autonomous Institute under the Dept. of Atomic Energy, Govt. of India. Bhubaneswar, PO: Jatani, Dist: Khurda, Odisha, 752050, India

\*Contact:jbhattacharjee@niser.ac.in

#### Category: Invited

Keywords: Geometric phases, Bloch electrons, Wannier functions, chemical bonding

Based on the geometric phases of Bloch electrons, we propose a scheme for the unambiguous spatial partitioning of charge in matter from first-principles, derivable directly from the Kohn–Sham states. Generalizing the fact that geometric phases acquired by electrons, due to the evolution of their crystal momentum k in any arbitrary direction throughout the Brillouin zone (BZ), render the location of their spatial localization with net minimum spread along the direction in real space reciprocal to that of the evolution of k, we find that the total charge can be meaningfully distributed into centers of a class of correlated hermaphrodite Wannier functions simultaneously contributed by electrons with their crystal momenta evolving linearly independently through each unique k across the BZ. The resultant map of charge centers readily renders not only the qualitative nature of interatomic as well as intra-atomic hybridization of electrons but also unbiased quantitative estimates of electrons that can be associated with atoms or shared between them, as demonstrated in a selected variety of isolated and periodic systems with varying degrees of sharing of valence electrons among atoms, including variants of multicentered bonds.

**References:** 

J. Phys. Chem. C, **128**, 42, 18102–18109 (2024)

<u>7</u>38

# Ligand Tunability of Emergent Non-collinear Magnetism in Cu-based Layered Hybrid Perovskites

Debakanta Samal Institute of Physics, Bhubaneswar, Odisha, India E-mail: dsamal@iopb.res.in

Transition metal based layered organic-inorganic hybrid perovskites (OIHPs) with their diverse structure and dimensionality exhibit compelling magnetic phenomena. This talk will illustrate a notable ligand tunability of magnetism in two new quasi 2D OIHPs (C<sub>7</sub>H<sub>9</sub>NBr)<sub>2</sub>CuX<sub>4</sub> (C<sub>7</sub>H<sub>9</sub>NBr=4-Bromobenzylammonium: A, X:Cl, Br) and provide a microscopic understanding through *ab initio* DFT calculations. Despite being isostructural, the Cl and Br analogs exhibit contrasting magnetic response; while A<sub>2</sub>CuCl<sub>4</sub> shows an in-plane ferromagnetic and out-of-plane antiferromagnetic like response, A<sub>2</sub>CuBr<sub>4</sub> follows the reverse trend; strikingly though the magnetic easy axis for both the systems lie in the plane (XY-type). The underlying origin of the observed magnetism is argued to stem from Dzyaloshinskii-Moriya interaction (DMI) present in these layered systems. Based on the competition between DMI and magnetocrystalline anisotropy, a complex-canted and a transverse conical spiral spin structures are proposed for A<sub>2</sub>CuCl<sub>4</sub> and A<sub>2</sub>CuBr<sub>4</sub> respectively; which explain the observed magnetic response. Further we construct the respective H-T phase diagrams revealing the evolution to distinct magnetic phases. Essentially this study provides a framework to tailor and understand the possible occurrence of non-collinear spin textures in the above class of OIHPs.

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# Resistive transition and superconductivity in V-doped MgTi<sub>2</sub>O<sub>4</sub> spinel

# <u>Debraj Choudhury</u>

Department of Physics, Indian Institute of Technology Kharagpur.

E-mail: <u>debraj@phy.iitkgp.ac.in</u>

MgTi<sub>2</sub>O<sub>4</sub> spinel oxide exhibits a rare concomitant magnetic (spin-singlet), structural and orbitalordering (tetramer orbital ordering) transition driven by Jahn-Teller active  $Ti^{3+}(3d^1)$  ions. In presence of a complimentary Jahn-Teller active ion (V<sup>3+</sup>(3d<sup>2</sup>)) doping, V-doped  $ATi_2O_4$  spinels exhibit a rare mixed-valent (containing  $Ti^{3+}$ ,  $V^{3+}$ ,  $Ti^{4+}$  and  $V^{2+}$  ions) ground state and it exhibits current-induced breakdown of their Mott insulating state to give way to a metallic state with extremely small threshold electric fields [1]. The Mg non-stoichiometric V-doped MgTi<sub>2</sub>O<sub>4</sub> (naturally stabilized as a surface layer on top of insulating bulk samples) exhibits superconductivity with the highest T<sub>C</sub> among spinel oxides and with very high critical-magnetic field [2].

# **References:**

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[2] A. Rahaman et al. Phys. Rev. B 107, 245124 (2023)

#### Interface driven magnetization in isovalent magnate heterostructures

Surendra Singh\*

Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085 India

\*Email: surendra@barc.gov.in

The distortion of corner-sharing octahedra in isovalent perovskite transition-metal oxide interfaces have proven to be an excellent way to tailor the electronic and magnetic properties of their heterostructures. The BO<sub>6</sub> oxygen octahedra, which are intimately correlated to orbital, charge, and spin order in perovskite oxides, enable the structural distortion by decreasing the B-O-B bond angles ( $\beta$ ) and increasing the B-O bond lengths (d). These structural modifications lead to a decrease in the electronic bandwidth (W), and directly change the electronic and magnetic properties. In the case of ABO<sub>3</sub> heterostructures, which offer additional means to tune the lattice structure, the oxygen octahedral rotation can be regulated either by interfacial strain or by interfacial oxygen octahedral coupling (OOC). The coexistence of phases (phase separation) is another important properties of complex oxide (isovalent manganites), which can be influenced by the non-uniform distribution of the B-O-B bond angles in chemically homogeneous systems. Here, I will discuss strong and asymmetric magnetic phase separation across the interfaces of isovalent La<sub>0.67</sub>Ca<sub>0.33</sub>MnO<sub>3</sub> (LCMO)/La<sub>0.67</sub>Sr<sub>0.33</sub>MnO<sub>3</sub> (LSMO) heterostructures due to modification in the octahedral rotations at the interfaces. Combining intrinsic property of polarized neutron reflectivity with other complementary techniques, which provide insight into the rich spectrum of phenomena present at the interfaces of complex oxide films, we will discuss evolution of asymmetric magnetism and magnetic phase separation across the transition temperature of LCMO [1, 2].

[1] Y. Kumar et al., Physical Review B 108, 174410 (2023).[2] S. Singh et al., unpublished (2024).

#### **Bimerons in Magnetic Topological Materials**

Oleg. A. Tretiakov<sup>1</sup>

<sup>1</sup> School of Physics, University of New South Wales, Sydney, Australia \*Contact: o.tretiakov@unsw.edu.au

Category: Invited

Keywords: Bimerons, skyrmions, Dzyaloshinskii-Moriya interaction, ferromagnets, antiferromagnets

I will discuss topological magnetic textures, such as skyrmions, half-skyrmions (merons), and bimerons, which constitute tiny whirls in the magnetic order. They are promising candidates as information carriers for next generation electronics, as they can be efficiently propelled at very high velocities employing current-induced spin torques [1]. First, I will talk about bimerons [2] in ferromagnetic systems coupled to heavy metals and topological materials. Then I will show that antiferromagnets can also host a variety of these textures, which have gained significant attention because of their potential for terahertz dynamics, deflection free motion [3], and improved size scaling due to the absence of stray fields. Finally, I will demonstrate that topological spin textures, merons and antimerons, can be generated at room temperature and reversibly moved using electrical pulses in thin film CuMnAs, a semimetallic antiferromagnet that is a test-bed system for spintronic applications [4].

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# Enhancing the performance of topological photonic devices through artificial intelligence

Abhishek Kumar<sup>1,2</sup> <sup>1</sup>International Centre for Materials Science (ICMS) <sup>2</sup>Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru abhishekkumar@jncasr.ac.in

Artificial intelligence (AI) is the most important new methodology in scientific research providing innovative, low-cost solutions for complex problems across various disciplines. In photonics, AI is particularly valuable, as it enables exploration beyond physical intuition and allows to explore the parameter space more efficiently to design and optimize the photonic devices with enhanced functionalities. Recently, topological photonic has emerged as promising candidate for developing on-chip photonic devices due to negligible scattering and bending losses. In this talk, I will show how AI based tools can be used to optimize and design the topological photonic devices with remarkable performance for high-speed on chip communication for 6G communication.

# Synthesis of Cu/CuO nanoparticles using laser ablation: effect of fluence and solvents

Rajesh Rawat<sup>a</sup>, Archana Tiwari<sup>b</sup>, Nimmala <u>Arun<sup>c</sup></u>, S.V.S Nageswara Rao<sup>c</sup>, S.Venugopal Rao<sup>d</sup>, A.P.Pathak<sup>e</sup>, Ajay Tripathi<sup>a</sup>, <sup>a</sup>Department of Physics, Sikkim University, Sikkim, Gangtok 737102, India

<sup>b</sup>Department of Physics, Banaras Hindu University, Varanasi, Uttar Pradesh

221005, India <sup>c</sup>Centre for Advanced Studies in Electronics Science and Technology (CASEST), School of Physics, University of Hyderabad, Hyderabad 500046, India

<sup>d</sup>Advanced Center of Research in High Energy Materials (ACRHEM), University of Hyderabad, Hyderabad 500046, India

<sup>e</sup>School of Physics University of Hyderabad, Hyderabad, 5000046, India E-mail: atripathi@cus.ac.in

#### Abstract:

Copper (Cu) being cheaper and had a vast potential in the field of medical and optical applications. In the present work, Cu/CuO nanoparticles were synthesized by ablating Cu target using nanosecond pulsed laser operating at 1064 nm with 8 ns pulse duration in three different solvents viz: ethylene-glycol (EG), deionized water (DI) and ethanol (Eth). The effects of these solvents at different laser fluence were investigated to study the stability and morphological transformation of nanoparticles using microscopic and spectroscopic techniques. We found that the along with the laser fluence, the physical properties of solvents (like viscosity, conductivity, polarity, and enthalpy) used in laser ablation also plays crucial role in shaping the morphology of these nanoparticles. In EG and DI, we have observed droplets like features (like a tadpole and necklace-like structure) of nanoparticles (as shown in figure 1) whereas in Eth hollow structure nanoparticles were observed. The growth mechanism of these morphologies during laser ablation will be discussed elaborately, which is the main highlight of the present work. In addition, on monitoring the sample for a long time we have seen the effect of polarity and dielectric constant of the solvent on the stability of Cu/CuO nanoparticles. This systematic study is expected to find application in the synthesis of nanostructures by tuning laser and liquid parameters.

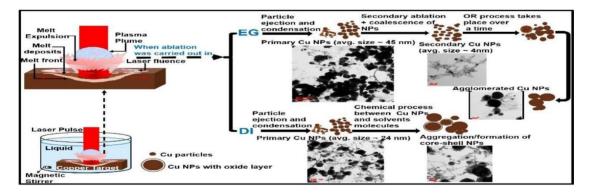


Figure 1 Schematic growth kinematics of Cu target ablated in EG and DI at a high laser fluence of 40 J/cm<sup>2</sup>

# Frustrated magnetism in 3d and 5d-based triple perovskite materials

T. Dey

Department of Physics, IIT (ISM) Dhanbad, Jharkhand -826004

Triple perovskite materials with the general formula  $A_3BM_2O_9$  provide an exciting platform for exploring quantum magnetism due to their unique structural and electronic properties. In these compounds, A is typically a nonmagnetic cation from the alkaline earth group (Group II), while B and M are magnetic ions from the d- or f-block elements. The B and M ions form an edge-sharing triangular lattice in the ab-plane, which can lead to magnetic frustration when these ions carry a magnetic moment. This frustration can give rise to novel phenomena like spin liquid behavior. We have synthesized both polycrystalline and single-crystalline samples of various  $A_3BM_2O_9$  compounds, incorporating a range of 3d and 5d magnetic elements, and have studied their structural and magnetic properties. In this presentation, I will discuss the novel magnetic behavior behaviors observed in some of these materials.

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# Quantum oscillations in the magnetization and density of states of

an interacting insulator

Abhisek Samanta<sup>1</sup>, Mohit Randeria<sup>1</sup> and Sumilan Banerjee<sup>2\*</sup>

1 Department of Physics, The Ohio State University, Columbus 43210, USA 2 Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India \*Contact: sumilan@iisc.ac.in

Category: Invited

Keywords: Kondo insulators, quantum oscillations

The Fermi surface, the defining characteristic of metals, leads to oscillatory behavior of various observables as a function of the inverse of magnetic field. It was thus a great surprise when such oscillations were seen in insulators without any Fermi surface, like in Kondo insulators. I will first briefly discuss a general theory [1] of quantum oscillations (QOs) in non-interacting hybridization-gap insulator and show that it exhibits distinct frequencies for Shubnikov deHass (SdH) and deHass-van Alphen (dHvA) oscillations for low-energy density of states and magnetization oscillations, respectively, unlike in a metal. Kondo insulators are, however, strongly correlated systems where the interaction effects cannot be a priori ignored. We generalize the periodic Anderson model to a solvable Sachdev-Ye-Kitaev (SYK)-like interactions for the f-electrons and study the effects of interactions, there are striking differences between SdH and dHvA oscillations, with the SdH amplitude strongly enhanced due to the renormalization of the effective gap. We also present an asymptotic low-temperature analysis to complement and analytically understand our numerical results.

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# Calcium Oxide nanoparticles prepared form waste Egg shell for potential applications from Semiconductor Electronics Material, Nano Medicine to Purification of water.

Dr. Rakesh Kumar Singh Head, School of Nanoscience and Nanotechnology Aryabhatta Knowledge University, Patna, Bihar, India Mail-rakeshsinghpu@gmail.com

Calcium oxide nanoparticles obtained from waste eggshell materials have several advantages, including non-toxicity to humans, green approach cost-effectiveness preparation, and its uses in energy & environment. The conversion of waste into wealth, knowledge and functional nanomaterials are prime focus of Government for sustained development. Prepared Calcium base Nano scale Powder from waste eggshell of Hen and its Physical properties are measured using modern scientific tools- XRD, SEM, Uv-Visible, FTIR, PL and Vibrating sample magnetometer for its multifunctional applications. The crystalline sizes are found less than 100 nm. Lemon juice/butter milk was used as an important ingredient in the preparation of these materials and no hazard gases emitted during preparation. Uv-Visible-NIR measurement indicates high energy band gape between 5-5.5 eV range, which are useful as semiconductor nanomaterials. Further this material emitted light in visible range upon excitation by LASER source, which supports its possible applications in optoelectronics devices. The antimicrobial studies showed prepared Cao as nanomedicine and is more effectual antifungal agent. Further prepared materials are found to remove arsenic from water, which highlights its applications in purification of water. Arsenic is major pollutant material in water, which causes various disease across the globe. In this talk I will discuss these functional properties of Calcium based nanomaterials obtained from waste egg shell reported by our research group at Nanoscience and nanotechnology center of Aryabhatta Knowledge university, Patna and by researcher at global level.

#### Catalogue of topological electronic materials and exploration of topological phonons

Tiantian Zhang Institute of Theoretical Physics, Chinese Academy of Sciences Contact: ttzhang@itp.ac.cn

Keywords: high-throughput calculation, topological material database, topological phonon

Topological materials play a crucial role in advancing the understanding of topological phases of matter, attracting significant attention in both fundamental and applied research. However, historically, identifying such materials has been coincidental. Collaboratively, <u>Zhang et al.</u> have devised comprehensive mappings from symmetry data to topological features (topological invariants, configurations, surface states, etc.), alongside developing symmetry-based indicator formulas for 230 space groups. Subsequently, <u>Zhang et al</u>. have developed an efficient algorithm capable of diagnosing all nonmagnetic materials in the database through highthroughput calculations [1], revealing that 24% of natural materials are topological. In the first part of the talk, <u>Zhang</u> will introduce her contributions to accelerating the discovery process of topological materials, and pioneering the establishment of the world's first searchable online database for topological materials, as depicted in Fig. 1.

<u>Zhang et al</u>. introduced topological band theory into the solid-state phonon spectrum and developed a method to calculate phonon topological invariants and surface states from first principles. <u>Zhang et al</u>. also proposed that topological information for phonons is encoded in the dynamical structural factor, detectable via x-ray or neutron scattering. In the second part of this talk, <u>Zhang</u> will introduce how to use this approach to successfully predict different topological phonon materials, including FeSi [2], BaPtGe, and MoB2 [3], all of which were experimentally validated.



Figure 1: Nonmagnetic topological material database<sup>[1]</sup>. (http://materiae.iphy.ac.cn/)

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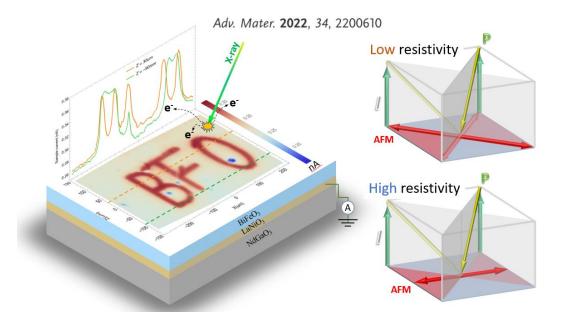
#### Study of Néel Vector in Room Temperature Multiferroic BiFeO<sub>3</sub>

Chang-Yang, Kuo

Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, 30010 Taiwan \*Contact: changyangkuo@nctu.edu.tw

#### Keywords: Spintronics, Optoelectronics, Sensors, Multiferroics

Multiferroics are materials in which two or more ordering parameters coexist and are coupled with each other. These coexisting order parameters and their inherent couplings form a rich playground, enabling the manipulation of intriguing properties to develop new functionalities. BiFeO<sub>3</sub>, which exhibits both ferroelectric and antiferromagnetic orders simultaneously at room temperature, has garnered significant attention over the last few decades due to its potential applications in multifunctional spintronic devices. However, most studies have predominantly focused on its ferroelectric properties, leaving its antiferromagnetic characteristics relatively underexplored. In this talk, I will present a systematic investigation of the Néel vector in epitaxially strained BiFeO<sub>3</sub> thin films. I will also propose strategies for controlling the Néel vector, highlighting their potential impact on future applications.



### Topological condensed matter & quantum

# Discovery and Deep Investigation of Novel Quasiparticles in Various Quantum Systems

Junzhang Ma

Department of Physics, City University of Hong Kong Contact: junzhama@cityu.edu.hk

Category: Invited / Prefer Online

Keywords: ARPES, Topological Physics, Quasiparticles, Quantum Materials

When atoms are orderly arranged into crystals, a plethora of rich and diverse quantum states emerge, such as topologically nontrivial states, superconductors, charge density waves, and various quasiparticle excitations. ARPES is an instrument that can directly probe the electronic structure of solids. It not only directly detects the single-electron spectral function in crystals but also reflects quasiparticle excitations, energy gaps and their symmetries, and the interactions between electrons and other degrees of freedom. Focusing on these scientific issues, we use the state-of-the-art ARPES to investigate the peculiar electronic structures formed by the interactions among charge, orbitals, spin, and lattice, aiming to explore novel states in condensed matter systems. In the talk, we will present our previous works of discovery and deep investigation of novel quasiparticles in various quantum systems including: The discovery and investigation of various quasiparticle fermions such as Weyl fermions in TaAs, hourglass fermions in KHgSb, three-component fermions and Fermi arcs in WC and MoP, fluctuating magnetic Weyl fermions, non-trivial magnetic Dirac fermions and axions in EuCd<sub>2</sub>As<sub>2</sub>, and unpaired singular Weyl Fermions in GaPt; Our research also extends to studying new quantum quasiparticles induced by electron-electron or electron-boson coupling in condensed matter. Examples of such studies include investigating mobile excitons in quasi-1D metallic material TaSe<sub>3</sub>, Cooper pairs and polarons in Iron-based superconductor Ba<sub>2</sub>Ti<sub>2</sub>Fe<sub>2</sub>As<sub>4</sub>O, and different quantum novel states in Kagome metals.

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### MAGNETISM & SUPERCONDUCTIVITY

#### **Evidence for multigap superconductivity in the Dirac semimetal PdTe**

<u>Amit Vashist<sup>1</sup></u>, Bibek Ranjan Satapathy<sup>1</sup>, Harsha Silotia<sup>1</sup>, Yogesh Singh<sup>2</sup>, and S. Chakraverty<sup>1</sup>

<sup>1</sup>Quantum Materials and Devices Unit, Institute of Nano Science and Technology, Sector-81, Punjab, 140306, India. <sup>2</sup>Department of Physical Sciences, Indian Institute of Science Education and Research Mohali, Sector 81, S. A. S. Nagar, Manauli, PO: 140306, India

\*Contact: amitvashist42@gmail.com

#### Category: Oral

Keywords: Dirac semimetal, Unconventional superconductor, dHvA oscillation

PdTe is a type-II superconductor and has recently been identified as a Dirac semimetal, which has generated significant research interest as a potential candidate for unconventional superconductivity based on ARPES measurement [1]. There are conflicting reports on whether it is a strongly or weakly coupled superconductor, depending on the quality of the crystals. The ARPES measurements also claimed it as a bulk nodal gap superconductor, which is in contrast to the recent thermal measurements, where it has been shown to be a multigap superconductor [2]. We use electrical transport and magnetization measurements to investigate the superconducting and Fermi surface properties of PdTe. The anisotropy in the upper critical magnetic field has been observed depending on the direction of applied magnetic field. The magnetic field vs temperature (H - T) phase diagram extracted using resistivity data shows an upward curvature similar to several multigap superconductors. Magnetization measurements show the presence of de Haas-Van Alphen (dHvA) oscillation. The Fourier transform of quantum oscillations revealed the presence of two Fermi pockets. Moreover, Landau fan diagram for a small Fermi pocket confirms the presence of non-trivial Beery phase  $\pi$ , consistent with the Dirac nature of PdTe.

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# Enhancing the hot corrosion resistance of nickel-based superalloy in real service environment via hafnium oxide nano-coating

Falak, Asif, Yousuf Digoo, Akeel Altaf Raja, Syed Suwaid Bukhari, Shafaq Ashraf Lone, Atikur Rahman\*

Department of Metallurgical and Materials Engineering, National Institute of Technology Srinagar, Hazratbal, Srinagar 190006, India

\* Corresponding Author: atikurrhmn@nitsri.ac.in

#### Abstract

In situ, analysis was conducted to analyse the behaviour of bare Superni 750 and HfO<sub>2</sub> coated Superni 750 superalloys in a medical waste incinerator. The study was conducted at  $850^{\circ}C \pm 50^{\circ}C$  for 1000 hours. The magnetron sputtering method was used to deposit the HfO<sub>2</sub> coating. The surface morphology of the hot corroded samples was determined with Scanning Electron Microscopy (SEM) analysis and elemental composition was ascertained with Energy Dispersive Spectroscopy (EDS). The phases present were identified using X-ray Diffraction (XRD). Weight changes were recorded to estimate the corrosion rate. The hot corrosion rate of the bare sample was found to be seven times higher than that of the coated sample. Based on this information, it can be concluded that the coated sample shows more corrosion resistance than the bare sample. The enhancement of oxidation resistance can be attributed to the presence of HfO<sub>2</sub>, which acts as a barrier between the environment and the underlying material. Moreover, the reduction in corrosion rate in the coated sample can be attributed to the presence of chromic oxide (Cr<sub>2</sub>O<sub>3</sub>) and spinel MgFe<sub>2</sub>O<sub>4</sub>. Corrosion resistance is further enhanced by spinel oxide NiCrMnO<sub>4</sub> which aids in the formation of a compact and adherent oxide scale.

Keywords: Incinerator, HfO<sub>2</sub> Coatings, Hot corrosion, Nano Structured coatings.

#### **Topological Properties in a Curved Space-Time Su-Schrieffer-Heeger Model**

Priyanuj Rajbongshi<sup>1</sup> and Ranjan Modak<sup>1</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517619, India

email: ph24d004@iittp.ac.in

Category: Poster

keywords: Su-Schrieffer-Heeger, topology, spacetime, symmetry, curvature.

The Su-Schrieffer-Heeger (SSH) model, a prime example of a one-dimensional topologically nontrivial insulator, has been extensively studied in flat space-time. However, the impact of curvature and gravitational effects on the topological properties of such systems remains an open question. In recent times, a lot of studies have been conducted to understand the low dimensional quantum material in curved spacetime by constructing synthetic gravitational event horizons. Here, we investigate the Curved Spacetime (CST) version of the SSH model by introducing a position-dependent hopping parameter, which includes the warping degree of spacetime in the Hamiltonian. We then observe the energy eigenvalues and probability densities, which are different from the flat spacetime counterpart, we also calculate the local topological marker for the lattice sites which indicates the CST version is also topologically nontrivial, thus calculating various other topologically invariant quantities such as winding number. We also observe the symmetries, such as whether the CST version of the SSH model belongs to the BDI symmetry class or not and how the traditional flat spacetime symmetries react to the nontrivial curvature. Our study will open the door to a whole novel class of curvature-adjustable topological quantum materials with its potential application and usage in a wide range of areas, including quantum computation and communication.

I.

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# Singlet, triplet, and mixed all-to-all pairing states emerging from incoherent fermions

Jagannath Sutradhar<sup>1,2, \*</sup>, Jonathan Ruhman<sup>1</sup>, and Avraham Klein<sup>2</sup> <sup>1</sup>Department of Physics, Bar Ilan University, Ramat Gan 5290002, Israel <sup>2</sup>Physics Department, Ariel University, Ariel 40700, Israel

\* sutradj@biu.ac.il

#### Category: Oral

Keywords: Superconductivity, all-to-all pairing, strongly correlated electrons, Y-SYK model

*Abstract:* The electron-electron and electron-phonon coupling in complex materials can be more complicated than simple density-density interactions, involving intertwined dynamics of spin, charge, and spatial symmetries. This motivates studying universal models with complex interactions, and whether BCS-type singlet pairing is still the "natural" fate of the system. To this end, we construct a Yukawa-SYK model with nonlocal couplings in both spin and charge channels. Furthermore, we provide for time-reversal-symmetry breaking dynamics by averaging over the Gaussian Unitary ensemble rather than the Orthogonal ensemble. We find that the ground state of the system can be an orbitally nonlocal superconducting state arising from incoherent fermions with no BCS-like analog. The superconductivity has an equal tendency to triplet and singlet pairing states separated by a non-Fermi liquid phase. We further study the fate of the system within the superconducting phase and find that the expected ground state, away from the critical point, is a mixed singlet/triplet state. Finally, we find that while at Tc the triplet and singlet transitions are dual to one another, below Tc the duality is broken, with the triplet state more susceptible to orbital fluctuations just by its symmetry. Our results indicate that such fluctuation-induced mixed states may be an inherent feature of strongly correlated materials. A summary of our model and result are shown in the figure below.

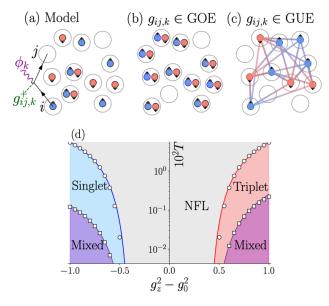


FIG. (a) Schematic of our model Hamiltonian. *N* fermionic orbitals (circles) coupled to *M* Bosons (wiggly line) via random coupling  $g_{ij,k}$ . The scattering occurs both in density ( $\sigma_0$ ) and spin channel ( $\sigma_z$ ) with variances  $g_0^2$  and  $g_z^2$ . (b) Earlier studies averaged  $g_{ij,k}$  over the GOE leading to intra-orbital singlet pairing. (c) In our study  $g_{ij,k}$  drawn from GUE results in an all-to-all inter orbital pairing. (d) The phase diagram for our model.

# **Topic: Topological condensed matter & quantum materials**

# Robustness of the Half-metallic Behavior under Disorder in Co<sub>2</sub>MnAl System

Subhadeep Datta<sup>1, \*</sup>, Sayari Ghatak<sup>1</sup>, and Dinesh Topwal<sup>1</sup> <sup>1</sup>INSTITUTE OF PHYSICS, P.O.: Sainik School, Bhubaneswar - 751005, INDIA \*Contact: subhadeep.d@iopb.res.in

## Category: Oral

Keywords: Heusler alloy, order-disorder, half metallicity, magneto-transport.

We are exploring the robustness of the half-metallic behavior under disorder in the Co<sub>2</sub>MnAl Heusler system as disorder plays a crucial role in governing various physical properties [1]. Cu<sub>2</sub>MnAl-type FCC L2<sub>1</sub> ordered full Heusler Co<sub>2</sub>MnAl undergoes a phase transition to disorder CsCl-type BCC B<sub>2</sub> structure around 950 K [2-3]. Ordered Co<sub>2</sub>MnAl experimentally exhibits half metallicity with high spin polarization and follows the Slater-Pauling rule for magnetization (4  $\mu_B$ /f.u.) and it undergoes ferromagnetic to paramagnetic transition at  $T_C \sim 726$  K. On the other hand, the disorder affects the magnetization (3.7  $\mu_B$ /f.u.) causing deviation from theoretical prediction and  $T_C$  at a lower temperature of ~685 K. Unlike ordered samples, disorder-induced e-e interaction or weak localization is predominant at low temperatures and transition from localized to itinerant ferromagnetic behavior is observed. Whereas, the transition gets shifted to a further lower temperature for the ordered sample. Intrinsic anomalous Hall contribution is the major factor for the large anomalous Hall conductivity in the system.

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## Effect of deposition temperature on the quality of Alq3 films and Alq3-Co interfaces

<u>Sambhunath Bera<sup>1, 2, \*</sup></u>, Kali Prasanna Mondal<sup>1</sup>, Ajay Gupta<sup>1, 3</sup>, Dileep Kumar<sup>4</sup>, Pooja Gupta<sup>5</sup>, Anil Gome<sup>4</sup>, V Raghavendra Reddy<sup>4</sup>, Pallavi Pandit<sup>6</sup>, and Stephan V Roth<sup>6</sup>

<sup>1</sup>Amity Centre for Spintronic Materials, Amity University, Noida, UP 201313, India
 <sup>2</sup>Present address: School of Engineering & Technology, BML Munjal University, Sidhrawali, Gurugram, Haryana, 122413, India
 <sup>3</sup>Present address: Department of Physics, University of Petroleum and Energy Studies, Dehradun, Uttarakhand 248007, India
 <sup>4</sup> UGC-DAE-CSR, Indore, MP 452017, India
 <sup>5</sup>Raja Ramanna Centre for Advanced Technology (RRCAT), Indore, Madhya Pradesh, 452013, India
 <sup>6</sup>Deutsches Elektronen-Synchrotron (DESY), Notkestrasse 85, D-22607 Hamburg, Germany

\*Contact: sambhunath.bera@bmu.edu.in

*Keywords:* Organic spintronics, Si/W/Alq3/Co/Alq3 multilayers, combined XRR & GIXSW, GISAXS, Co diffusion into Alq3

Organic semiconductor Alq<sub>3</sub> thin films were deposited at four different substrate temperatures ranging from 30 °C to 90 °C. X-ray reflectivity (XRR) studies reveal good-quality Alq<sub>3</sub> films with smooth surfaces. Electron density gradually increases with increasing deposition temperature, which indicates continual reduction of porosity in the films. Grazing-incidence small-angle scattering (GI-SAXS) studies demonstrate that with increasing deposition temperature pore separation increases and pore depth decreases progressively in the films. Co diffusion into the Alq<sub>3</sub> layer in four Si/W/Alq<sub>3</sub>/Co/Alq<sub>3</sub> multilayers were investigated using XRR and grazing-incidence x-ray standing wave (GI-XSW) measurements together. The Alq<sub>3</sub> layers in the multilayers were deposited at the four different substrate temperatures as mentioned above. It was found that with increasing growth temperature of Alq<sub>3</sub> layer, penetration of Co into Alq<sub>3</sub> through Alq<sub>3</sub>/Co interface gradually reduces. This study demonstrates that by modulating the deposition temperature of Alq<sub>3</sub> film, quality of Alq<sub>3</sub> films and interface of Co-Alq<sub>3</sub> heterostructures can be improved significantly, which is required for better performance of organic spintronic devices.

#### **TOPOLOGICAL CONDENSED MATTER & QUANTUM**

#### **Topological Nodal Line Features in NiSe Semimetal**

Sharadnarayan Pradhan<sup>1</sup>, Sanand Kumar Pradhan<sup>1</sup>, Priyanath Mal<sup>2</sup>, P. Rambabu<sup>1</sup>, Archana Lakhani<sup>3</sup>, Bipul Das<sup>4</sup>, Bheema Lingam Chittari<sup>5</sup>, G. R. Turpu<sup>1</sup> and <u>Pradip Das<sup>1</sup></u>\*

<sup>1</sup>Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur-495009, C. G., India.

<sup>2</sup>Department of Physics and Photon Science, Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea.

<sup>3</sup>UGC-DAE CSR, University Campus, Khandwa Road, Indore, 452001, India.

<sup>4</sup>Department of Physics, National Taiwan Normal University, 162, Section 1, Heping E. Rd., Taipei City 106, Taiwan. and

<sup>5</sup>Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India.

\*Contact: pradipd.iitb@gmail.com

#### Category: Oral

Keywords: Topological nodal line semimetal, Electronic transport, Weak antilocalization, Hall effect.

The next generation of low-dissipation electronics and spintronics may make use of the linear band touching at one-dimensional lines or rings that characterize a nodal line semimetal phase. This has generated a lot of interest in research. Here, we used temperature-dependent resistivity data fitted to the Bloch-Gruneisen-Mott formula to show the existence of multiple scattering processes within a single crystal of NiSe, including electron-phonon (e-p) and Mott's interband scattering. The observation of transverse magnetoresistance (MR) data that revealed both a deviation from and a well-scaled extended Kohler's rule further confirmed multiple scattering mechanisms. Temperature-dependent resistivity under different magnetic fields suggests that NiSe is topological semimetal. Weak antilocalization (WAL), as described by the modified HLN model, is confirmed by the observed negative magnetoconductivity. The -ln(B) scaling behavior of weak field magnetoconductivity validates the topological nodal line feature, even though the Fermi surface is not perfectly toroidal in shape. The experimental realization of electron dominance comes from the observation of non-linear Hall resistivity with negative slope. Based on the results of DFT calculations, five different types of nodal lines with  $\pi$ -Berry phase without spin orbit coupling (SOC) are presented: two with six-fold rotational symmetry, one with threefold rotational symmetry, one endless, and one diamond-shaped. Except for the nodal line with a diamond shape, all nodal lines stack perpendicular to the crystallographic c-axis. In the presence of SOC, the two nodal lines that are still protected are also shown by the DFT calculations.

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## **DEVICES**

# Resistively detected electron spin resonance and g factor in few-layered exfoliated MoS<sub>2</sub> devices

<u>Chithra H. Sharma<sup>1,2\*</sup></u>, Appanna Parvangada Pemmaiah<sup>2</sup>, Lars Tiemann<sup>2</sup>, Kai Rossnagel<sup>1</sup>, Jens Martin<sup>3</sup>, Robert H. Blick<sup>2,4</sup>

<sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

<sup>2</sup>Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper Chaussee 149, Hamburg 22761 Germany. <sup>3</sup>Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany

<sup>4</sup>Material Science and Engineering, University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA.

\*Contact: Sharma@physik.uni-kiel.de

Category: Oral

Keywords: Electron-spin-resonance, MoS<sub>2</sub>, g factor, Transport, Transition-metal-dichalcogenides

Electron spin resonance (ESR) is a powerful technique to investigate the behavior of electron spins and extract information such as g factor, spin-relaxation times and spin-orbit interaction strength. While using resistively detected ESR (RD-ESR), manipulation of the electron spins in a device environment can be studied. [1,2] This is an important tool for the development of spintroic devices, qubits etc.

 $MoS_2$  has recently evolved as a material with great potential for hosting quantum devices and spintronic applications. Hence, the demonstration of RD-ESR and the determination and improved physical understanding of the *g* factor is of great importance. Nevertheless, its application has been limited so far by highly resistive contacts to  $MoS_2$ . Here, we exploit n-doped few-layered  $MoS_2$  devices with tin (Sn) contacts demonstrating ohmic behavior at low temperatures. By means of RD-ESR, we determine the *g* factor in multi-layered  $MoS_2$  and observe that the *g* factor value is independent of the charge carrier density within the limit of our measurements.

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# Multifunctional Resistive Switching in Magnetization-graded Ni/NiMnIn/V2O5 Flexible Heterostructure towards Brain-inspired Neuromorphic Computing

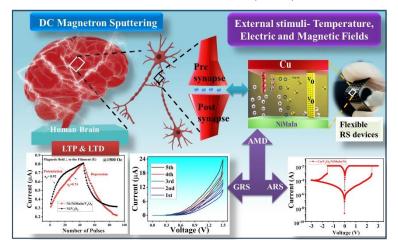
Kumar Kaushlendra<sup>1</sup>, and Davinder Kaur<sup>1\*</sup>

Functional Nanomaterials Research Laboratory (FNRL), Department of Physics and Centre for Nanotechnology, Indian Institute of Technology Roorkee, Uttarakhand, India \*Corresponding author: davinder.kaur@ph.iitr.ac.in

Keywords: Neuromorphic, RRAM devices, thin film, 2D materials, functional materials

## Abstract

Bio-inspired neuromorphic computing (NC) is attracting significant research interest due to the imitation of the human brain functioning in electronic devices. The current study describes a flexible  $Cu/V_2O_5/NiMnIn$  based memory device fabricated using the DC magnetron sputtering technique on flexible Ni substrate. It manifests the simultaneous existence of analog and abrupt switching characteristics, making it promising for neuromorphic applications. The switching behavior has been explained through the proposed analytical model. In abrupt resistive switching, the device displays a reasonably high OFF/ON resistance ratio of ~4.1×103, endurance (~5000 cycles), and data retention time (~4500 s). The tunability of the device has been investigated by studying the influence of external stimuli, such as temperature and magnetic field anisotropy, on the SET voltage. The realization of LTP and LTD synaptic functions in analog switching demonstrates the nonlinear and asymmetric features of the device. The effect of temperature on LTP, LTD, and memory window has been thoroughly investigated. The strain generated in the NiMnIn layer during the first-order martensite transformation aids in tuning the LTP and LTD of the device. The negative and positive piezomagnetic coefficients of Ni and NiMnIn lead to magnetization-graded ferromagnetic assembly and enhance the linearity of LTP and LTD. Additionally, the memory device exhibits outstanding flexibility. The current work opens up new possibilities for upcoming neuromorphic applications.



## **Table of Contents (TOC)**

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## Structural and Magnetic Studies of Mn2-xNixM03O8 Polar Magnetic Material

Tarun Pratap Singh<sup>1</sup>, <u>G.R. Turpu<sup>1</sup></u>, P. Rambabu<sup>1</sup>, Pradip Das<sup>1</sup>, V. Raghvendra Reddy<sup>2</sup>
1 Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya, Bilaspur 495009, India 2 UGC-DAE-CSR, University Campus, Khandwa Road, Indore 452001, India \*Contact: dr.tgreddy@gmail.com

Keywords: Multiferroics, Polar Magnet, Magnetization,

Multiferroicity in condensed matter has been an active area of research to explore the physics involved in there [1]. Polar magnetic oxides form a new class of multiferroic materials and being studied intensely in recent times [2]. Here we report the structural, and magnetic properties of polar magnetic oxide  $Mn_{2-x}Ni_xMo_3O_8$  (x = 0, 0.5, 0.75). These compounds were prepared through solid state route. Rietveld refined RT-XRD confirms hexagonal structure (P6<sub>3</sub>mc) for  $Mn_{2-x}Ni_xMo_3O_8$  (x = 0, 0.5, 0.75). Temperature dependence of magnetization measurements emerges with L-type ferrimagnetic (FiM) ordering at temperature T<sub>C</sub> ~ 40K for  $Mn_2Mo_3O_8$ , and for  $Mn_{1.5}Ni_{0.5}Mo_3O_8$  and  $Mn_{1.25}Ni_{0.75}Mo_3O_8$ , T<sub>C</sub> are 27.05 and 26.97K, respectively. Isothermal magnetization at 2K shows a nonlinear behavior suggest a possible spin orientation or spin flop transition due to applied magnetic field in  $Mn_2Mo_3O_8$ .

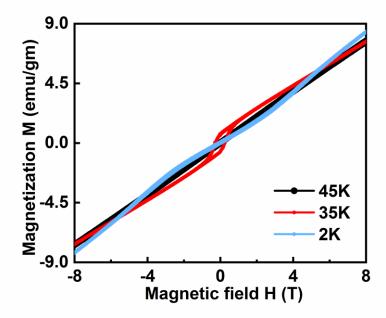


Fig:(1) Isothermal magnetization of Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>

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# **Theme:** DEVICES (ELECTRONICS, SPINTRONICS, OPTOELECTRONICS, SENSORS & ACTUATORS)

## Nucleation to Motion: Skyrmions in Pd/Fe Multilayers

Tamali Mukherjee<sup>1\*</sup>, Banasree Sadhukhan<sup>2</sup>, and V Satya Narayana Murthy<sup>1</sup>

<sup>1</sup>Birla Institute of Technology and Science, Pilani, Hyderabad Campus, India <sup>2</sup>SRM Institute of Science and Technology, Chennai, India

\*Contact: p20220034@hyderabad.bits-pilani.ac.in

#### Category: Poster

Keywords: Magnetic skyrmions, Spintronics, Micromagnetic simulation, PdFe bilayer.

Skyrmions are small swirling topological defects in ferromagnetic materials that show promising features to be used as a 'bit' of information in future spintronic devices. We use a PdFe bilayer (of dimension 200 x 200 nm<sup>2</sup> and thickness 1 nm) on Ir (111) to study skyrmion formation by applying a magnetic field and electric current and its dynamics by applying an electric current pulse. From the spin-spiral initial state, the skyrmion phase in the ferromagnetic background is achieved at the threshold magnetic field of 1.7 T applied in the +z direction. With the increasing strength of the magnetic field, the number of skyrmion increases, and their diameters are reduced. Skyrmions get annihilated at 5 T of the magnetic field, and the layer becomes ferromagnetic. Instead of the magnetic field, if a nano-second current pulse is applied to induce the required spin transfer torque (STT) to change the initial spin-spiral phase, we get the final relaxed state as a skyrmion of opposite core magnetization nucleated in a spin-spiral background. The threshold current pulse to observe skyrmion formation is  $10^{11}$  A/m<sup>2</sup> applied in the +z direction. After nucleation, the skyrmion dynamics are studied by applying STT or spin-orbit torque (SOT) provided by a nano-second current pulse. A proper arrangement of skyrmions in the sample must be implemented to be convenient in the context of spintronic devices. Different desired arrangements like T-shape,  $\pi$ -shape, L-shape, and so on can be formed by modulating the magnitude and pulse width of the current density pulse applied in specific directions. The magnetization dynamics of the PdFe free layer is given by the Landau-Lifshitz-Gilbert (LLG) equation and solved by Mumax3.

$$\frac{d\overrightarrow{m}_{free}}{dt} = -\gamma \overrightarrow{m}_{free} \times \overrightarrow{H}_{eff} + \alpha \overrightarrow{m}_{free} \times \frac{d\overrightarrow{m}_{free}}{dt} + \overrightarrow{\tau}_{STT} + \overrightarrow{\tau}_{SOT}$$

The material parameters used to carry out the simulation are, saturation magnetization ( $M_s$ ) = 6.3 x 10<sup>5</sup> A/m, Gilbert constant ( $\alpha$ ) = 0.023, exchange constant ( $A_{ex}$ ) = 2.269 x 10<sup>-12</sup> J/m, interfacial DMI ( $D_{int}$ ) = 3.64 x 10<sup>-3</sup> J/m<sup>2</sup>, first order anisotropy constant ( $Ku_1$ ) = 1.4 x 10<sup>6</sup> J/m<sup>3</sup> and easy axis is taken in (0, 0, 1) direction.

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# **Asian Pacific**

# Magneto-phonon Raman spectroscopy of Graphene (C13) encapsulated by Graphene (C12)

<u>Mrityunjay Pandey</u><sup>1</sup>, Corinne Steiner<sup>1</sup>, Taoufiq Ouaj<sup>1</sup>Lutz Waldecker<sup>1</sup>, Bernd Bechoten<sup>1</sup>, Christoph Stampfer<sup>1</sup>

1 1JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, D-52074 Aachen, Germany

\*Contact: Mrityunjay.pandey@physik.rwth-aachen.de

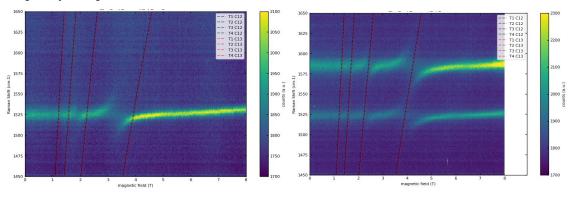
### Category: Oral/Poster

Keywords: Landau Level spectroscopy, electron-phonon coupling, many body effect

Abstract

The influence of the substrate on electron-phonon coupling (EPC) and electron-electron interactions in graphene is substantial for a variety of fundamental physical phenomena, such as superconductivity or room temperature electronic transport. Raman spectroscopy is a powerful tool to investigate EPC and el-el interactions the influence of the dielectric screening of the environment on the electron and phonon dispersion is not fully understood magneto-Raman measurements allow to study the resonant coupling between the optical phonons of the Raman G-mode and the Landau-Levels [1] from the B-field position of the transition the Fermi velocity can be extracted electron-electron interactions renormalize the Fermi velocity and it is therefore sensitive to dielectric screening observation of T transitions up to n = 3. Extraction of the Fermi velocity for various system using the T transition: strongest reduction of the Fermi velocity for graphene (C13) encapsulated by graphene (C12). However fermi velocity in C13 without encapsulation is found to be larger than encapsulated.

(a) Magneto Raman spectroscopy of C13 without encapsulation (b) Magneto Raman Spectroscopy of C13 encapsulated by C12. (dashed line indicating the fitting of Fermi velocity for the c13 completely encapsulated in c12).



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# Soft condensed matter

# Temperature Dependent Diffusion of Cationic Lipids and DNA-NPs in Lipid Bilayers

Sakiko Nakata<sup>1</sup>, <u>Chandan Kumar<sup>1\*</sup></u>, Miho Tagawa<sup>1,2</sup>, Shunta Harada<sup>1,2</sup> and Toru Ujihara<sup>1,2</sup>

1 Institute of Materials and Systems for Sustainability, Nagoya University, Furo Cho, Chikusa ku, Nagoya, Aichi, Japan 464 8601

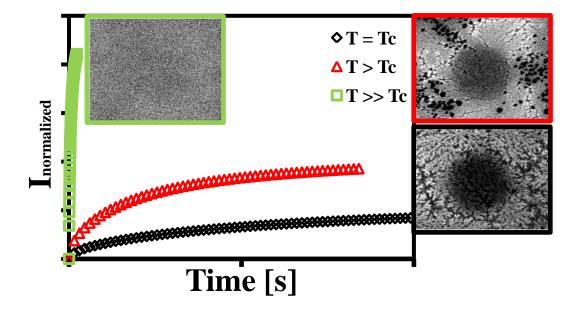
2 Department of Materials Process Engineering, Furo cho, Chikusa ku, Nagoya University, Aichi, Japan 464 8601

\*Contact: <u>kumar.chandan.x2@f.mail.nagoya-u.ac.jp</u>, <u>tagawa.miho.z5@f.mail.nagoya-u.ac.jp</u>

## Category: Oral

Keywords: Cationic lipid, Lipid bilayer, Nanoparticle diffusion

We investigate the complex relationship between cationic lipid diffusion and the mobility of DNAfunctionalized gold nanoparticles (DNA-NP) within a supported lipid bialyer. Employing advanced techniques such as fluorescence recovery after photobleaching (FRAP) and atomic force microscope (AFM), we meticulously examine the temperature-dependent diffusion and the structural changes of the complex system. Our findings reveal a pronounced influence of temperature on the lateral diffusion coefficient of both lipid and DNA-NP with significant enhancement in diffusivity at near bilayer phase transition temperatures and temperatures above phase transition. Conversely, below phase transition temperatures, a decreased diffusivity was observed. AFM analysis further corroborated the self-organization of DNA-NPs on the bilayer surface, providing valuable insights into the structural implications of nanoparticle diffusion. This comprehensive study offers a deeper understanding of the interplay between nanoparticle mobility and lipid bilayer behavior, shedding light on the fundamental processes governing their assembly dynamics.



## Hyperbolic Phonon Polariton for Molecular Sensing

Rohit Kumar<sup>1</sup>, Nihar Ranjan Sahoo<sup>1</sup>, Parul Sharma<sup>1</sup>, Ikshvaku Shyam<sup>1</sup>, Abhay Anand VS<sup>1</sup>, Janhavi Khunte<sup>1</sup>, Brijesh Kumar<sup>1</sup>, and Anshuman Kumar<sup>1,\*</sup> <sup>1</sup> Laboratory of Optics of Quantum Material, Indian Institute of Technology Bombay, India \*anshuman.kumar@iitb.ac.in

#### Category: Oral/Poster

Keywords: Hyperbolic Material, Phonon Polaritons, van der Waals crystal, molecular sensing

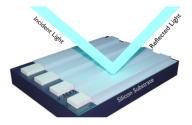


Figure 1: Far field interaction of molecules and HPhPs in  $\alpha - MoO_3$  grating structures.

Hyperbolic phonon polaritons (HPhPs), arising from the strong coupling between photons and phonons in hyperbolic materials, provide a promising approach for confining electromagnetic waves beyond the diffraction limit. These polaritons offer extreme sub-wavelength confinement, making them highly beneficial for sub-wavelength focusing, quantum photonics, polarization optics, and sensing[1][2]. The unique properties of HPhPs, including their hyperbolic isofrequency surface, anisotropic dispersion, and tunable field confinement[3], make them as versatile candidates for advancements in nano-photonics and mid-infrared photonics.

In this study, we explore the tunable field confinement of HPhPs to achieve molecule detection. Conventional spectroscopy techniques are often constrained in this regime due to low signal-to-noise ratios when probing molecules at subwavelength scales. The enhanced confinement provided by HPhPs, however, allows for ultrasensitive detection at low concentrations that standard spectroscopic methods cannot achieve. Hyperbolic isofrequency contours in hyperbolic materials lead to a significant momentum mismatch between photons and HPhPs, preventing direct far-field excitation. To address this issue, we apply nanostructuring to provide the additional momentum required. Specifically, we employ a grating structure of in-plane hyperbolic van der Waals (vdW) material,  $\alpha - MoO_3$ , as a thin film on a silicon substrate to enable far-field excitation of HPhPs.

In this work, we show that by tuning the HPhP resonators to couple with molecular resonances, we observe significant spectral shifts and enhanced molecular interaction signatures. These spectral changes indicate effective coupling between the HPhPs and molecular resonances, confirming the sensitivity of the system to molecular interactions at low concentrations. Overall, the results demonstrate that grating-structured  $\alpha$ -MoO<sub>3</sub> thin films provide an effective platform for far-field excitation of HPhPs, enabling sensitive detection of molecular interactions via enhanced spectral signatures. The tunability of the HPhP resonators in this configuration facilitates coupling with various molecular resonances, paving the way for advancements in sensing and subwavelength molecular detection.

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## **Quantum materials**

# Growth mechanism of Colloidal MoS<sub>2</sub> Quantum Dots: Influence of reaction time and precursor concentration

Geetika Sahu<sup>1,\*</sup>, Chanchal Chakraborty<sup>2</sup>, Subhadeep Roy<sup>1</sup> and Souri Banerjee<sup>1</sup>

1 Dept. of Physics, BITS Pilani Hyderabad Campus, Telangana 500078 India 2 Dept. of Chemistry, BITS Pilani Hyderabad Campus, Telangana 500078 India \*Contact: p20210061@hyderabad.bits-pilani.ac.in

Category: Oral presentation

Keywords: Quantum dots, reaction time, precursor concentration, fractal analysis

We aim to investigate the growth mechanism of molybdenum disulfide quantum dots<sup>1</sup> (MoS<sub>2</sub> QDs) under hydrothermal reaction conditions by exploring two important parameters that control the growth process – reaction-time<sup>2</sup> and precursor-concentration. This fundamental study focuses on tuning the particle size, impacting the optical and electronic properties due to the quantum confinement effect, also monitoring the spatial growth of QD-sheets prepared through the aggregation of individual QDs. Among the mentioned two parameters, the former dictates the duration of aggregation while the latter controls the aggregation rate. The hydrothermally synthesized QDs have been analyzed through morphological and optical tools, and we used fractal analysis<sup>3</sup> to understand the growth process.

With increasing reaction time  $\tau$  (at a constant precursor concentration  $\approx 73mM$ ), the growth process shows a crossover from a bottom-up to a top-down process at  $\tau = 14$  hours. A non-monotonic behavior of average QD size ( $\bar{d}$ ) is observed, which is supported by morphological studies like TEM and STEM, as well as optical studies. Higher QD sizes correspond to lower bandgap and significant redshift in the PL spectra. The fractal dimension ( $d_f$ ) of the QD clusters shows a sudden drop from 1.92 at this particular time  $\tau = 14$  to 1.82 and saturates at this value afterward. This signifies the onset of the fragmentation of the clusters due to the unavailability of active precursors and to validate this, we have carried out the concentration-based studies keeping the reaction-time constant. We observe a similar non-monotonic behavior in QD size (maximum size at  $\approx 73mM$ ) supported by the morphological and optical studies as the precursor concentration varies from 22mM ( $\bar{d} = 10nm$ ) to 125mM ( $\bar{d} = 7nm$ ). This is in agreement with fractal analysis, where the maximum  $d_f$  of 1.97 is observed at 73mM which decreases at both higher and lower concentration. This impact of precursor concentration is consistent for all reaction times. Finally for better understanding of growth process we have also replicated the system through numerical simulations of the random walk process on a 2D square lattice.

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# **Theme: Nano and Functional Materials**

# Magnetoelastic and magnetodielectric coupling in the solid solution system $(1-x)Ba(Fe_{1/2}Nb_{1/2})O_3-xLaFeO_3$ (x = 0.50)

Arun Kumar<sup>1\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Science Education and Research (IISER) Pune-411008, India

\*Contact: Email ID: arun.kumar@acads.iiserpune.ac.in

## Category: Poster/Oral

Keywords: Perovskites, Magnetic phase transitions, Magnetoelastic coupling and magnetodielectric coupling

Perovskite oxides with the general formula  $ABO_3$  (where A is an alkaline earth or rare-earth cation, and B is a transition metal cation) continue to be a focal point of research in condensed matter physics due to their intriguing electronic and magnetic properties [1]. The formation of solid solutions between perovskites allows for fine-tuning of material properties to meet specific technological demands, such as in microelectronic devices, ceramic capacitors, piezoelectric sensors, actuators, and memory devices [2].

In this work, we investigate the new solid solution system  $(1-x)Ba(Fe_{1/2}Nb_{1/2})O_3-xLaFeO_3$  with x = 0.50, abbreviated as BFN-0.50LF, using a combination of macroscopic and microscopic techniques to explore structure-property correlations. The system crystallizes in a cubic structure with the space group *Pm-3m*. Temperature-dependent magnetization measurements reveal successive magnetic transitions at ~175 K and ~30 K. Our analysis of temperature-dependent X-ray diffraction and dielectric data highlights two key features of the BFN-0.50LF system: (i) magnetoelastic coupling linked to the magnetic transitions, evident from changes in the unit cell volume, and (ii) magnetodielectric coupling, as indicated by anomalies across the two transitions. This study offers insights into designing environmentally friendly, lead-free perovskites with potential technological applications.

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# Unified analytical prescription for flat band engineering in a class of quasi-one dimensional networks

Atanu Nandy\*

\*Contact: atanu@apccollege.ac.in

## Category: Oral

Keywords: flat band, decimation, slow light, compact localized state

The specific topology of the lattice has a strong influence on the overall spectrum and in certain cases it can induce exotic spectral features through a set of macroscopically degenerate dispersionless flat bands. The momentum independence of the single particle eigenstates brings the flavor of divergent effective mass leading to the immobility of the incoming excitation. The extremely low group velocity of the wave packet causes a singularity in the density of states. This divergence plays a crucial role in the context of thermoelectric devices to enhance their thermopower and low-thresold laser device. The methodology to discern the flat band modes in some quasi-one dimensional networks is reported within the tight-binding framework following the real space decimation scheme. Analytical calculations regarding the decoupling scheme to demonstrate the localizing character of those non-dispersive states have been reported. Dispersion relation and two-terminal transport of those systems have been worked out using the analytical method. Tight-binding analogy provides a smooth platform to map our electronic problem onto the corresponding photonic scenario. The analytical technique of this one-to-one mapping is discussed elaborately. In the context of photonic flat band modes, concept of slow light is also introduced. Slow light is a very promising solution for optical delay line or optical buffering and advanced time-domain optical signal processing. It is also anticipated to enhance linear and nonlinear effects and so miniaturize functional photonic devices, as slow light compresses optical energy in space that eventually increases the light-matter interaction.

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# Anisotropic Magnetocaloric Effect Driven by Spin Nematic Fluctuations

in Multiferroic Sr<sub>2</sub>CoGe<sub>2</sub>O<sub>7</sub>

T. Kihara<sup>1\*</sup>, M. Aakaki<sup>2</sup>, K. Mitsumoto<sup>3</sup>, M. Kimata<sup>2</sup>, A. Miyake<sup>2</sup>, and M. Tokunaga<sup>4</sup>

 Research Institute for Interdisciplinary Science, Okayama University 2 Institute for Materials Research, Tohoku University
 Graduate School of Arts and Sciences, The University of Tokyo 4 Institute for Solid State Physics, The University of Tokyo \*Contact: tkihara@okayama-u.ac.jp

## Category: Oral

Keywords: Multiferroics, Spin nematic, Magnetocaloric effect, Specific heat, High magnetic field

Solid-state cooling based on magnetocaloric, electrocaloric, or elastocaloric/barocaloric effect can potentially offer higher energy efficiency than traditional vapor-compression refrigeration systems. To achieve a large caloric effect, exploiting different degrees of freedom such as spin, electron, and lattice systems is crucial. In this context, multiferroic materials, with their strong coupling between magnetic, electric, and structural degrees of freedom, can exhibit giant caloric effects, and therefore, they have been the focus of much research [1]. However, the detailed mechanism of cross-coupling between the different degrees of freedom in multiferroic materials and its contribution to the caloric effect remains veiled.

Because direct measurement of the caloric effect can provide a deeper understanding of the complex crosscoupling in multiferroic materials, we, in this study, performed magnetocaloric effect (MCE) measurements for the multiferroic  $Sr_2CoGe_2O_7$ . This material exhibits magnetoelectric effects in the antiferromagnetic ordered phase below  $T_N = 6.5$  K [2]. As shown in the left panel of Fig. 1, magnetic Co ions are tetrahedrally coordinated by four oxygen ions, and the hybrid orbitals formed by the Co 3d orbitals and O 2p orbitals exhibit directional dependence on the Co spin (S = 3/2). Consequently, an electric polarization along the c-axis emerges when the spins align along the [110] direction, while the polarization vanishes when the spins align along the [100] direction [2]. The right panel of Fig. 1 shows the MCE results measured under pulsed high magnetic fields along the [100] and [110] directions. Despite the magnetization processes are nearly identical for the two directions, a clear difference in the adiabatic temperature change was observed just

below the saturation magnetization. Because the magnetic anisotropy of  $Sr_2CoGe_2O_7$  is isotropic within the ab-plane, the observed anisotropy in the MCE is attributed to magnetoelectric cross-correlation. This anisotropic entropy change was also confirmed by the specific heat measurements up to 25 T. Additionally, the Monte Carlo simulations revealed a significant role for the anisotropic spin nematic fluctuations.

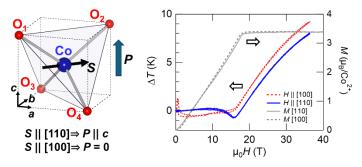


Fig. 1 (left)  $CoO_4$  tetrahedron. (right) Magnetizations and magnetocaloric effects measured under the pulsed high fields.

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# Rashba-like spin splitting at the interface of Antiferromagnet-WS $_2$ van der Waal heterostructure

Purba Dutta<sup>\*</sup> and Nirmal Ganguli<sup>†</sup>

Department of Physics, Indian Institute of Science Education and Research Bhopal, Bhauri, Bhopal 462066, India

(Dated: 29 October 2024)

Magnetic van der Waals (vdW) materials with intrinsic magnetic properties provide an ideal platform for exploring magnetism in the two-dimensional limit, where new physical phenomena are expected, creating many opportunities for both the discovery of interesting new physics and the development of innovative device concepts. Effects like magnetic proximity effects are highly sensitive to interfacial electronic properties, such as electron wave function overlap and band alignment. The recent emergence of magnetic two-dimensional materials opens new possibilities for exploring proximity effects in van der Waals heterostructures, which feature atomic thicknesses and form atomically sharp interfaces, are an attractive platform to realize and harness the proximity effect. The aim of this work is to explore how to control and enhance the functionalities of 2D vdW layered materials using heterostructures with magnetic layers for application in next-generation electronic and spintronic devices. By interfacing Tungsten disulphide with MnPS<sub>3</sub>, the proximity-induced exchange field gives rise to spontaneous Zeeman splitting. In addition, a type-II band structure forms at the heterostructure interface with the lowest conduction band from MnPS<sub>3</sub>. This work will provide insights into the magnetic proximity effects of a vdW magnetic heterostructure by utilizing the multiple magnetic and electronic properties.

<sup>&</sup>lt;sup>†</sup> Email: NGanguli@iiserb.ac.in



<sup>\*</sup> Email: Purba19@iiserb.ac.in

## Fermi Level of Intrinsic and Extrinsic Semiconductors in q-deformed calculus

Pintu Bhattacharya<sup>1</sup>

1 Department of Physics, L. N. College, Bhagwanpur, Vaishali A constituent Unit of B. R. A. Bihar University, Muzaffarpur.Bihar-844114

#### \*Contact: pbhattacharya89@gmail.com

*Abstract:* Quantum calculus, termed as q-calculus is an unconventional branch of mathematics that does not involve the concept of limit. In the last decades, q-calculus especially q-deformed calculus has expanded explosively as a bridge between physics and mathematics [1]. A number of studies have been done to understand the thermoelectric properties of q-deformed electron gas and other useful statistical parameters [2]. Recently, q-deformed ideal Fermi gas in 2d, and 3-D space is studied extensively as in ref. [1, 2]. It is remarkable that q-deformation will unveil some important characteristics different from those found ordinarily in conventional statistical physics [1, 3].

In this paper, we use q-deformed fermion algebra and the associated distribution to deduce the expression of Fermi level for intrinsic semiconductors. Expression of hole concentration in the valence band, law of mass action, and intrinsic carrier concentration will also be deduced using q-deformed calculus. In addition, the Fermi level for extrinsic semiconductor will be studied in view of q-deformed quantum statistics. As a consequence, it is found that, at high temperature, q-deformed statistics reduces to undeformed conventional statistical mechanics. Thus, we can infer the q-deformed calculus changes their form as they are in ordinary statistical systems.

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## Electron energy in nanowires and rectangular nanorods in q-deformed calculus

Pintu Bhattacharya<sup>1\*</sup>, <u>Md. Naiyar Perwez<sup>2</sup></u> and Joydip Ghosh<sup>3</sup>

Department of Physics, L. N. College, Bhagwanpur, B. R. A. Bihar University, Muzaffarpur, Bihar-844114
 Department of Physics, R. N. College, Hajipur, B. R. A. Bihar University, Muzaffarpur, Bihar-844101
 Department of Physics, R. D. S. College, B. R. A. Bihar University, Muzaffarpur, Bihar-842001
 \*Contact: pintu@lncollege.ac.in

## Keywords: q-calculus, q-deformed calculus, q-analog, nanowire, nanorod

Quantum calculus, known as q-calculus is an intreguing expansion of classical calculus without limit. It brings the idea of "q-analogs" for a variety of mathematical as well as physical entities. Recently, q-deformed quantum mechanics provides a rich landscape for deeper exploration and understanding of Fermi energy with a general energy spectrum [1-3].

In this paper, we have derived the expression of energy levels for a quantum nanowire and a rectangular nanorod using q-deformed calculus. More specifically, the energy spectrum of an electron in a quantum wire using one electron approximation has been revisited and then extend it for a rectangular nano rod in view of q-deformed calculus. Thus, the influence of the actual cross-sectional shape along with the 'q-parameter' is studied theoretically using q-deformed Schrödinger equation. Effort has also been made to realize the modification of the energy levels with the appearance of 'q' as a general consequence q-deformed calculus.

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# Designing Hybrid Quantum Devices Using Photon-Photon Coupling for Quantum Technologies.

### Rakesh Kumar Nayak, Abhishek Maurya, Meghana Mishra, Rajeev Singh, Biswanath Bhoi\*.

Nano-Magnetism and Quantum Technology Laboratory, Department of Physics, Indian Institute of Technology (BHU), Varanasi, 221005, Uttar Pradesh ,India.

Email of Presenting Author: rakeshkumarnayak.rs.phy22@itbhu.ac.in

\*Email of corresponding author: <u>biswanath.phy@iitbhu.ac.in</u>

Category: Poster

Keywords: Photon-Photon Coupling, Level Attraction, Level Repulsion .

In recent decades, research in quantum information science has increasingly focused on controlling and manipulating electromagnetic waves, uncovering intriguing phenomena such as photon-photon coupling and leading to significant advancements across various quantum technology fields. Photon-photon coupled hybrid systems hold substantial promise for improving quantum processing technologies [1]. This study investigates the crucial role of managing photon mode interactions, including different anti-crossings, to develop information processing devices with optimal tunability and scalability.

A framework is introduced that facilitates photon-photon coupling with the ability to switch between level repulsion (LR) and level attraction (LA). These advancements have enabled the realization of quantum gates and quantum hybrid devices paving the way for more robust and scalable quantum communication networks and quantum computing systems.

We carried out numerical simulations, illustrate these switching features in two distinct photon-photon mode, demonstrating how dynamic adjustments between LR and LA can improve the performance and versatility of quantum devices [2]. The findings highlight the importance of precise control over photon-photon interactions for creating scalable and adaptable quantum technologies, paving the way for progress in quantum computing, communication, and sensing applications.

Furthermore, the study examines the characteristic features of these photon mode interactions through a quantum mechanical model. This model allows for fine-tuning of parameters and enables the observation of interactions at room temperature. The results emphasize the potential of these hybrid systems to develop versatile and scalable quantum devices, which are crucial for the progress of quantum technology.

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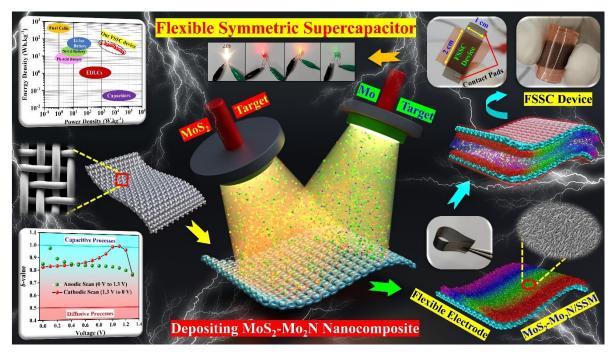
## Pseudocapacitive Kinetics in Synergistically Coupled MoS<sub>2</sub>-Mo<sub>2</sub>N Nanowires with Enhanced Interfaces towards All-Solid-State Flexible Supercapacitors

Bhanu Ranjan and Davinder Kaur\*

<sup>1</sup>Functional Nanomaterials Research Laboratory (FNRL), Department of Physics, Indian Institute of Technology Roorkee (IIT Roorkee), Roorkee-247667, Uttarakhand, India \*Contact: davinder.kaur@ph.iitr.ac.in

*Keywords:* Flexible supercapacitor; High energy density; Molybdenum disulfide (MoS<sub>2</sub>); Molybdenum nitride (Mo<sub>2</sub>N); Nanocomposite.

Pseudocapacitive kinetics in rationally engineered nanostructures can deliver higher energy and power densities simultaneously. The present report reveals a high-performance all-solid-state flexible symmetric supercapacitor (FSSC) based on MoS<sub>2</sub>-Mo<sub>2</sub>N nanowires deposited directly on stainless-steel mesh (MoS<sub>2</sub>-Mo<sub>2</sub>N/SSM) employing direct current (DC) Reactive Magnetron Co-sputtering technology. The abundance of synergistically coupled interfaces and junctions between MoS<sub>2</sub> nanosheets and Mo<sub>2</sub>N nanostructures across the nanocomposite results in greater porosity, increased ionic conductivity, and superior electrical conductivity. Consequently, the FSSC device utilizing polyvinyl alcohol-sodium sulfate (PVA-Na<sub>2</sub>SO<sub>4</sub>) hydrogel electrolyte renders an outstanding cell capacitance of 252.09 F.g<sup>-1</sup> (44.12 mF.cm<sup>-2</sup>) at 0.25 mA.cm<sup>-2</sup> and high rate performance within a wide 1.3 V window. Dunn's and *b*-value analysis reveals significant energy storage by surfacecontrolled capacitive and pseudocapacitive mechanisms. Remarkably, the symmetric device boosts tremendous energy density ~10.36  $\mu$ Wh.cm<sup>-2</sup> (59.17 Wh.kg<sup>-1</sup>), superb power density ~6.5 mW.cm<sup>-2</sup> (37.14 kW.kg<sup>-1</sup>), ultrastable long cyclability (~93.7% after 10,000 galvanostatic charge-discharge (GCD) cycles) and impressive mechanical flexibility at 60°, 90°, and 120° bending angles.



- Bhanu Ranjan and Davinder Kaur, "Pseudocapacitive Kinetics in Synergistically Coupled MoS<sub>2</sub>-Mo<sub>2</sub>N Nanowires with Enhanced Interfaces towards All-Solid-State Flexible Supercapacitors" ACS Applied Materials & Interfaces, 16 (12), 14890-14901 (2024).
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## **Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)**

# Analytical Model for Plasmonic Waves and Charge Density in Ternary AlScN/AlN/GaN Heterostructures

Neha Pande<sup>1,2</sup>, Kavita T. Upadhyay<sup>2,3</sup> and Manju K. Chattopadhyay<sup>4\*</sup>

1 School of Instrumentation Devi Ahilya University, Indore, Madhya Pradesh, India 2 Department of Electronics and Telecommunication Engineering, Institute of Engineering and Technology, Devi Ahilya University, Indore, Madhya Pradesh, India

3 Department of Electronics and Communication Engineering, IPS Academy, Institute of Engineering and Science, Indore, Madhya Pradesh, India

4 School of Instrumentation Devi Ahilya University, Indore, Madhya Pradesh, India

\*Contact: mkorwal@yahoo.com

## Category: Oral

Keywords: high electron mobility transistors (HEMT), Terahertz, plasmon frequency, polarization.

Over time, THz-related technologies have seen extensive application across various domains, encompassing THz mixers, frequency multipliers, imaging systems, transceivers, and sensors [1-3]. We present an analysis of the plasmon frequency and 2DEG of ScAlN/AlN/GaN high electron mobility transistors (HEMTs). We investigate the influence of HEMT parameters on the plasmon frequency and the sheet charge density of the 2DEG. Notably, the ScAlN/AlN/GaN heterostructure induces plasmon oscillations in the Terahertz (THz) range, surpassing frequencies observed in other semiconductor compounds. Furthermore, our study reveals substantial sensitivity in tuning these frequencies, particularly through adjustments in applied gate voltage. We optimize structural parameters to identify conditions that maximize the plasmon frequency for a given doping concentration. The potential applications of the interaction between radiation and plasmons span various fields, including developing detectors, mixers, and THz wave generators.

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# Soft Condensed Matter

# Unravelling the structure and dynamics of nano-bio interfaces and liquid surfaces by X-ray scattering

Rajendra P Giri<sup>1,\*</sup>, Bridget M Murphy<sup>2</sup>, Sajal K Ghosh<sup>3</sup> and Mrinmay K Mukhopadhyay<sup>4</sup>

1 Department of Physics, IIT (ISM) Dhanbad, Jharkhand 826004, India

2 Institute for Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany

3 Department of Physics, Shiv Nadar Institution of Eminence, Uttar Pradesh 201314, India

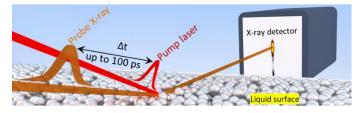
4 SP&MS Division, Saha Institute of Nuclear Physics, Kolkata 700064, India \*Contact: rpgiri@iitism.ac.in

## Category: Oral

Keywords: Biological membrane, Nano-bio interface, X-ray scattering, Pump-probe, Liquid

Nanoparticles (NPs) are currently being widely used in nanomedicine, disease diagnosis, biosensing, and environmental research. However, their biocompatibility and effectiveness are of great concern. Comprehending their molecular interactions with the first barrier of cell, i.e., the biomembrane, is pivotal to understanding the physiological effects of nanomaterials. Liquids are also essential to life because liquid surfaces and interfaces host most of the essential biological processes, and chemical reactions for maintaining the dynamic nature of life. The critical dynamic processes, such as thermally induced capillary waves and optically induced electron solvation at the liquid surfaces, occur in short timescales, typically, on sub-nanosecond to second.

Here, our experimental results<sup>1,2</sup> on the self-assembly, membrane mechanics and thermodynamics of the interaction of protein, cholesterol, and synthetic and biologically relevant NPs with biomimetic model membranes will be discussed. Also, the elucidation of the underlying non-equilibrium ultrafast physics at the liquid surfaces and interfaces along with our recent developments of an optical pump – X-ray probe setup<sup>3</sup> (Figure 1), which is first of its kind for liquid surface investigations, at the LISA P08 beamline of DESY synchrotron (Germany) will be demonstrated. The capability of the developed facility and its accessibility to the international researchers will also be discussed.



**Fig. 1**: Schematic of the optical pump – X-ray probe setup we have developed at the PETRA-III X-ray synchrotron of DESY (Germany).

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# Many-body correlation effects in quasi one-dimensional quantum wire

Vinod Ashokan<sup>1, \*</sup>

<sup>1</sup>Department of Physics, National Institute of Technology, Jalandhar, Punjab 144011, India \*Contact: ashokanv@nitj.ac.in

## Category: Oral

Keywords: Tomonaga-Luttinger liquid, Quantum wire, Electrons Correlation, Wigner Crystal

The many-body correlation effects in quasi-one-dimensional ferromagnetic and paramagnetic electron quantum wires influence the electronic properties of emergent quantum materials. We investigate how these correlation effects impact the ground state properties of ferromagnetic and paramagnetic electron quantum wire systems across different wire widths b and electron densities  $r_s$  using the quantum Monte Carlo method. Specifically, we calculate the ground-state energy, correlation energy, pair-correlation function, static structure factor, and momentum density of ferromagnetic and paramagnetic quasi-one-dimensional electron gases. Moreover, we extract the Tomonaga-Luttinger liquid (TLL) parameter from the momentum density and examine how finite wire widths affect this TLL parameter. Our findings indicate that as the wire width decreases, electron correlations strengthen. For the paramagnetic electron gases, we explore how the wire width and electron density influence the crossover in the static structure factor peak from  $2k_F$  to  $4k_F$ . The onset of a quasi-Wigner crystal phase is known to depend on electron density and the crossover occurs in the lowdensity regime. Our results show that, for a given electron density, the crossover in the charge structure factor from a dominant peak at  $2k_F$  to one at  $4k_F$  occurs as the wire width decreases. This crossover appears to result from the interplay between  $r_s$  and b. The prominent peaks in the charge and spin structure factors at  $4k_F$  and  $2k_F$ , respectively, highlight the decoupling of charge and spin degrees of freedom. Furthermore, the wire-width dependence of the electron correlation energy and the TLL parameter is found to be significant.

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# Photoluminescence properties of Eu<sup>3+</sup> and Dy<sup>3+</sup> doped SrCO<sub>3</sub> nanophosphors synthesized by hydrothermal method

Swati Rani<sup>1,\*</sup>, Indranil Maity<sup>2</sup>, Anil K. Yadav<sup>1</sup>, Ajay D. Thakur<sup>2</sup> <sup>1</sup>Department of Physics, Ch. Charan Singh University Meerut, UP 250004, India <sup>2</sup>School of Basic Sciences, Indian Institute of Technology, Patna 801106, India

#### \*Contact: swatirani1320@gmail.com

Keywords: RE doped phosphors; strontium carbonate phosphors; hydrothermal method.

Photoluminescence materials, also known as phosphors, have versatile applications in various fields such as display devices, optical storage, in-vivo bio-imaging, color LEDs, flat panel displays, etc. Phosphors convert ultraviolet (UV) or blue light into a broad visible spectrum and, hence can be utilized to produce desired light suitable for various lighting applications. Phosphors typically consist of a host material, providing space for the luminescence mechanism, doped with activators that influence their luminescence properties. Among various host materials, strontium carbonate (SrCO<sub>3</sub>) has got lot of attention due to their excellent stability and unique optical properties as compared to other sulfide-based phosphors. Lots of research is going on towards the enhancement of luminescence properties of SrCO<sub>3</sub> by doping rare earth elements. However, the emission color, intensity, and afterglow time of RE doped SrCO<sub>3</sub> phosphors have not been explored much. In this work, we have synthesized SrCO<sub>3</sub>: Eu<sup>3+</sup>, Dy<sup>3+</sup> nanophosphors by hydrothermal method, and their structural, morphological, and luminescence properties were studied by X-ray diffraction (XRD), and Field effect scanning electron microscopy (FESEM), and photoluminescence emission (PL) spectroscopy. The X-ray diffraction (XRD) analysis indicates that the synthesized sample possesses an orthorhombic phase with the Pmcn space group. FESEM images reveal that the SrCO<sub>3</sub> nanophosphors exhibit pseudospherical shapes with an irregular morphology. Photoluminescence (PL) emission spectra, recorded at various excitation wavelengths, show emission peaks at 608 nm. This red light emission is attributed to the hypersensitive forced electric dipole transition  ${}^{5}D_{0}-{}^{7}F_{2}$  of Eu<sup>2+</sup> ions. Here, Eu<sup>3+</sup> functions as the luminescent center responsible for the red emission, while  $Dy^{3+}$  serves as a trap center to enhance the afterglow duration within the SrCO<sub>3</sub> host lattice. These red phosphors with strong absorption in the blue region are promising candidates for manufacturing flat panel displays, and LEDs.

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## Polyvinyl alcohol and Barium Hexaferrite Nanoparticle Composites for Electromagnetic Pollution Reduction Applications

Mayank Mausam<sup>1</sup>, Nakuleshwar Dut Jasuja<sup>2</sup> and Sunil Kumar<sup>1\*</sup>

<sup>1</sup>University Department of Electronic Science, Babasaheb Bhimrao Ambedkar Bihar University Muzaffarpur, Bihar-842001,India

<sup>2</sup>Professor, Vivekananda Global University, Jaipur, Rajasthan, 303012, India

\*Email:<u>sunil.iitpatna@gmail.com</u>

Electromagnetic interference (EMI) poses a growing challenge in modern electronics due to the surge in wireless communication and electronic devices. Effective EMI shielding materials are crucial to ensuring device performance, reducing signal disruption, and promoting environmental safety. This research explores polyvinyl alcohol (PVA) and barium hexaferrite (BHF) nanocomposites as advanced EMI shielding materials. Barium hexaferrite nanoparticles, known for their superior magnetic properties and high dielectric constant, were synthesized via the sol-gel method, ensuring uniform particle distribution and improved crystallinity. These nanoparticles were embedded in a PVA matrix using a solution-cast method, creating nanocomposites with tunable properties by varying BHF concentrations (x=0.00, 0.02, 0.05, 0.1). The structural and chemical interactions within the composites were analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). Electrical properties were characterized through impedance measurements, revealing that the 5% BHFdoped composite exhibited the highest conductivity, lowest impedance, and reduced dielectric constant. Using a vector network analyzer in the 8-12 GHz (X-band) range, the PVA-BHF nanocomposites demonstrated excellent EMI shielding effectiveness, exceeding 30 dB. The shielding mechanism stemmed from the synergistic effects of dielectric loss, magnetic loss (attributed to BHF), and conductive loss, while PVA enhanced flexibility and processability. These findings highlight the potential of PVA-BHF nanocomposites, particularly the 5% BHF formulation, as next-generation EMI shielding materials. Their applications extend to aerospace, telecommunications, and defence industries, where flexibility, high conductivity, and strong EMI absorption are critical.

Keywords: Polyvinyl alcohol, EMI, XRD, FTIR, Vector Network Analyzer

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## **Topological Condensed Matter and Quantum Materials**

# Berry curvature driven Anomalous (Hall, Nernst) effects in half-metallic FeRu-CrSi: A first principles study

Monika Rana<sup>1</sup>, Bheemalingam Chittari<sup>2</sup> and P. Rambabu<sup>1,\*</sup>

1 Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, C. G. - 495009.

2 Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India. \*Contact: rams.hcu@gmail.com

Category: Oral

Keywords: Berry Cuvrature, Anomalous Hall effect, Anomalous Nernst Effect, Magneto-optic Kerr effect

Heusler alloys were discovered in the early 20<sup>th</sup> century by Fritz Heusler. These fascinating class of materials are found to have remarkable applications in the field of spintronics, thermoelectricity, topological materials, magnetic tunnel junctions, spin filtering devices, superconductivity, magneto-caloric effect, shape memory alloys etc.

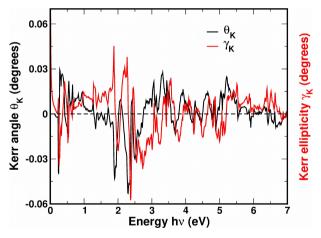


Figure 1. The Kerr angle and Kerr ellipticity of FeRuCrSi (with spin-orbit coupling) as a function of photon energy.

The Density functional theory (DFT) simulations are performed on half-metallic ferromagnetic Heusler alloy FeRuCrSi to study electronic, magnetic and topological features. The compound is found to be stable mechanically and dynamically. The spin-orbit coupling (SOC) induced Berry Curvature driven Anomalous (Hall, Nernst) effect are thoroughly investigated. The maximum Anomalous Hall Conductivity (AHC) and the Anomalous Nernst Conductivity (ANC) values are determined within the range of  $\pm 300$ meV around Fermi level  $E_F$  respectively. Also, the variation of ANC with temperature and chemical potential is investigated. The maximum value of polar Kerr angle ( $\theta_k$ ) is estimated. These properties may suggest the FeRuCrSi compound to be a suitable candidate for practical applications.

## Role of scattering processes in lattice thermal conductivity of MgB<sub>2</sub>

Nitin P.  $Singh^*$ 

Department of Physics, Jaipur National University, Jaipur, India \*Contact: Email ID: nprajpph@jnujaipur.ac.in

Keywords: Lattice thermal conductivity, phonons, relaxation time, scattering process, Callaway's model.

#### Abstract:

The contribution of various scattering mechanisms namely; combined boundary scattering, impurity scattering, anharmonic phonon processes, electron-phonon interactions and interference scattering to thermal conductivity of superconductors has been analyzed below and above  $T_c$ . It is observed that various scattering processes play an important role at different temperatures. The significance of BRT function has also been estimated in determining the best agreements between experimental and theoretical results. BRT theory calculates the electronic thermal conductivity when the dominant scatters are impurities as well as the effect of electrons on the thermal conductivity of unconventional superconductors.

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# Theme: Renewable Energy (Conversion & Storage)

## Cobalt Ferrite as a Promising Material for High-Performance Lithium-Ion Batteries

Author: <u>Dr. Sweety Supriya</u>, Assistant Professor Affiliation: Department of Electronics, LS College, Muzaffarpur Email: sweety.supriya.lscollege@gmail.com

#### Category: Oral Presentation

**Keywords:** Cobalt Ferrite, Lithium-ion Batteries, Anode Materials, Energy Storage, Electrochemical Performance.

#### **Abstract:**

The escalating demand for clean and renewable energy sources underscores the critical need for advanced energy storage technologies. Lithium-ion batteries, as a cornerstone in this domain, require high-performance anode materials to meet the growing energy storage needs. This study delves into the potential of cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>) as a promising anode material.

By employing hydrothermal synthesis and a combination of characterization techniques including Xray diffraction (XRD), scanning electron microscopy (SEM), and electrochemical impedance spectroscopy (EIS), this research aims to elucidate the underlying mechanisms governing lithium-ion storage in  $CoFe_2O_4$  and optimize its electrochemical performance. The synthesized  $CoFe_2O_4$ nanostructures exhibited high specific surface area, porous morphology, and uniform particle distribution, which are critical for efficient lithium-ion storage and transport.

Electrochemical evaluation demonstrated a high specific capacity, excellent rate capability, and improved cycling stability. These findings suggest that the unique structural and electronic properties of cobalt ferrite contribute significantly to its superior electrochemical performance. The high specific surface area and porous morphology facilitate better electrolyte penetration and lithium-ion diffusion, while the robust crystal structure ensures stability during repeated charge-discharge cycles.

Thus, this study provides a comprehensive understanding of cobalt ferrite as a promising anode material for high-performance lithium-ion batteries. The findings offer valuable insights for the rational design of advanced anode materials and contribute to the development of sustainable energy storage solutions. By highlighting the advantages of CoFe<sub>2</sub>O<sub>4</sub>, this research paves the way for its practical application in next-generation lithium-ion batteries, aiming to enhance energy density, efficiency, and longevity.

\*\*\*\*

## Enhanced physical properties of BiFeO<sub>3</sub>-modified Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> thin film

## prepared by pulsed laser deposition technique for memristor devices

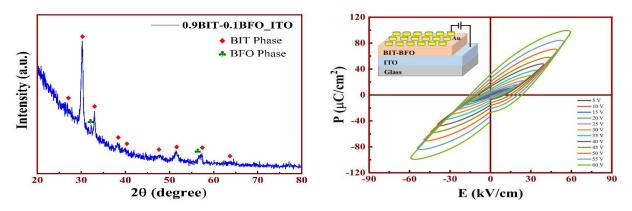
Priyanka Mitra<sup>1\*</sup> and B. Harihara Venkataraman<sup>1</sup>

1 Department of Physics, BITS-Pilani, Hyderabad Campus, Jawahar Nagar, Shameerpet, Telangana-500078, India \*Contact: p20190457@hyderabad.bits-pilani.ac.in

#### Category: Oral

Keywords: Multiferroic composite thin film, Pulsed laser deposition, GIXRD, Ferroelectric properties.

In the digital era, multiferroic materials are attractive owing to their simultaneous coupling of the ferroelectric and ferromagnetic order parameters. The urge to stimulate the magnetoelectric effect has driven researchers to utilise these materials for various applications like capacitors, sensors, spintronics, actuators and NVRAM devices. Usually, these material classifications exist in single or composite forms; however, due to the inherent characteristic limitations, single-phase materials may not be suitable for electronic applications compared to hybrid-phase. Keeping this in view, the 0.9Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> (BIT) - 0.1BiFeO<sub>3</sub> (BFO) diphasic composite thin film has been prepared using the Pulsed Laser Deposition (PLD) technique. This thin film sample was grown on the ITO-coated glass substrate using the KrF laser (248 nm). Deposition time is crucial in obtaining a highquality multiferroic composite thin film, among other deposition conditions like oxygen gas pressure, repetition frequency, and substrate temperature deposition. The as-grown hetero-structured thin film was characterized by Grazing Incident X-ray Diffraction (GIXRD), Field Emission Scanning Electron Microscopy (FeSEM), Atomic Force Microscope (AFM), X-ray Photoelectron Spectroscopy (XPS), and Electric Field-Dependent Polarization (P-E) techniques. The XRD pattern confirmed the co-existence of the diphasic composite thin film with a significant phase from the orthorhombic BIT and a minor Bragg reflection from the BFO (rhombohedral) phase. A sharp characteristic peak at  $2\theta \sim 30.08^{\circ}$  has confirmed the phase formation of a bismuth titanate associated with a low intense peak at  $2\theta \sim 32.10^{\circ}$  of the bismuth ferrite phase. The presence of all the constituent elements of BIT and BFO crystalline phases is validated by XPS analysis. The roomtemperature ferroelectric analysis exhibited a hysteresis loop with an enhanced magnitude of  $2P_r$  (~65  $\mu$ C/cm<sup>2</sup>) and  $2E_c$  (~ 38 kV/cm) than their bulk counterpart. Hence, this uniformly deposited di-phasic composite thin film configuration could be exploited as a better candidate for memory-based device applications.



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## **Nano and Functional materials**

# Impact of Aluminium Doping on the Nanocrystalline La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> as an Electrode Material for Supercapacitor Applications

<u>Aliva Panigrahi<sup>1</sup></u>, Amod Kumar<sup>1</sup>, Yaswant Kashyap<sup>2</sup>, Piyali Biswas<sup>3</sup>, Rakesh Kumar Pandey<sup>2</sup>, Manoranjan Kar<sup>3</sup>, Pawan Kumar<sup>1</sup>\*

> <sup>1</sup>Department of Physics, Mahatma Gandhi Central University, Bihar-845401, India. <sup>2</sup>Department of Chemistry, Mahatma Gandhi Central University, Bihar-845401, India. <sup>3</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna-801103, India \*Contact: pawankumarmgcub@gmail.com

Category: Oral

Keywords: Perovskite, XRD, Rietveld, Supercapacitor

The choice of stable and effective electrode material is crucial for the development of supercapacitor devices. Several classes of materials have proved their potential to become electrodes in supercapacitors. Among them, perovskite oxide electrodes are widely studied because of their high energy and power density. The ionic size of both cations in ABO<sub>3</sub>-type perovskite materials affects the stability or symmetry of the material, which has a significant effect on how well it works overall. However, cyclic stability has been a major setback for their wide-scale application as an electrode for supercapacitors. This can be resolved by partially substituting the cations with a suitable dopant whose ionic sizes and valency will impact the electrochemical performance of perovskites such as LaMnO<sub>3</sub> [1-3]. In the present investigation, the effect of Al and Sr doping in the nanocrystalline LaMnO<sub>3</sub> has been studied to optimize its electrochemical properties for the supercapacitor device application. The X-ray diffraction (XRD) patterns show that all the samples are essentially in the  $\alpha$ phase of Lanthanum strontium manganite, which could be indexed to  $R\overline{3}c$  (# 167) space group in hexagonal symmetry. The Rietveld refinement of all XRD patterns was carried out to access the corresponding change in the lattice parameters and unit cell volume with the replacement of La<sup>3+</sup> with  $Sr^{2+}$ , which has a greater ionic radius, and  $Mn^{3+}$  with  $Al^{3+}$ , which has a similar ionic radius. The supercapacitor devices were fabricated on the graphite sheet and characterized using a three-electrode and two-electrode electrochemical cell design. In an aqueous potassium hydroxide (KOH) electrolyte solution, experiments on cyclic voltammetry (CV), galvanostatic charge-discharge techniques (GCD), and electrochemical impedance spectroscopy (EIS) were conducted at room temperature. The electron transfer studies were performed to study the effect of doping on the electron transfer rate. These findings aid in the strategic design of optimized solid-state supercapacitors, broadening the application of Lanthanum Manganite as a stable and effective electrode material in various electrochemical energy storage systems.

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# **Renewable Energy (Conversion & Storage)**

# Low Lattice Thermal Conductivity-Driven Promising Thermoelectric Figure of Merit in NaSrSb and NaBaSb Zintl Phases

C. K. Vishwakarma<sup>1</sup>, <u>M. Zeeshan<sup>2,\*</sup></u> and B. K. Mani<sup>3,\*</sup> Department of Physics, Indian Institute of Technology, New Delhi 110016, India \*Contact: ird600132@physics.iitd.ac.in

#### Category: Oral

Keywords: Thermoelectricity, Energy.

Zintl phases have excellent thermoelectric prospects to put the waste heat to good use. In the quest for the same, using first-principles methods combined with Boltzmann transport theory, we explored two recent phases, NaSrSb and NaBaSb. We found remarkably low lattice thermal conductivities of 0.7 (2.1) and 0.4 (1.4) W m<sup>-1</sup> K<sup>-1</sup> at 900 K (300 K) for NaSrSb and NaBaSb, respectively, which are of the same order as other potential Zintl phases such as  $Sr_3AlSb_3$  and BaCuSb. We find that such low values could be attributed to the short phonon lifetimes and small phonon group velocities in the lattice. The calculated electrical transport properties reveal a large Seebeck coefficient for both materials. Furthermore, combining low lattice thermal conductivity with electrical coefficients, we obtained a high figure of merit of ZT ~ 1.9 at 900 K for n-type NaSrSb. On the other hand, the figure of merit of NaBaSb reaches the unity. We are optimistic about our findings and believe that our work sets a basis for future experimental investigations.

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## Investigation of Grain Boundary Segregation and Short Range Chemical Ordering in Multi Principal Element Alloy

Md. Lokman Ali

Department of Physics, Pabna University of Science and Technology, Pabna-6600, Bangladesh

#### Abstract

The segregation of the grain boundary (GB) and chemical short-range order (CSRO) influences the evolution of the microstructure and mechanical properties of multi principal element alloys. GB segregation and CSRO production at GB in NiCoCr medium entropy alloy (MEA) at various GBs have not been extensively researched. In this study, we looked into GB segregation and CSRO production at GB in a NiCoCr MEA alloy. A Semi Grand Canonical Monte Carlo (SGCMC) technique was used to construct thermodynamically equilibrium tilt GB structures of  $\Sigma 5$  and  $\Sigma 9$ . We confirmed GB segregation by evaluating the distribution of chemical composition perpendicular to the GB, which shows that less Ni is located in the GBs. Furthermore, the in-plane partial radial distribution function (RDF) in the GB region was used to explore the CSRO at GBs. We discovered that GB-specific CSRO structures can form in the GB region, which differs from CSRO in the bulk region. Furthermore, we study the impact of lattice relaxation on the CSRO at GB. By elucidating the production of CSRO at GB in multi-principal element alloys, the current work advances understanding of GB segregation and GB CSRO in multi-principal element alloys, enriching the knowledge base for materials design.

**Keywords**: Medium entropy alloy, Chemical ordering, Grain boundary segregation, Semi Grand Canonical Monte Carlo simulation

# Josephson diode effect in a quantum dot junction

## Debika Debnath<sup>1</sup>, Paramita Dutta<sup>1</sup>

<sup>1</sup> Physical Research Laboratory, Navrangpura, Ahmedabad–380009, India

We theoretically study the Josephson diode effect (JDE) in a quantum dot (QD)–based Josephson junction (JJ) in the presence of an external magnetic field and Rashba spin-orbit interaction (RSOI). In order to achieve the diode effect in the JJ we break the time-reversal symmetry through the Zeeman field and the inversion symmetry is broken by RSOI. We calculate the Josephson current using the Keldysh nonequilibrium Green's function technique. Our QD with RSOI induces JDE in the heterojunction with a large rectification coefficient (RC) that can be tuned to be as high as 70% by an external gate potential, indicating a giant JDE in our QD junction. Our result also shows that the rectification property could be enhanced with the inclusion of chirality in the QD. Interestingly we find that the sign and magnitude of the RC are highly controllable by the magnetic field and RSOI. We also investigate the role of electronelectron correlation to the Josephson diode by incorporating an interacting QD as the intermediate tunneling medium. Our proposed QD–based Josephson diode (JD) has the potential to be an efficient superconducting device component.

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## NANO AND FUNCTIONAL MATERIALS

# Atomic Switch Networks of Ag-Ag<sub>2</sub>S Core-Shell Nanoparticles for Neuromorphic computing

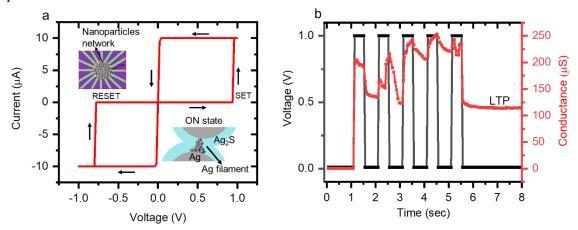
Samapika Mallik<sup>1,2</sup>, Thien Tan Dang<sup>1</sup>, Yusuke Nakaoka<sup>1</sup>, Yuki Usami<sup>1,2</sup>, Hirofumi Tanaka<sup>1,2</sup> <sup>1</sup> Graduate School of Life Science and Systems Engineering, Kyushu Institute of Technology (Kyutech), 2-4 Hibikino, Wakamatsu, Kitakyushu, 808-0196, Japan <sup>2</sup> Research Center for Neuromorphic AI Hardware, Kyutech, Kitakyushu, 808-0196, Japan \*Contact: mallik.samapika146@mail.kyutech.jp

#### Category: Invited

Keywords: Neuromorphic Computing, Atomic Switch Network, Core-Shell Nanoparticles, Synaptic Plasticity

Atomic switch networks (ASNs), made of interconnected switches, mimic synaptic plasticity and enable memory functions similar to the human brain, combining individual memristive properties with large-scale system features<sup>1</sup>. These networks play a vital role in neuromorphic computing by supporting dynamic adaptation, parallel processing, and energy-efficient computation. In this work, we demonstrate the synaptic behavior of an ASN using Ag-Ag<sub>2</sub>S core-shell nanoparticles.

Ag-Ag<sub>2</sub>S nanoparticles were synthesized using a modified Brust-Schiffrin method<sup>2</sup>. The device structure (inset, Figure 1a) features 16 electrodes with nanoparticles drop-cast into a circular gap. Figure 1a shows the typical current-voltage (I-V) characteristics of the network at room temperature. Under the sweeping of positive bias from 0 to 1 V with a voltage step of 20 mV, the device exhibited a SET process at 0.94 V from the OFF to the ON state (Inset of Figure 1a). When the voltage was swept back from 1 V to -1 V, the device RESET at -0.8 V, indicating bipolar resistive switching, which is the basis for non-volatile memories. Figure 1b shows that the increased conductance under applied voltage pulses persisted even after the pulses were removed, indicating long-term potentiation (LTP). Our results reveal stable switching behavior and quantized conductance states at integer multiples of  $2e^2/h$  (G<sub>0</sub>). Repeated voltage sweeps and pulse applications triggered a transition from volatile to non-volatile switching, analogous to the shift from short-term to long-term memory in biological synapses. By sweeping to higher voltages, we successfully achieved a longer retention time of 92 minutes, indicating the potential of the Ag-Ag<sub>2</sub>S nanoparticle network for long-term memory applications. These findings suggest that the nanoparticle network could be promising candidate for neuromorphic system development.



**Figure:** (a) I-V characteristics of the Ag-Ag<sub>2</sub>S nanoparticle network. Inset (upper left): schematic of the device structure (green: electrodes, gray: nanoparticles); lower right: schematic of the ON state. (b) Increased conductance under voltage pulses, maintained after pulse removal, demonstrating long-term potentiation (LTP).

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## **Renewable Energy (Conversion & Storage)**

# Boosting the performance Li ion battery electrode and Electrocatalytic Water splitting via MXene based heterostructures

<u>Shubham Sahoo<sup>1</sup></u>, Dr. Soumya Jyoti Ray<sup>2</sup> <sup>1,2</sup>Indian Institute of Technology Patna, Bihta, Bihar, 801103

Shubhamsahoo4u@gmail.com

## Category: Poster

Keyword: HER, OER, DFT, heterostructure, Gibbs free energy

We investigated the electrochemical performance and electro catalytic mechanism<sup>1</sup>, specifically the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) of heterostructures(HS) of two dimensional MXene Ti<sub>3</sub>C<sub>2</sub>X<sub>2</sub> (X= F,O,OH) and Fe<sub>2</sub>O<sub>3</sub>. We investigated the electrochemical performance and water-splitting mechanism for Ti<sub>3</sub>C<sub>2</sub>F<sub>2</sub>, Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub>, Ti<sub>3</sub>C<sub>2</sub>F<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub> and Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub> heterostructures with Density functional theory<sup>2</sup> (DFT) frame work. The lowest adsorption energy was observed on top of the carbon of MXene. The terminating functional F of MXF is inactive for the H atom with a value of 1.97 eV, attributed to the difficulty of hydrogen atom adoption due to the electronegativity of the fluorine atom. The calculated Gibbs free energy difference  $\Delta G_{H}$  is 1.23 eV, 1.14 eV, -0.18 eV and -0.15 eV for MXF, XMFFO HS, MXO and MXOFO heterostructure (Fig 1.b). On the other hand, Li ion faced vary low diffusion barrier of 0.06 eV at the interface of the HS (Fig 1.a) which is very low as compared to barrier faced on Fe<sub>2</sub>O<sub>3</sub> (3.1 eV). The studies reveal Ti<sub>3</sub>C<sub>2</sub>X<sub>2</sub> helps to improve the electrochemical performance while Fe<sub>2</sub>O<sub>3</sub> helps in overall water splitting mechanism.

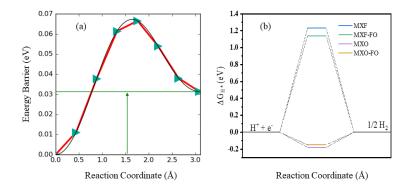


Fig 1: (a) Diffusion barrier at interface (b) Gibbs free energy variation with reaction coordinate during Volmer-Heyrovsky mechanism of  $Ti_3C_2(OH)_2 - Fe_2O_3$  HS.

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## Multifunctional Resistive Switching in Magnetization-graded Ni/NiMnIn/V2O5 Flexible Heterostructure towards Brain-inspired Neuromorphic Computing

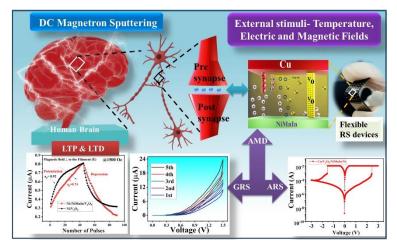
Kumar Kaushlendra<sup>1</sup>, and Davinder Kaur<sup>1\*</sup>

Functional Nanomaterials Research Laboratory (FNRL), Department of Physics and Centre for Nanotechnology, Indian Institute of Technology Roorkee, Uttarakhand, India \*Corresponding author: davinder.kaur@ph.iitr.ac.in

Keywords: Neuromorphic, RRAM devices, thin film, 2D materials, functional materials

## Abstract

Bio-inspired neuromorphic computing (NC) is attracting significant research interest due to the imitation of the human brain functioning in electronic devices. The current study describes a flexible Cu/V<sub>2</sub>O<sub>5</sub>/NiMnInbased memory device fabricated using the DC magnetron sputtering technique on flexible Ni substrate. It manifests the simultaneous existence of analog and abrupt switching characteristics, making it promising for neuromorphic applications. The switching behavior has been explained through the proposed analytical model. In abrupt resistive switching, the device displays a reasonably high OFF/ON resistance ratio of ~4.1×103, endurance (~5000 cycles), and data retention time (~4500 s). The tunability of the device has been investigated by studying the influence of external stimuli, such as temperature and magnetic field anisotropy, on the SET voltage. The realization of LTP and LTD synaptic functions in analog switching demonstrates the nonlinear and asymmetric features of the device. The effect of temperature on LTP, LTD, and memory window has been thoroughly investigated. The strain generated in the NiMnIn layer during the first-order martensite transformation aids in tuning the LTP and LTD of the device. The negative and positive piezomagnetic coefficients of Ni and NiMnIn lead to magnetization-graded ferromagnetic assembly and enhance the linearity of LTP and LTD. Additionally, the memory device exhibits outstanding flexibility. The current work opens up new possibilities for upcoming neuromorphic applications.



## **Table of Contents (TOC)**

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### The MnAl-alloy Nanoparticles Incorporated PVDF-based Piezoelectric Nanogenerator as a Self-powered Real-time Pedometer Sensor

Tupan Das<sup>1</sup> and Manoranjan Kar<sup>1, \*</sup> <sup>1</sup>Indian Institute of Technology Patna, Bihta, Bihar, 801106 \*Contact: mano@iitp.ac.in

Keywords: Nanogenerator, Nanofiber, Alloy, Electrospinning, Piezoelectric nanogenerator

This study introduces a flexible, sensitive, and cost-effective hybrid piezoelectric nanogenerator (PENG) by integrating MnAl-alloy nanoparticles into a PVDF nanocomposite film. The MnAl-alloy nanoparticles serve as a nucleating agent for promoting the formation of the electroactive  $\beta$ -phase. It is observed that the electro-active  $\beta$ -phase, dielectric permittivity, saturation polarization and output performance of the device are becoming promising with the incorporation of the MnAl-alloy nanoparticles up to 7.5 wt% in the PVDF matrix. Hence, in this work, we report a MnAl-alloy-based optimized piezoelectric nanogenerator device using a free-standing nanofiber mat (7.5 wt% MnAl-alloy) prepared by the electrospinning technique. The as-fabricated piezoelectric nanogenerator effectively channels charges generated by mechanical stress to the electrodes, resulting in an impressive output voltage of approximately 16V and an output current of around 7.1µA, yielding a power of 47 µW across 4.5 MΩ resistor. Furthermore, energy harvesting from human movements such as jogging, knee bending and walking is demonstrated for practical application. A piezo potential of approximately 8V generated during walking showcases the development of a self-powered pedometer. Furthermore, tapping the PENG charges a capacitor of 0.1µF up to approximately 1V, demonstrating the potential application for the power up of small portable electronic devices.

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### Ti-Cr-N Nanopyramid/Nitrogen-Doped Carbon Quantum Dot/Stainless Steel Mesh as a Flexible Supercapacitor Electrode

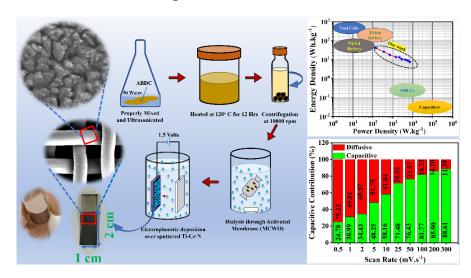
Rajesh Kumar, Bhanu Ranjan, Krishan Kumar, Satyam Shankhdhar and Davinder Kaur\*

Functional Nanomaterials Research Laboratory (FNRL), Department of Physics and Centre for Nanotechnology, Indian Institute of Technology Roorkee, Uttarakhand, India \*Corresponding author: davinder.kaur@ph.iitr.ac.in

*Keywords:* Titanium chromium nitride nanopyramids; Nitrogen-doped carbon quantum dots; Pseudocapacitive storage; Flexible supercapacitor electrode; High energy density.

### Abstract

Nitrogen-doped carbon quantum dots (N-CQDs) incorporated into highly conductive transition metal nitride offer enhanced electrochemical performance, delivering high energy density and outstanding electrochemical stability. The present study reports a high-performance supercapacitor electrode consisting of electrophoretic anchored zero-dimensional N-CQDs with reactively co-sputtered titanium chromium nitride nanopyramids (Ti-Cr-N) thin film on flexible stainless-steel mesh (SSM) substrates. The nanopyramids of N-CQDs/Ti-Cr-N offer remarkable electrochemical performance through Li<sup>+</sup> storage, ascribed to the abundant electroactive sites and enhanced synergism between the high specific surface area of N-CQDs and higher conductivity of Ti-Cr-N. Subsequently, the N-CQDs/Ti-Cr-N/SSM electrode in 1M Li<sub>2</sub>SO<sub>4</sub> aqueous electrolyte exhibits an excellent gravimetric capacitance of 393.8 F.g<sup>-1</sup> at a specific current density of 0.32 A.g<sup>-1</sup>. Further, the N-CQDs/Ti-Cr-N/SSM heterostructure outperforms other multi-cationic-based supercapacitors with a maximum energy density of 41.41 Wh.kg<sup>-1</sup> and a superior power density of 7.0 kW.kg<sup>-1</sup>. Impressive electrochemical stability of ~88.6% is retained by the heterostructure even after 5000 continuous charge-discharge cycles. Insights into charge-storage mechanisms highlight the dominance of surface-limited capacitive and pseudocapacitive kinetics, with fewer contributions from diffusion-controlled faradaic processes. Furthermore, an exemplary mechanical stability of ~99.98% over 1200 bending cycles demonstrates the N-CQDs/Ti-Cr-N/SSM heterojunction's excellent resilient structural strength, validating the present electrode potential for high-performance flexible supercapacitor application.



### **Graphical Abstract**

- R. Kumar, B. Ranjan, K. Kumar, S. Shankhdhar, D. Kaur, Ti-Cr-N Nanopyramid/Nitrogen-Doped Carbon Quantum Dot/Stainless Steel Mesh as a Flexible Supercapacitor Electrode, ACS Applied Nano Materials, 7 (7), 7663-7673, 2024.
- R. Kumar, B. Ranjan, D. Kaur, Pseudocapacitive performance of reactively co-sputtered titanium chromium nitride nanopyramids towards flexible supercapacitor with Li-ion storage, J. Energy Storage.
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### Lattice distortion driven electrocaloric and optical properties of rare earth modified of leadfree perovskite materials

Jyotirekha Mallick

Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Powai, Maharashtra , India-400076

#### \*Contact: 20004022@iitb.ac.in

Keywords: Electrocaloric effect, Lead-free Perovskites, Optical Bandgap, Solid state refrigeration

Environment-friendly solid-state refrigeration based on the Electrocaloric effect (ECE) is the best mechanism in advanced cooling technology for microelectronic cooling devices. Moreover, ferroelectric materials also exhibit interesting photosensitive properties which enable it for multi-functional applications. In this respect, structural, electrocaloric effect and optical properties of A site rare earth modified Ba<sub>0.8</sub>Sr<sub>0.2</sub>TiO<sub>3</sub>(BSTO) have been thoroughly investigated. The deduction of tetragonality of Sm<sup>3+</sup> modified BSTO is the main reason behind the diminished electrocaloric performance of Ba<sub>0.8-</sub>xSm<sub>x</sub>SrO<sub>.2</sub>TiO<sub>3</sub> (BSmSTO). The relaxor behavior of the synthesized compound has been confirmed through temperature variation dielectric and ferroelectric measurements that show characteristic temperature-dependent responses. The highest electrocaloric parameters such as isothermal entropy change ( $\Delta S$ ), adiabatic temperature change ( $\Delta T$ ), and electrocaloric strength  $\Delta T/\Delta E$ were found to be 1.230 Jkg<sup>-1</sup>K<sup>-1</sup>, 0.862 K, and 0.028 73 K cm/kV at 316 K, respectively, for Ba<sub>0.77</sub>Sm<sub>0.03</sub>Sr<sub>0.2</sub>TiO<sub>3</sub>[1]. The optical band gap of all synthesized samples has been estimated by using the Tauc plot method and concluded that the band gap decreases from 3.13 eV to 2.97 eV with the increase in  $\text{Sm}^{3+}$ concentration due to the structural disorder induced in the lattice because of the formation of A-site vacancies and distortions in octahedral clusters (TiO6) [2]. Basically, this A site vacancy produces shallow defects in the band gap of BSmSTO and reduces its value. This comprehensive study gives an idea about the correlation between the crystal structure and the electrical-optical properties of BSmSTO, providing valuable insights into the design of multifunctional ferroelectric materials for advanced cooling applications and optoelectronic devices.

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### **Nano and Functional materials**

## Synthesis and Characterization of La<sub>2</sub>BMnO<sub>6</sub> (where B = Co, Ni, Cu) for Energy Storage Applications

<u>Amod Kumar<sup>1</sup></u>, Yaswant Kashyap<sup>2</sup>, Tupan Das<sup>3</sup>, Rakesh Kumar Pandey<sup>2</sup>, Manoranjan Kar<sup>3</sup>, Pawan Kumar<sup>1</sup>,\*

<sup>1</sup>Department of Physics, Mahatma Gandhi Central University, Bihar-845401, India. <sup>2</sup>Department of Chemistry, Mahatma Gandhi Central University, Bihar-845401, India. <sup>3</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna-801103, India \*Contact: pawankumarmgcub@gmail.com

### Category: Oral

Keywords: Double perovskites, Sol-gel, XRD, Rietveld, Supercapacitor

The technological and industrial development that has emerged in recent decades often implies excessive energy consumption, and currently, most of the energy sources used are non-renewable. This research investigates the potential of double perovskite oxides  $La_2BMnO_6$  (where B = Co, Ni, Cu) as electrode materials for energy storage applications. These materials offer promising properties due to their structural flexibility, tunable electronic structures, and high theoretical capacity. Perovskite oxides have attracted significant attention in energy storage performances because of their eccentric physical and chemical features [1]. Herein, we aim to study the electrochemical characterization of double perovskite  $La_2BMnO_6$  (where B = Co, Ni, Cu) prepared through a facile sol-gel route. The synthesized materials were characterized using various techniques, including X-ray diffraction (XRD) and electrochemical impedance spectroscopy (EIS). The Rietveld refinement of all XRD patterns was performed to evaluate changes in lattice parameters, unit cell volume, and crystal structure. The electrochemical performance of the nanocomposites of double perovskite materials (70 wt %), Graphene oxide (10 wt%), Polypyrrole (10 wt%), and the PVDF binder (10 wt %) on graphite sheet as substrate, have been evaluated through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electron transfer rate measurements. At first, the electrochemical studies of the working electrodes have been carried out in a three-electrode setup, followed by a two-electrode setup for energy storage applications. The results demonstrate the influence of the B-site cation on the structural, electronic, and electrochemical properties of the double perovskites. The findings provide valuable insights into designing and optimizing electrode materials for advanced energy storage devices.

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### Unveiling different structural orderings in Fe5-xGeTe2

<u>Vaibhav Walve<sup>1\*</sup></u>, Piyush Parakh<sup>1</sup>, Umashankar Rajput<sup>1</sup>, Akash S<sup>2</sup>. Mhase, Kirandeep Singh<sup>2</sup>, and Aparna Deshpande<sup>1</sup> 1 STM and Atom Manipulation Lab, IISER Pune, India 2 Physical and Material Chemistry Division, CSIR-NCL Pune, India \*Contact: Vaibhav.walve@students.iiserpune.ac.in

### Keywords: van der Waals itinerant ferromagnet, STM, STS.

We investigate the metallic van der Waals itinerant ferromagnet  $Fe_{5-x}GeTe_2$  with atomic scale, spatially resolved low-temperature scanning tunneling microscopy (STM), and spectroscopy (STS). STM images unveil a new structural order  $2a \times 1a$  along with the known order  $\sqrt{3}a \times \sqrt{3}a$  manifesting as non-uniform domains<sup>[1]</sup>. STS shows spatial and energy resolved local density of states that reveal the crucial influence of Fe(1) site occupancy on the system's electronic interactions. Our magnetization measurements show magnetic anomalies at lower temperatures and identify a Curie temperature (T<sub>c</sub>) surpassing room temperature. Collectively, our results elucidate the intricate nature of  $Fe_{5-x}GeTe_2$  and underscore its potential for tunability of spintronics and high-temperature magnetic applications.

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## **Two Dimensional (2D) Materials**

### **Superconducting Diode Effect in Van der Waals Josephson Junctions**

<u>Annu Anns Sunny</u>, Parvathy Gireesan, Madhu Thalakulam\* Indian Institute of Science Education and Research, Thiruvanathapuram, Kerala, 695551, India Email:madhu@iisertvm.ac.in

### Category- Poster

Keywords –Superconducting Diode effect, Josephson Junction, Niobium Diselenide

A lot of attention has been drawn to the recently discovered superconducting diode effect (SDE), also known as the rectification of supercurrents, from a theoretical standpoint as well as in terms of novel device applications in superconducting electronics, superconducting spintronics, and quantum information and communication technology<sup>1</sup>. To put in simple words, the diode effect in superconductors occurs when the critical current  $I_c$  depends on the current sweep direction. When both inversion and time-reversal symmetries are broken,  $I_c$  can be nonreciprocal<sup>2</sup>. Van der Waals materials (Two-dimensional materials(2D)) with high crystal quality and tunable transition temperatures can be a promising candidate for superconducting Josephson Junction devices, which possess broken inversion and time reversal symmetries.

Van der Waals heterostructure, which consists of Niobium Diselenide NbSe<sub>2</sub>, a superconducting Transition Metal Dichalcogenide (TMDC material) which has a transition temperature of T<sub>c</sub> 7K, can be an excellent device that demonstrates superconducting diode effect. In this work, NbSe<sub>2</sub> Josephson junction is fabricated by micromechanical exfoliation of layered NbSe<sub>2</sub> flakes and vertically stacking them by dry transfer technique on prepatterned Cr-Au metalized probes and followed by etching to control the junction area. An NbSe<sub>2</sub> flake with an odd number of layers can be a reason for broken inversion symmetry, and the application of an in-plane magnetic field can break the time-reversal symmetry of the Josephson junction. From the Current-voltage characteristics and magnetotransport measurements at temperatures lower than the critical temperature,  $I_{c+} \neq |I_{c-}|$  at a definite in-plane magnetic field where  $I_{c+}$  is the critical current in the forward directions and  $I_c$  is the critical current in backward directions. Second harmonic resistance measurements and half-wave rectification using square waves at different magnetic fields are also carried out to confirm the superconducting diode effect.

Our study demonstrates that low-dimensional crystalline superconductors like NbSe<sub>2</sub> are promising systems to realize the effects like superconducting diode effect and, consequently, valuable for additional device applications.

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## **Two-Dimensional (2D) Materials**

### Probing Surface defects on bulk semiconductor CrSBr

Subhrajit Dalai<sup>1</sup>, V. Walve<sup>1,</sup> and A. Deshpande<sup>1\*</sup>

1 Department of Physics, Indian Institute of Science Education and Research, Pune, India

\*Contact: aparna.d@iiserpune.ac.in

### Category: Poster

### Keywords: Spintronics, Scanning tunneling microscopy, van der Waals (vdW)

The discovery of exfoliated graphene in 2004 ignited a new wave of research into two-dimensional van der Waals (vdW) materials, which exhibit significantly different physical properties compared to their bulk counterparts. This also inspired the discovery of 2D vdW magnets for potential use in spintronics, magnonics and quantum information application. Some examples of such magnets are CrI<sub>3</sub>, Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub>, VSe<sub>2</sub> and Fe<sub>3</sub>GeTe<sub>2</sub>, many of them have great sensitivity to ambient conditions posing a significant barrier to integrate in practical device [1].

The vdW material CrSBr has recently emerged as a highly stable antiferromagnetic material at ambient conditions, featuring an intriguing semiconducting quasi-one-dimensional electronic structure (band gap of 1.5 eV) and a high magnetic ordering temperature ( $T_N = 132$  K). This material hosts strong coupling between its electronic and magnetic properties[2]. Defects in CrSBr are inevitably present and can significantly alter band gap and local magnetic property making it an interesting topic to study.

The experimental identification of defects of CrSBr at atomic level is still lacking. In this study, we performed an atomic investigation of these defects using scanning tunneling microscopy (STM) and spectroscopy (STS), identifying three types, i.e., Br vacancy ( $V_{Br}$ ), S vacancy ( $V_S$ ), and Cr Vacancy ( $V_{Cr}$ ) with distinct spatial distributions of the localized defect states [3]. This will be extremely useful for designing a novel 2D magnet with a tunable band gap through defect engineering.

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## **Electron and Phonon Hydrodynamics in Graphene**

<u>Subhalaxmi Nayak</u><sup>\*</sup>, Cho Win Aung, Thandar Zaw Win, Ashutosh Dwibedi, Sabyasachi Ghosh Sesha Vempati<sup>5</sup>

Department of Physics, Indian Institute of Technology Bhilai, Kutelabhata, Durg, Chhattisgarh,491002, India.

\*Contact: subhalaxmin@iitbhilai.ac.in

### Category: Poster

*Keywords:* Hydrodynamics, Specific Heat, Einstein's theory of specific Heat, Lorenz ratio, electron-phonon scattering

Phonons are the quantum of lattice vibration energy that behave like quasiparticles. The interacting phonons depict hydrodynamic behavior at low frequencies and extended wavelength limits. Phonon hydrodynamics has become popular because it strongly contributes to electrical properties and heat transport phenomena in crystalline materials like graphene. In the case of phonon hydrodynamics, the phonon-phonon scattering is predominant among boundary, impurity, and defect-mediated scattering. Here, we analytically calculated and compared various thermodynamic quantities like energy density, number density, pressure, and specific heat per particle for both phonon and electron in the hydrodynamics regime for graphene. We have analyzed the specific heat capacity versus temperature for various cases and compared it with the traditional Dulong Petit law and Einstein's theory of specific heat. This results in the electron and phonon contributions to the specific heat dominating over the conventional behavior of metal in the low-temperature region. The fluid behavior of electrons and phonons may also violate the Wiedemann-Franz law for the graphene system.

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## **Topological condensed matter & quantum materials**

## Nano-Porous Carbon-Based Kagome Topological Insulator with Tunable Electronic and Topological Properties

Shashikant Kumar<sup>1</sup> and Prakash parida<sup>1,\*</sup> <sup>1</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Bihar, 801106, India <sup>\*</sup>Contact : pparida@iitp.ac.in

Category : Poster

Keywords : Kagome, Graphene, Spin-orbit coupling, Berry Curvature, Topological Insulator.

We present a carbon-based two-dimensional (2D) kagome topological insulator with a nanoporous structure arranged in a graphene-like kagome-honeycomb pattern. Inspired by recent bottom-up synthesis techniques by Galeotti et al., pore sizes are systematically varied, leading to a transition in the material from metallic to semiconducting. A key finding of this study is the ability to control both electronic and topological properties of the system. As pore size increases, the band structure remains stable near the Fermi energy, showing a zero band gap. However, the Fermi energy shifts from the Dirac band to a flat band. In graphene, the introduction of holes or pores, commonly called anti-dots, typically results in the formation of a non-zero gap in the electronic structure. Schmidt et al. demonstrated the effectiveness of helium ion beam milling for creating smaller pores, fabricating pores of 3 to 4 nm with a pitch of 10 nm. Similarly, this study achieves tunable pore sizes ranging from 1 to 4 nm, enabling precise control over electronic properties. The inclusion of spin-orbit coupling introduces a small bandgap, enhancing the topological properties of the material. The non-zero Chern number derived from the Berry curvature confirms the topological insulating behavior. These findings provide valuable insights into the design and development of tunable 2D topological insulators for applications in quantum computing and advanced spintronic devices.

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### **Two-dimensional (2D) materials**

## Unveiling the Potential of TiO<sub>2</sub>, a high-K dielectric in few layer MoS<sub>2</sub> based Field Effect Transistor for Advanced Electronic Applications

Samiksha<sup>1,\*</sup> and Pramod Kumar<sup>1</sup>

1 Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India. \*Contact: <u>samikshabhatia@iitb.ac.in</u>

Category: Poster

Keywords: TMDs, FET, Dielectric engineering, MoS<sub>2</sub>, TiO<sub>2</sub>.

In this study, we have investigated the impact of using a high-K gate oxide TiO<sub>2</sub> (K $\approx$  80) on the electric performance of the back gated  $MoS_2$  field effect transistor (FET). It is observed that the mobility has been significantly increased from 19 cm<sup>2</sup>/V·s to 67 cm<sup>2</sup>/V·s (~ 3.5 times). While TiO<sub>2</sub> has been used as an interfacial layer between the MoS<sub>2</sub> channel and metal contacts to mitigate Fermi-level pinning and reduce the effective Schottky barrier height [1], there have been lack of experimental studies focusing on its role as a gate dielectric. High-k dielectrics significantly reduce coulombic scattering through the dielectric screening effect. Divya et al. [2] predicted in simulation studies that TiO<sub>2</sub> could offer better electrical performance than the more widely studied Al<sub>2</sub>O<sub>3</sub> (K  $\approx$  9.3) and HfO<sub>2</sub> (K  $\approx$  25) making experimental investigation of TiO<sub>2</sub> as a gate dielectric crucial. A 20 nm of  $TiO_2$  has been deposited using radio-frequency (RF) sputtering on thermally grown 200 nm SiO<sub>2</sub> on highly doped Si substrate and a backgated 5-layer exfoliated MoS<sub>2</sub> FET has been fabricated using the Photolithography and Sputter techniques. We observed a 3.5 fold increment in mobility, maximum  $I_{on}$  current at  $V_d = 100$  mV has been improved from 0.35  $\mu$ A/ $\mu$ m to 0.78  $\mu$ A/ $\mu$ m, however  $I_{off}$  current has also been increased from 2.4 pA to 78 nA which decreased the  $I_{on/off}$  ratio from  $4.3 \times 10^5$  to  $1.4 \times 10^3$ . This degradation in the I<sub>on/off</sub> ratio may be attributed to the leakage in sputter-deposited TiO<sub>2</sub>. This study demonstrates that TiO<sub>2</sub> has the potential to significantly enhance mobility in MoS<sub>2</sub> FETs. However, to fully realize its benefits, further research is essential to focus on reducing the off current which can potentially be addressed by using ALD-deposited TiO<sub>2</sub> or incorporating a buffer layer over TiO<sub>2</sub>.

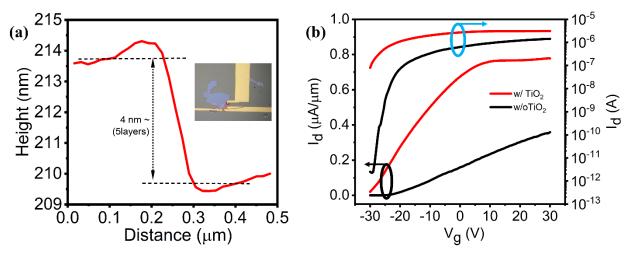


Figure 1: (a) AFM height profile, inset; Optical image of the fabricated FET and (b) Transfer characteristics in log and linear scale at  $V_d = 0.1$  V with and without TiO<sub>2</sub>.

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### Rumi De

# Department of Physical Sciences, IISER Kolkata Mohanpur, Nadia 741246, West Bengal, India Email: rumi.de@iiserkol.ac.in

**Title:** The dynamics of evasion and pursuit in prey swarms and the emergence of various escape strategies during a predator attack.

Abstract: Cohesive group formation has been observed in diverse species, such as a flock of birds, a school of fishes, and a swarm of insects. In nature, swarming behavior has generally been found in search of food, for breeding, to avoid predators, etc. It is quite intriguing how a large number of individuals self-organize to form collective groups and generate complex organized patterns. In this talk, I will discuss how simple computational models, specifically self-propelled particle models, help get an insight into the underlying dynamics of a prey swarm under a predator attack. Our study shows that varying ranges of interaction strongly influence the trajectory of prey when chased by a predator. As seen in nature, diverse escape patterns emerge, such as circling, chasing, maneuvering into an arc, dividing into subgroups, and merging again into a single group to avoid the predator attack. We also find that inertia plays a pivotal role in the survival dynamics of the prey swarm. Our research reveals the existence of three distinct regimes based on the predator-to-prey mass ratio: (i) frequent chase and capture leading to the non-survival of the prey swarm, (ii) the survival regime without the capture of prey, and (iii) an intermediate regime where competition between pursuit and capture occurs, resembling an arms race as seen in natural ecosystems. Interestingly, our study demonstrates the existence of a favorable predator-prey mass ratio for efficient predation, which corroborates with the field studies.

### Understanding and Study of the Kagome Metal CsV<sub>3</sub>Sb<sub>5</sub> with AFM and Raman spectroscopy

<u>Rajashri Renuse<sup>1</sup></u>, Vaibhav Walve<sup>1</sup>, Luminita Harnagea<sup>2</sup>, and Aparna Deshpande<sup>1</sup> 1 STM and Atom Manipulation Lab, IISER Pune, India 2 I-HUB Quantum Technology Foundation, IISER Pune, India \*Contact: Email ID

### Keywords: Kagome metal, AFM, Raman spectroscopy

Kagome lattices have gathered significant attention over the past few decades due to their corner-sharing triangular geometry, which induces geometric frustration and hosts exotic phases such as the quantum spin liquid phase. The recent discovery of new kagome materials, which are layered, air-stable, and exfoliable, has further intensified interest in this area<sup>[1]</sup>. This frustration in the kagome lattice gives rise to intriguing band structure features, including Van Hove singularities, Dirac cones, and flat bands<sup>[2]</sup>. In this study, we focus on the characterization of the kagome metal  $CsV_3Sb_5$  using Atomic Force Microscopy (AFM) and Raman spectroscopy on exfoliated flakes. Optimal exfoliation was achieved by initially using Scotch tape, followed by a transfer to blue tape, minimizing glue residue and improving yield. Time-dependent AFM measurements revealed a notably slow oxidation process in the exfoliated flakes, while Raman spectroscopy showed the second peak to be highly sensitive to sample quality, serving as a reliable indicator of the material quality.

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## Theme: Topological condensed matter & quantum materials

## Atomically thin obstructed atomic insulators in group-Va monolayers

Rahul Verma<sup>1,\*</sup> and Bahadur Singh<sup>1</sup>

<sup>1</sup>Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Mumbai 400005, India \*Contact: rahul.verma@tifr.res.in

### Category: Oral

Keywords: Obstructed Atomic Insulators, Quasi-symmetry, Spin-Hall conductivity, Spintronics devices

Understanding the electronic properties and topological states of quantum materials is crucial for both fundamental research and the development of topological electronic technologies. In this work, we demonstrate the presence of robust edge states in phosphorene and group-Va monolayers with puckered lattices [1]. By carefully analyzing the symmetry of the occupied atomic sites, we predict obstructed atomic insulator states in these monolayers. We show that despite having topologically trivial, phosphorene has occupied virtual Wyckoff positions. Cleaving through these sites generates partially occupied edge modes. These edge modes exhibit Rashba-type spin splitting with Rashba parameter ( $\alpha$ ) as large as 1.52 *eV* Å. We also domonstrate a topological phase transition induced by strain or doping, transforming the obstructed insulator phase into a phase with enhanced spin-Berry curvature. This transition results in a double quantum spin Hall state with a large quantized spin-Hall conductivity of  $4e^2/h$ , exceeding the value in any known materials. The experimental accessibility of phosphorene and other group-Va monolayers could validate the obstructed atomic states and enhanced spin-Berry curvature effects delineated in this study.

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### Theme: Other emerging areas

### Electric field induced emergent volatile resistive switching (RS) in Mott insulator titanate spinel

### Priyanka Maji<sup>1</sup>, Ayan Roy Chaudhuri<sup>2,\*</sup> and Debraj Choudhury<sup>1,\*</sup>

<sup>1</sup> Department of Physics, Indian Institute of Technology Kharagpur, W.B. - 721302, India <sup>2</sup> Materials Science Centre, Indian Institute of Technology Kharagpur, W.B. - 721302, India

### \*Contact : <u>priyankamaji2294@kgpian.iitkgp.ac.in</u>, <u>ayan@matsc.iitkgp.ac.in</u>, <u>debraj@phy.iitkgp.ac.in</u>;

### **Category: Poster**

### Keywords: Threshold field, Volatile resistive switching, Forming free switching, Selectors

Materials exhibiting a transition from an insulating to conducting state under the application of a small threshold current/electric field are extremely promising for a plethora of potential applications in the field of electronic devices and memory technology. Furthermore, they can provide unique platform to study the non-equilibrium phenomena and underlying microscopic mechanism in such systems. However, manifestation of resistive switching with very small threshold field (Eth) (~ few kV/cm) have rarely been achieved in transition metal spinel oxides//chalcogenides [1-2]. Mott breakdown with a small threshold field has recently been identified in the family of spinel oxides, more precisely in Vdoped MgTi<sub>2</sub>O<sub>4</sub> with  $E_{th} \sim 40$  V/cm at 50 K [3]. High-current-induced charge transfer from Ti<sup>3+</sup> to V<sup>3+</sup> softens the Jahn-Teller(JT)-effect-driven structural transition, which gives rise to metallicity. Here, we have investigated the resistive switching properties of magnesium titanate oxides. The system undergoes the breakdown at a much smaller threshold field (~ 60 V/cm at 40 K) than the Zener breakdown limit (~kV/cm). The electric-field induced low resistive state is metastable and the system returns to its initial high resistive state when the applied field or voltage is turned off manifesting volatile resistive switching (VRS). Interestingly, our system demonstrates a forming free and stable threshold switching with negligible cycle to cycle variations in switching voltages. Further, systematic investigations predict a non-thermal origin for the observed switching phenomena. Also the very low threshold field requirement in our system will benefit in terms of low power consumptions. Our study underlines that the current- or electric field-induced phase transition provides useful pathways to create tunable resistors/selector based on titanate spinels for low-temperature applications. Threshold switching devices also have shown potentials in imitating the imperative neural characteristics to be implemented as artificial neurons in the neuromorphic engineering.

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### **Two-dimensional (2D) materials**

## A first principles study of inducing magnetism in bilayers WSe<sub>2</sub> by 3d transition metal atom doping

Paras Poswal<sup>1</sup>\*, Neeraj Shukla<sup>1</sup>\*

1 Department of Physics. National Institute of Technology Patna, Patna, Bihar 800005, India \*Contact: neerajs@nitp.ac.in, poswalparas@gmail.com

### Category: Poster

Keywords: TMDs, Tungsten diselenide (WSe2), Density Functional Theory, 2D Material, Spintronics

In this study, first principles calculations have been performed for investigation regarding the structural stability, electronic and magnetic properties of pristine and transition metal doped bilayer tungsten diselenide (WSe<sub>2</sub>) [1]. Spin-polarized calculation using the Generalize Gradient Approximation with Hubbard correction (GGA+U) have been used to accurately capture the electronic correlations. Two different staking configuration, AA and AA', of bilayer WSe<sub>2</sub> have been considered, with AA' sequence identified as energetically most favorable and dynamically stable. To induce magnetism, doping of 3d transition metal atom has been done in one layer to achieve the configuration MSe<sub>2</sub>-WSe<sub>2</sub> (M= (M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn) [2]. The transition metal atoms exhibit strongly binding with nearest Se atoms, having binding energy ranging from -2.732 eV to -6.365 eV, indicating robust structural stability. Our calculations reveal that, TMs doping induce magnetization in the structure, with Mn-doped structure attaining maximum magnetic moment of order 3.63  $\mu$ B, which makes it a promising magnetic 2D material. Density of States (DOS) and band structure calculation identify the phase transition from semiconductor to metallic in doped configuration MSe<sub>2</sub>-WSe<sub>2</sub>. Especially, the Fe doped structure exhibit high degree of spin polarization of 75%, dominating by spin down states in the fermi level. This study opens up possibilities for the utilization of bilayer WSe<sub>2</sub> in advanced electronic and magnetic device application.

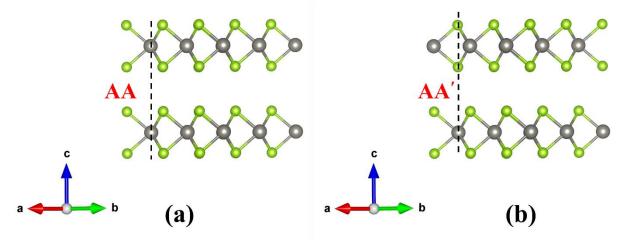


Figure. Stacking sequence of WSe2 bilayer (a) AA configuration, (b) AA' configuration

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## **Two-Dimensional (2D) Materials**

## **Thermal Transport in 2D materials**

Nikhil Joseph Joy<sup>1</sup>, Ranjuna M K<sup>1</sup>, and Jayakumar Balakrishnan<sup>1</sup>

Indian Institute of Technology Palakkad \*Contact: jayakumar@iitpkd.ac.in

Category: Invited

Keywords: 2D Materials, edge thermal transport, Graphene, MoS2

The effect of phonon-boundary scattering on the thermal transport in 2D materials is less explored. Here, we explore experimentally the thermal transport near graphene edges -zig zag and arm chair [1]. The microscopic roughness at the boundaries lead to dominant diffuse reflections, there by significantly reducing the thermal conductivity- at least by 50% near the edges in our samples. The results are in good agreement with the recent theoretical predictions [2]. Finally, I will also briefly discuss our results on other 2D materials like MoS<sub>2</sub> [3].

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# Cholesterol modulates the interaction of sodium salt with negatively charged phospholipid membrane

Kalyan Kumar Banerjee<sup>1</sup> and Sanat Karmakar<sup>\*</sup>

Soft matter and Biophysics Laboratory, Department of Physics, Jadavpur University, 188, Raja S. C. Mallick Road, Kolkata 700032, India.

<sup>1</sup>Email: kalyanbanerjee802@gmail.com \*Email: sanat.karmakar@jadavpuruniversity.in

Keywords: Membrane, cholesterol, zeta potential, ITC, NaI, Fluorescence spectroscopy.

We present a systematic study on how alkali metal salts, like NaCl and NaI, affect negatively charged phospholipid vesicles using a range of experimental methods. Our goal was to find out how chain saturation and cholesterol affect the interaction between the ions and the membrane. An isothermal titration calorimetry study on large unilamellar vesicles made from dimyristoyl phosphatidylcholine (DMPC) revealed that Na+ shows higher binding affinity to the DMPC membrane phase at 15 °C compared to the fluid phase at 30 °C. Further, cations also show stronger affinity to the membrane in the fluid composed of saturated lipids than that of unsaturated lipids. The binding affinity of Na+ with anionic vesicles prepared from a mixture of DMPC and DMPG was found to decrease significantly with increasing cholesterol as well as salt concentrations, as revealed by the zeta potential study. Besides the binding constant, the Gouy Chapman theory based on the electrostatic double layer shows that cholesterol reduces the surface charge density without altering the significant area per molecule. Further, the effect of counter-ions was investigated using fluorescence spectroscopy of an environmentsensitive lipophilic dye, nile red. Although cholesterol alters the emission properties of nile red significantly, there is no significant change in the presence of ions. This result suggests that anions do not bind significantly to anionic vesicles. The main striking feature of the ion-membrane interaction in the presence of cholesterol is that membranes with saturated lipids exhibit a completely opposite trend from membranes with unsaturated lipids.

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## Analytical tools in condensed matter

# Entanglement Dynamics of Many-body System With Evolving System Conditions

Devanshu Shekhar\*, Pragya Shukla

Indian Institute of Technology, Kharagpur \*E-mail: <u>devanshu2096@kgpian.iitkgp.ac.in</u>

### Category: Oral

Keywords: Entanglement, random matrix theory, many-body localization

*Abstract:* The entanglement analysis of a pure state of a many-body quantum system requires prior information about its density matrix / state matrix, obtained in principle by solving the Hamiltonian matrix. However, the missing information due to the complexity of the many-body interactions renders it necessary to consider an ensemble of Hamiltonian and, thereby, an ensemble of pure states, leaving a statistical description of the entanglement measures as the only option. We theoretically analyze the effect of varying system conditions on the entanglement statistics and identify a single functional of the system parameters that reveals a deep web of connection underlying different quantum states. We calculate the linear entropy and the von Neumann entropy as entanglement measures for various system sizes, and study their average and variance as a function of the single parameter. We also study the random-field Heisenberg model, which is believed to showcase many-body localization transition, by exactly diagonalizing the Hamiltonian, for numerical verification of our claims.

## **Two-dimensional (2D) materials**

# O<sub>2</sub>-assisted phase transition from mixed oxide phases of Mo to stable MoO<sub>3</sub> phase

Athira C<sup>1</sup>, \* Subhashis Gangopadhyay

1 Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031, India<sup>1,2</sup> \*Contact: subha@pilani.bits-pilani.ac.in

### Category: Oral

Keywords: Nanostructures, TMO, phase transition, thermal oxidation.

Nanostructured transition metal oxides (TMO), known for their unique electronic, magnetic, and optical properties at the nanoscale, have emerged as leaders in revolutionizing electronic applications [1]. At the nanoscale, these compounds undergo significant structural changes with widescale morphologies, resulting in the emergence of novel electromagnetic phenomena, which are not present in their bulk counterparts [2]. Among various TMOs, molybdenum oxides (MoOx) are one of the most appealing metal oxides because of their unique structural properties. Versatile applications of  $MoO_3$ and  $MoO_2$  span across several domains, encompassing electrochemical supercapacitors, lithium-ion batteries, electrocatalysis, sensors, and field emission devices [3]. Mo oxides usually appear in a mixed oxide phase which can undergo different phase transitions under specific growth conditions. In this work we aim to address a major challenge of the selective growth of a single oxide phase with an enhanced crystallinity of different oxide nanostructures. High purity MoO<sub>3</sub> films are deposited on quartz substrates, using a vacuum assisted thermal evaporation technique ( $\sim 10^{-5}$  mbar). Afterwards, thermal oxidation in controlled ambient is performed at various temperatures to obtain a selective oxide phase. Structural, morphological, chemical, and electrical properties of these oxide layers are investigated using various surface characterization techniques such as XRD, SEM, Raman spectroscopy, and XPS. XRD results show high crystalline quality of the oxide films. Orthorhombic MoO<sub>3</sub> phase is usually observed for oxidation temperatures up to 500°C. FESEM imaging depicts two distinct nanostructured morphologies such as large, faceted clusters of elongated shape and homogeneous distribution of small granular islands. At a certain growth condition, asymmetric growth of 1D nanorods are also formed. Oxidation states of these nanostructures are carefully analyzed with the help of XPS to obtain an oxide film with a single oxide phase.

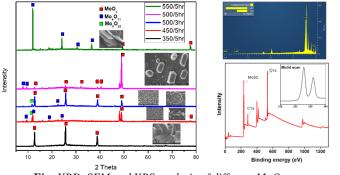


Fig: XRD, SEM and XPS analysis of different MoO<sub>x</sub> nanostructures

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## Physical properties of LaBO<sub>3</sub> (B = Mn, Fe, Co) thin films fabricated on SrTiO<sub>3</sub> using pulsed laser deposition

Bibek Ranjan Satapathy, Amit Vashist, Suvankar Chakraverty

1. Quantum Materials and Devices unit, Institute of Nano Science and Technology, Mohali, Punjab-140306, India.

Category: Poster

Keywords: Oxide heterostructure, Negative Magnetoresistance, Anomalous Hall effect, Spin polarised

Achieving the correct stoichiometry in oxide thin films is a notable challenge in materials science. The growth dynamics and kinetics can lead to thin films exhibiting different physical properties compared to their bulk counterparts. In our research, we examine thin films of LaBO<sub>3</sub> (where B = Mn, Fe, Co), deposited on SrTiO<sub>3</sub> (001) substrates using pulsed laser deposition under various thermodynamic conditions. X-ray Photoelectron Spectroscopy (XPS) analysis reveals the presence of multiple valence states, resulting in weak ferromagnetism in these films at room temperature. Furthermore, the interface between LaFeO<sub>3</sub> and SrTiO<sub>3</sub> (LFO-STO) exhibits conductivity and spin-polarization features, such as negative magnetoresistance and anomalous Hall resistivity above 150 K, which persist up to room temperature. Below 150 K, however, the system shows positive magnetoresistance and a normal Hall effect. Notably, the LFO-STO interface is nearly transparent across the visible light spectrum. Our findings hold promise for the field of transparent oxide spintronics, opening up new possibilities for research and technological innovation.

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## **Theme: Artificial Intelligence and Machine learnings in Physics**

## Classification of Wetting States of the Droplet Placed on Rectangular Textured Surfaces Using Machine Learning

Ganesh Sahadeo Meshram $^{1,\,*},$  Suman Chakraborty $^1$  and Partha P Chakrabarti $^2$ 

1 Department of Mechanical Engineering, IIT Kharagpur, Kharagpur, India 721302 2 Department of Computer Science & Engineering, IIT Kharagpur, Kharagpur, India 721302 \*Contact: ganeshmeshram.iitkgp@gmail.com

### Category: Poster

Keywords: Machine learning, Classification, Wetting states, Contact angle

The accurate categorization and anticipation of wetting conditions on surfaces with texture play a crucial role in the advancement of specialty materials that possess customized characteristics suitable for various applications, such as self- cleaning surfaces, anti-fouling coatings, and fluid manipulation technologies [1]. The conventional approaches for assessing wetting states (Wenzel state, Cassie state, and Cassie-Baxter state), predominantly relying on contact angle measurements, encounter constraints in terms of operational efficiency, scalability, and responsiveness, especially when confronted with textured surfaces. The present study investigates the use of machine learning (ML) models [2] to address these obstacles, presenting an ML strategy for the automated categorization and predictive modeling of wetting phenomena on rectangular textured surfaces. The experimentation on ML models provide evidence of the accurate and effectives in properly classifying Wenzel state, Cassie state, and Cassie-Baxter state, resulting in a substantial reduction in the time and effort required compared to conventional estimation techniques. From this present study, it has been found that Random Forest and XGBoost models are found to be more accurate in classifying the surfaces based on droplet spreading.

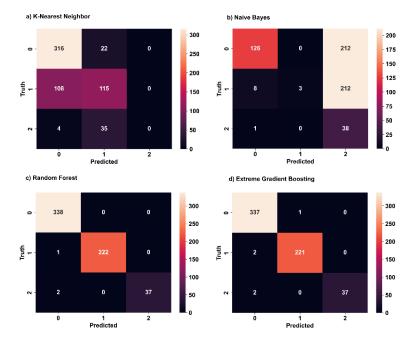


Figure 1 Confusion matrix comparison of the models. Here, 0, 1, and 2 denotes for Wenzel state, Cassie state, and Cassie-Baxter state, respectively.

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#### Anomalous electrical transport in Co7Zn8Mn5 single crystal

<u>Sharadnarayan Pradhan<sup>1</sup></u>, Sanand Kumar Pradhan<sup>1</sup>, Priyanath Mal<sup>2</sup>, P. Rambabu<sup>1</sup>, Archana Lakhani<sup>3</sup>, Niharika Mohapatra<sup>4</sup>, Bipul Das<sup>5</sup>, Bheem Lingam Chittari<sup>6</sup>, G.R. Turpu<sup>1</sup>, Pradip Das<sup>1, \*</sup>

<sup>1</sup> Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya, Bilaspur 495009, C.G., India

<sup>2</sup>Department of Physics and Photon Science, Gwangju Institute of Science and Technology (GIST), Gwangju 61005,

Republic of Korea

<sup>3</sup> UGC-DAE-CSR, University Campus, Khandwa Road, Indore 452001, India

<sup>4</sup>School of Basic Sciences, Physics, Indian Institute of Technology Bhubaneswar, 752050, India

<sup>5</sup>Department of Physics, National Taiwan Normal University, 162, Section 1, Heping E. Rd., Taipei City 106, Taiwan

<sup>6</sup>Department of Physical Science, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West

Bengal, India.

\*Contact: pradipd.iitb@gmail.com

Keywords: Electrical transport, Negative magnetoresistance, Anomalous Hall effect, Magnetization.

A new class of chiral magnets harboring skyrmion spin texture has drawn special attention to  $\beta$ -Mn-type Co-Zn-Mn (x + y + z =20) alloys. In this work, we report the successfully growth of  $\beta$ -Mn-type Co<sub>7</sub>Zn<sub>8</sub>Mn<sub>5</sub> single crystals and explore their magnetic and transport properties. Co<sub>7</sub>Zn<sub>8</sub>Mn<sub>5</sub> single crystals were grown through modified Bridgemen technique. Cubic crystal structure *P4*<sub>1</sub>*32* for Co<sub>7</sub>Zn<sub>8</sub>Mn<sub>5</sub> confirms through Rietveld refinement of polycrystalline XRD data. Temperature dependent resistivity curve shows the metallic nature. Positive magnetoresistance observed at 2 K, however between 5 K to 300 K negative magnetoresistance is observed. Hall resistivity at different temperature suggests anomalous Hall effect in Co<sub>7</sub>Zn<sub>8</sub>Mn<sub>5</sub>. The detailed electronic transport and magnetization will be presented.

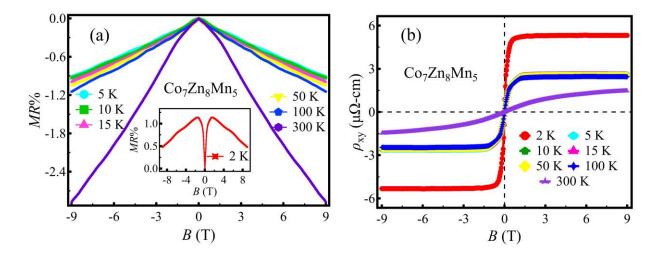


Fig. (a) Transverse magnetoresistance at different temperature. Inset: transverse magnetoresistance at 2 K, (b) Magnetic field dependent Hall resistivity at different temperature.

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### Growth and Characterisation of CdSe Nanolayers by Chemical Vapor Deposition

Priyanka Kumari<sup>1</sup> and Satchidananda Rath<sup>1</sup> 1 School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India E.Mail: S22PH09008@iitbbs.ac.in

Keywords: 2D material, chemical vapor deposition, nanolayers,

### **Abstract**

Materials of the II-VI type semiconductor, cadmium chalcogenides (Two-dimensional (2D) materials) are becoming a significant family for photovoltaic and optoelectronic devices because of their direct band-gap, high absorbance coefficients, high solar energy conversion, gas sensors, heterogeneous photocatalysis, etc. The direct band gap of cadmium selenide (CdSe), one of the important members of this family, allows it to be valuable in numerous technological applications, including optoelectronic devices. The present paper reports the structural and optical characteristics of CdSe nanolayers (NLs) grown by the cost-effective chemical vapor deposition (CVD) method. Field Emission Scanning Electron Microscopy (FESEM) was used to examine the morphology of the developed samples, revealing the development of nanolayers. The structural characteristics of CdSe NLs were investigated using the Raman spectra and X-ray diffraction (XRD). The XRD analysis reveals that the generated samples have a hexagonal structure and a 40 nm crystallite size. The optical properties of NLs are characterised by the UV-VIS spectrometer, which shows a direct allowed transition of CdSe NLs with a band gap of approximately 1.69 eV. The CdSe nanolayers may find use in photovoltaic and optoelectronic devices at the nanoscale. This paragraph starts the text section of the abstract.

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# Comprehensive studies of GaGeTe single crystal: Insights from structural, vibrational, and electronic transport properties

Sanand Kumar Pradhan<sup>1</sup>, Sharadnarayan Pradhan<sup>1</sup>, Priyanath Mal<sup>2</sup>, P. Rambabu<sup>1</sup>, Dinesh Kumar<sup>3</sup>, Bipul Das<sup>4</sup>, Bheem Lingam Chittari<sup>5</sup>, G.R. Turpu<sup>1</sup>, Pradip Das<sup>1,\*</sup>

<sup>1</sup> Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya, Bilaspur 495009, C.G., India

<sup>2</sup>Department of Physics and Photon Science, Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea

<sup>3</sup>Central Research Facility, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India.

<sup>4</sup>Department of Physics, National Taiwan Normal University, 162, Section 1, Heping E. Rd., Taipei City 106, Taiwan

<sup>5</sup>Department of Physical Science, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West

Bengal, India.

\*Contact: pradipd.iitb@gmail.com

Keywords: Single crystal, Raman spectra, magnetoresistance, Hall measurement

This study examines the synthesis, structural, vibrational, and electronic transport properties of high-quality GaGeTe single crystals. Phase purity of the studied compound is revealed by Rietveld refinements. The orientation along the (*OOl*) plane in the X-ray diffraction patterns indicates the easy growth direction is crystallographic *c*-axis. Temperature dependent Raman spectroscopy is used to record the vibrational spectra. The four notable room temperature Raman modes in theoretical calculations agree well with the experimental findings. The blue shift at low temperatures and the red shift at high temperatures are observed by analysis of temperature-dependent Raman spectra. There is no anharmonic phonon-phonon interaction, as indicated by the linear fit to Raman shift and the full-width at half maximum as a function of temperature. Measurements of Hall resistivity show that the majority of charge carriers are hole-type. The negative magnetoresistance (MR) curve in  $B \perp c$ , indicates weak-localization. On the other hand, the MR curve  $B \parallel c$  exhibits positive MR at temperatures below 10 K, but as temperatures rise, negative MR appears; this could be because of chiral anomaly effects.

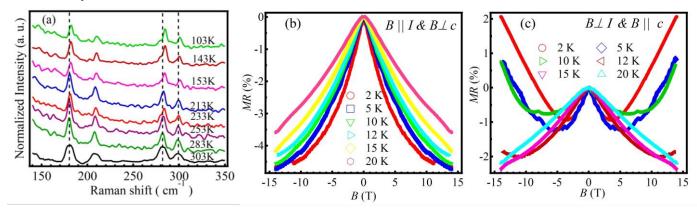


Fig. 1(a) Temperature-dependent Raman spectra of GaGeTe single crystal. (b) In-plane MR (%) as function of magnetic field  $(B \perp c)$  at different temperature. (c) Out-of-plane MR(%) versus magnetic field  $(B \parallel c)$  at different temperature.

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### Theoretical study on induced metallic state in Graphene/h-BN Hetero junction: A Tight Binding Model approach

Sivabrata Sahu<sup>1</sup>, G. C. Rout<sup>2,\*</sup>

 <sup>1</sup>School of Basic Science (Physics), NIIS Institute of Information Science and Management, Bhubaneswar, Odisha, India
 <sup>2</sup>P.G. Department of Applied Physics and Ballistics, Fakir Mohan University, Balasore, Odisha, India
 Corresponding email: \*profgcrout@gmail.com,sivabratasahu@gmail.com

*Keywords:* Graphene/h-BN system, Tight-binding method, Green's function, Electron band dispersion, Coulomb potential

Abstract. We address here the electronic band dispersion of graphene/h-BN hetero junction in a transverse applied electric field. The system is described by kinetic energy with nearest neighbor electron-hopping with hopping energy  $t_1$  and gate potential V across the two layers. The electron Green's functions are calculated by Zubarev's Green's function technique and electron band dispersion is found by equating the denominator of the Green's function to zero. It is observed that the graphene/h-BN system exhibits the band dispersion, where the two bands form a small gap and other two bands form a large gap near the Dirac point. Again we will show that, in contrast to this consensus, in a van der Waals heterostructure consisting of graphene and hexagon boron nitride (h-BN), the onsite Coulomb repulsion will at first destroy the localized state. This is due to the fact that the onsite Coulomb repulsion tends to suppress the asymmetry between neighboring carbons induced by h-BN substrate. We corroborate this surprising phenomenon by solving a tight-binding model with onsite Coulomb repulsion treated with Hartree Fock approximation, where hopping parameters are derived from density functional theory calculations based on the graphene/h-BN heterostructure. Our results indicate that both gapless and gapped states observed experimentally in graphene/h-BN heterostructures can be understood after a realistic value of the onsite Coulomb repulsion, as well as different interlayer distances, is taken into account. Finally, we propose ways to enhance the gapped state which is essential for potential application of graphene to next-generation electronics. Furthermore, we argue that band gap suppressed by many-body effect should happen in other van der Waals heterostructures.

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## Theme: Soft condensed matter

# Cholesterol modulates the membrane-membrane interaction induced by an antimicrobial peptide, Magainin 2 in phospholipid vesicles

Surajit Das<sup>1\*</sup>, Rajeev Jain<sup>2</sup>, Kalyan Kumar Banerjee<sup>1</sup> and Sanat Karmakar<sup>1#</sup>

<sup>1</sup>Soft matter and Biophysics Laboratory, Department of Physics, Jadavpur University, 188, Raja S. C. Mallick Road, Kolkata 700032, INDIA

<sup>2</sup>Structural Biology & Bio-Informatics Division, CSIR, Indian Institute of Chemical Biology, Kolkata 700032, INDIA

\* Email - surajitphys@gmail.com, Phone - 8918265754

<sup>#</sup>Corresponding author: Email: sanat.karmakar@jadavpuruniversity.in

Category: Poster

### Abstract

Antimicrobial peptides (AMPs) are part of innate immune response in all animal and human body against invading pathogens, like viruses, fungi, bacteria, etc. The AMPs target the bacterial membrane, especially negatively charged surface and create defects, such as pores, leading to disruption of the membrane. In this work, we have systematically investigated the interaction of an antimicrobial peptide Magainin 2 with the bacteria mimicking model membranes. We intend to understand mechanism of transmembrane pore formation and the role of cholesterol on the antimicrobial activity. Large unilamellar vesicles and giant unilamellar vesicles, composed of anionic lipid DOPG and zwitterionic lipid DOPC for different cholesterol concentration were prepared as model membrane. Electrostatics of anionic membranes containing cholesterol in the presence of Magainin 2 have been studied using dynamic light scattering (DLS) and zeta potential. Owing to their large size, GUV were observed directly under phase contrast microscope in order to investigate the evidence of pores. This study shows that Magainin 2 can create pores in both anionic and zwitterionic phospholipid membranes. However, adding cholesterol to the membrane reduces Magainin 2's ability to form pores. Also, our research shows how cholesterol plays an important role in changing the antibacterial effect of magainin 2 on lipid membranes.

Keywords-Model membrane, Phase contrast microscopy, Electroformation, Antimicrobial peptide, Cholesterol

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# Co-assembly of Two Carboxylic Acid Based Molecules with Dissimilar Symmetries and Sizes

<u>Debasish Behera</u> and Avijit Kumar<sup>\*</sup> 1 Department of Physics, School of Basic Sciences, Indian Institute of Technology Bhubaneswar, 752050, Odisha, India Email ID: avijitkumar@iitbbs.ac.in

Keywords: TMA, H<sub>4</sub>BPTA, molecular assembly, ambient condition STM, HOPG

Multi-component molecular self-assembly involving two or more type of molecules on surfaces leads to an increased complexity due to additional inter-molecular interactions among various types of molecules<sup>1</sup>. This leads to a rich and complex network of co-assembly on the underlying surfaces which needs to be explored to understand intermolecular interactions and various phases of co-assembly<sup>2</sup>. We present co-assembly on a HOPG surface at liquid-solid interface of two kinds of molecules with dissimilar symmetries and sizes: (i) three-fold symmetric trimesic acid (TMA) and (ii) two-fold symmetric 4,4',4",4"'-([1,1'-biphenyl]-4,4'-diylbis(azanetriyl)) tetrabenzoic acid (H<sub>4</sub>BPTA). Ambient condition Scanning Tunneling Microscope (STM) imaging demonstrates existence of two kinds of phases. At relatively lower concentration of TMA with respect to H<sub>4</sub>BPTA, one or two TMA occupy the pores of H<sub>4</sub>BPTA network. At relatively higher concentration of TMA, the co-assembly shows a porous phase with both TMA and H<sub>4</sub>BPTA molecules become part of the network. This phase consists of variety of pores generated by different arrangement of TMA around the small networks of H<sub>4</sub>BPTA molecules. While the former phase may be attributed to small size of TMA molecules compared to H<sub>4</sub>BPTA pores, the later phase may be attributed to the comparable length and the same symmetry of TMA dimers with that of H<sub>4</sub>BPTA molecules. The result provides an insight into two-component molecular self-assembly of molecules with dissimilar symmetries and sizes.

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## **Two-dimensional (2D) materials**

# Unraveling the electronic structure of GeS correlated with optical and transport anisotropy

Rahul Paramanik<sup>1</sup>, Tanima Kundu<sup>1</sup>, Soumik Das<sup>1</sup>, and Subhadeep Datta<sup>1</sup>\*

1 Indian Association for the Cultivation of Science, 2A & B Raja S. C. Mullick Road, Jadavpur, Kolkata, India

\*Contact: <u>sspsdd@iacs.res.in</u>

### Category: Poster

*Keywords:* vdW materials, electronic structure, optical anisotropy, transport anisotropy, polarized Raman spectroscopy,

In the fast-growing two-dimensional (2D) vdW materials family, low symmetry group IV-V monochalcogenides exhibit unique in-plane anisotropy leading to diverse optoelectronic properties. Herein, we present the influence of such intrinsic anisotropic structure on the in-plane electrical and optical properties of 2D Germanium sulfide (GeS), a group IV monochalcogenide with puckered orthorhombic morphology and *p*- type semiconducting behavior. We systematically investigate the angle-resolved photoemission spectroscopy (ARPES), field-effect transport measurements and angle-resolved polarization Raman spectroscopy (ARPRS) to systematically characterize both electrical and optical anisotropy of multilayered GeS. Micro-ARPES study on a freshly cleaved GeS single crystal resembles the anisotropic band structure along two perpendicular in-plane orientations that well agrees with the theoretical band structure calculated by density functional theory. The corresponding effective mass ratio along armchair and zigzag direction estimated from the band dispersion is 0.5 and anisotropic ratio of the hole mobility measured from the FET characteristics is as high as 3.3, superior to most 2D anisotropic materials. Angle-resolved polarization Raman spectroscopy offers an efficient way to identify the crystal orientations easily. This unique structural motif offers a new degree of freedom in the field of photoconductor and detectors as well as next-generation device electronics.

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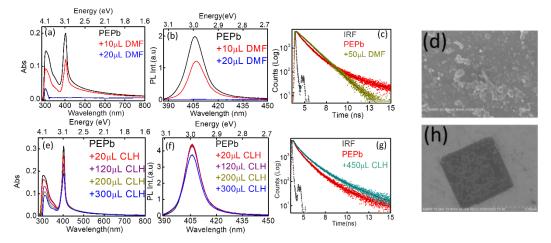
### Solvent engineering on Organic Inorganic Hybrid Perovskites

<u>Soumi Dutta</u>, \* Sankalan Mondal<sup>,</sup> and Manas Kumar Sarangi Department of Physics, IIT Patna, Bihta Campus, Bihta, Patna 801106

\*Contact:soumi\_2221ph26@iitp.ac.in

#### Keywords: PEA, HOIP, Solvent.

In the era of inorganic perovskites, hybrid organic-inorganic perovskites (HOIPs) have been emerged as an excellent class of materials for the optoelectronic applications because of their extremely high absorption coefficients, bandgap tunability and several other properties etc.<sup>1,2</sup> In this work, an organic cation phenylethyl ammonium (PEA) has been used as A site cation to get a 2D layered perovskite structure. The layered perovskite with composition (PEA)<sub>2</sub>PbBr<sub>4</sub> is formed due to the interaction between the layered inorganic Pb octahedra and the organic layers.<sup>3</sup> We have studied the behaviour of the (PEA)<sub>2</sub>PbBr<sub>4</sub> in the presence of different solvent environments (DMF, Hept., Hex., ACN, AcTn etc). After addition of 5% of DMF with high Guttman Donor Number (DN) 26.6, the crystal gets completely disintegrated whereas after adding 22.5% Cyclohexane with 0 DN no. solvent, the crystal structure remains undistorted and provides stability also, shown in figure below. This will give a new insight in revealing the interaction and the long-term stability of these materials in their colloidal forms and will also help us to delve into the interactions between the Pb complexes and the A site cation.<sup>3</sup>



**Figure 1:** Uv-vis,PL and Lifetime after addition of DMF in a) ,b) and c) respectively, and in Cyclohexane in e),f), g) respectively. d) and h) is the corresponding FESEM images in these solvents

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# **Two-dimensional Materials**

## Controlled growth of large area few-layer Molybdenum sulfide(MoS<sub>2</sub>) via chemical vapor deposition

Deepak Kumar Sahu<sup>1</sup>, Shreyasi Das<sup>2</sup>, Samit K, Ray<sup>1\*</sup>

1 Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal, 721302
2 School of Nanoscience and Technology, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal, 721302

\*Contact: physkr@phy.iitkgp.ac.in

### **Category: Poster**

Keywords: 2D materials, MoS2, CVD growth, van -der -Waals force

### Abstract:

Transition metal dichalcogenides (TMDs) are layered semiconducting two-dimensional (2D) materials with strong in-plane and weak out-of-plane van-der-Waals force<sup>1</sup> and thickness-dependent tunable band gap<sup>2</sup>, exhibiting exceptional mechanical, electronic, optoelectronic, spintronic, and valleytronic properties. Among all the synthesis techniques of 2D TMDs, Chemical Vapor Deposition (CVD) is a highly versatile and powerful technology for producing considerable sizes of good quality, highly stable mono to few layers of TMDCs in large quantities, suitable for industrial CMOS application. This technique involves several growth parameters to play around with to achieve controlled growth, as well as to carry out vast research on growth dynamics. Here, we have grown MoS<sub>2</sub> flakes by atmospheric pressure CVD (APCVD) by varying the carrier gas flow rate, growth temperature, precursor quantity, chamber conditioning, and growth time and we investigated their interrelation to form larger MoS<sub>2</sub> flakes. Further, the variation of these growth parameters changes the ratio of local concentration of MoO<sub>3</sub> and Sulfur, thus interestingly producing MoS<sub>2</sub> flakes of different shapes like triangles, hexagons, truncated triangles, dendritic triangles, and flower-like flakes, including recently explored Wuff structures ( butterfly shapes) containing many grain boundaries, all resulting from varying local density of precursor vapors at various locations on the same substrate (SiO<sub>2</sub>/Si). The obtained MoS<sub>2</sub> flakes are bilayer, confirmed by optical microscopy, Raman spectroscopy, Field Emission Scanning Electron Microscopy, Atomic Force Microscopy, and Photoluminescence Spectroscopy characterizations. Moreover, the formation of triangles with various stacking orders like AA, AB, ABA, or a few flakes without stacking on the same substrate are also observed, making these observations very impressive and attributed to the relatively high-temperature growth. Our study explores controlled conditions for growth of different sizes, shapes, and multiple stacking. configurations of MoS<sub>2</sub> flakes, providing a new avenue for the development of future electronic and optoelectronic devices.

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## Soft Condensed Matter

## Unravelling the structure and dynamics of nano-bio interfaces and liquid surfaces by X-ray scattering

Rajendra P Giri<sup>1,\*</sup>, Bridget M Murphy<sup>2</sup>, Sajal K Ghosh<sup>3</sup> and Mrinmay K Mukhopadhyay<sup>4</sup>

1 Department of Physics, IIT (ISM) Dhanbad, Jharkhand 826004, India

2 Institute for Experimental and Applied Physics, Kiel University, 24118 Kiel, Germany

3 Department of Physics, Shiv Nadar Institution of Eminence, Uttar Pradesh 201314, India

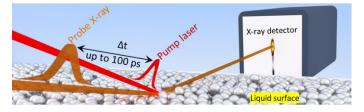
4 SP&MS Division, Saha Institute of Nuclear Physics, Kolkata 700064, India \*Contact: rpgiri@iitism.ac.in

### Category: Oral

Keywords: Biological membrane, Nano-bio interface, X-ray scattering, Pump-probe, Liquid

Nanoparticles (NPs) are currently being widely used in nanomedicine, disease diagnosis, biosensing, and environmental research. However, their biocompatibility and effectiveness are of great concern. Comprehending their molecular interactions with the first barrier of cell, i.e., the biomembrane, is pivotal to understanding the physiological effects of nanomaterials. Liquids are also essential to life because liquid surfaces and interfaces host most of the essential biological processes, and chemical reactions for maintaining the dynamic nature of life. The critical dynamic processes, such as thermally induced capillary waves and optically induced electron solvation at the liquid surfaces, occur in short timescales, typically, on sub-nanosecond to second.

Here, our experimental results<sup>1,2</sup> on the self-assembly, membrane mechanics and thermodynamics of the interaction of protein, cholesterol, and synthetic and biologically relevant NPs with biomimetic model membranes will be discussed. Also, the elucidation of the underlying non-equilibrium ultrafast physics at the liquid surfaces and interfaces along with our recent developments of an optical pump – X-ray probe setup<sup>3</sup> (Figure 1), which is first of its kind for liquid surface investigations, at the LISA P08 beamline of DESY synchrotron (Germany) will be demonstrated. The capability of the developed facility and its accessibility to the international researchers will also be discussed.



**Fig. 1**: Schematic of the optical pump – X-ray probe setup we have developed at the PETRA-III X-ray synchrotron of DESY (Germany).

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## Theme: Two Dimensional (2D) Matterials

## Enhancement of wetting of Multi-layered 2D MXene (Mo<sub>2</sub>TiC<sub>2</sub>Tx) using Low Energy Ion Beam

Durga Madhab Pani, Shyamal Chatterjee\*

School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Jatni, Odisha – 752050

\*Email: <u>shyamal@iitbbs.ac.in</u>

### Catagory:Poster

### Keywords: 2D Mxene, TRI3DYN simulation, Hydrophilic, Hydrophobic

This study examines the effects of low energy argon ion exposure on the electrical conductivity and surface characteristics of Mo<sub>2</sub>TiC<sub>2</sub>T<sub>x</sub> MXene Nanosheets [1, 2]. The 2D MXene was synthesized through the chemical etching of its MAX phase. The characterization revealed the elimination of Al from precursors, resulting in a layered structure enriched with metal carbides. MXene were deposited onto a conductive silicon substrate via a spin coating process. The coated films underwent irradiation with 10 keV Ar<sup>+</sup> ions at three distinct fluences of  $5 \times 10^{15}$ ,  $1 \times 10^{16}$ , and  $3 \times 10^{16}$  ions.cm<sup>-2</sup>. The pristine and irradiated samples were characterized through X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), and X-ray photoelectron spectroscopy (XPS). As ion fluence increases, the MXene sheets establish a cohesive welded structure. The TRI3DYN simulation facilitates the examination of surface modifications in  $Mo_2TiC_2T_x$  following irradiation at two distinct fluences (1  $\times$  10<sup>16</sup> and 3  $\times$  10<sup>16</sup> ions.cm<sup>-2</sup>). Mo<sub>2</sub>TiC<sub>2</sub>T<sub>x</sub> MXene is primarily hydrophilic because they have surface terminal groups like -O, -OH, F etc. Irradiation with low-energy Ar+ ion at  $3 \times 10^{16}$  ions.cm<sup>-2</sup> fluence convert hydrophilic to hydrophobic ones. Furthermore, a significant improvement in electrical conductivity has been observed with an increase in ion fluence, which can be ascribed to the preferential sputtering of functional groups and the structural alteration of Mo<sub>2</sub>TiC<sub>2</sub>T<sub>x</sub> MXene.

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### **Topological condensed matter & quantum materials**

### Field-induced strongly correlated state in BiSb

<u>Masashi Tokunaga<sup>1</sup></u>

1 The Institute for Solid State Physics, The University of Tokyo \*Contact: tokunaga@issp.u-tokyo.ac.jp

### Category: Invited

Keywords: topological semimetal, quantum limit state, semimetal-semiconductor transition

Recent extensive research on topological semimetals has led to a paradigm shift in understanding the band electrons. Since charge carriers in these materials have small effective masses, we usually utilize the band theory, which ignores the effects of electron correlation, to describe their electronic states. We aim to introduce the electron correlation effects by applying high magnetic fields to these topological semimetals.

Applying a sufficiently high magnetic field realizes a quantum limit state where all carriers occupy only the lowest Landau subband. Further increasing the magnetic field in this state of three-dimensional materials continuously reduces the bandwidth toward zero. Therefore, a strongly correlated state is realized in a sufficiently high magnetic field in which the Coulomb interaction between carriers dominates the bandwidth. It has yet to be clarified what kind of quantum states are realized by electron correlation in the ultra-quantum limit state of three-dimensional systems [1].

We have investigated the high-field properties of  $Bi_{1-x}Sb_x$  alloys near the semimetal-semiconductor transition to realize this ultra-quantum limit state. For a topological insulator sample with  $x \sim 0.10$ , we applied a magnetic field along the trigonal axis of the crystal. The bulk band gap collapses to a semimetallic state in a magnetic field of about 11 T. We applied higher magnetic fields from this state to continuously increase the number of electrons and holes by increasing the band overlap. Then, the system exhibits an insulating behavior below  $\sim$ 4 K in a magnetic field of about 20 T (Fig. 1) [2]. This insulating behavior cannot be explained by the shift of Landau subbands, suggesting the importance of many-body effects. In this situation, the realization of an excitonic phase has long been expected [3]. Our estimation of exciton binding energy and the condensation temperatures suggests the possible emergence of the excitonic phase.

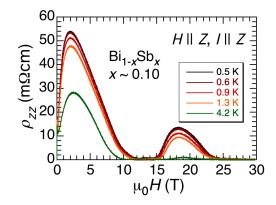


Fig. 1 Longitudinal magnetoresistace of  $Bi_{1-x}Sb_x$  with  $x \sim 0.10$ ,

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### Polyvinyl alcohol and Barium Hexaferrite Nanoparticle Composites for Electromagnetic Pollution Reduction Applications

Mayank Mausam<sup>1</sup>, Nakuleshwar Dut Jasuja<sup>2</sup> and Sunil Kumar<sup>1\*</sup>

<sup>1</sup>University Department of Electronic Science, Babasaheb Bhimrao Ambedkar Bihar University Muzaffarpur, Bihar-842001,India

<sup>2</sup>Professor, Vivekananda Global University, Jaipur, Rajasthan, 303012, India

\*Email:sunil.iitpatna@gmail.com

Keywords: Polyvinyl alcohol, EMI, XRD, FTIR, Vector Network Analyzer

Electromagnetic interference (EMI) poses a growing challenge in modern electronics due to the surge in wireless communication and electronic devices. Effective EMI shielding materials are crucial to ensuring device performance, reducing signal disruption, and promoting environmental safety. This research explores polyvinyl alcohol (PVA) and barium hexaferrite (BHF) nanocomposites as advanced EMI shielding materials. Barium hexaferrite nanoparticles, known for their superior magnetic properties and high dielectric constant, were synthesized via the sol-gel method, ensuring uniform particle distribution and improved crystallinity. These nanoparticles were embedded in a PVA matrix using a solution-cast method, creating nanocomposites with tunable properties by varying BHF concentrations (x=0.00, 0.02, 0.05, 0.1). The structural and chemical interactions within the composites were analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR). Electrical properties were characterized through impedance measurements, revealing that the 5% BHFdoped composite exhibited the highest conductivity, lowest impedance, and reduced dielectric constant. Using a vector network analyzer in the 8-12 GHz (X-band) range, the PVA-BHF nanocomposites demonstrated excellent EMI shielding effectiveness, exceeding 30 dB. The shielding mechanism stemmed from the synergistic effects of dielectric loss, magnetic loss (attributed to BHF), and conductive loss, while PVA enhanced flexibility and processability. These findings highlight the potential of PVA-BHF nanocomposites, particularly the 5% BHF formulation, as next-generation EMI shielding materials. Their applications extend to aerospace, telecommunications, and defence industries, where flexibility, high conductivity, and strong EMI absorption are critical.

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## Berry curvature driven Anomalous (Hall, Nernst) effects in half-metallic FeRu-CrSi: A first principles study

Monika Rana<sup>1</sup>, Bheemalingam Chittari<sup>2</sup> and P. Rambabu<sup>1,\*</sup>

1 Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, C. G. - 495009.

2 Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India. \*Contact: rams.hcu@gmail.com

Category: Oral

Keywords: Berry Cuvrature, Anomalous Hall effect, Anomalous Nernst Effect, Magneto-optic Kerr effect

Heusler alloys were discovered in the early 20<sup>th</sup> century by Fritz Heusler. These fascinating class of materials are found to have remarkable applications in the field of spintronics, thermoelectricity, topological materials, magnetic tunnel junctions, spin filtering devices, superconductivity, magneto-caloric effect, shape memory alloys etc.

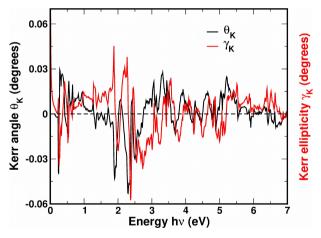


Figure 1. The Kerr angle and Kerr ellipticity of FeRuCrSi (with spin-orbit coupling) as a function of photon energy.

The Density functional theory (DFT) simulations are performed on half-metallic ferromagnetic Heusler alloy FeRuCrSi to study electronic, magnetic and topological features. The compound is found to be stable mechanically and dynamically. The spin-orbit coupling (SOC) induced Berry Curvature driven Anomalous (Hall, Nernst) effect are thoroughly investigated. The maximum Anomalous Hall Conductivity (AHC) and the Anomalous Nernst Conductivity (ANC) values are determined within the range of  $\pm 300$ meV around Fermi level  $E_F$  respectively. Also, the variation of ANC with temperature and chemical potential is investigated. The maximum value of polar Kerr angle ( $\theta_k$ ) is estimated. These properties may suggest the FeRuCrSi compound to be a suitable candidate for practical applications.

### Role of scattering processes in lattice thermal conductivity of MgB<sub>2</sub>

Nitin P. Singh\*

Department of Physics, Jaipur National University, Jaipur, India \*Contact: Email ID: nprajpph@jnujaipur.ac.in

Keywords: Lattice thermal conductivity, phonons, relaxation time, scattering process, Callaway's model.

### Abstract:

The contribution of various scattering mechanisms namely; combined boundary scattering, impurity scattering, anharmonic phonon processes, electron-phonon interactions and interference scattering to thermal conductivity of superconductors has been analyzed below and above  $T_c$ . It is observed that various scattering processes play an important role at different temperatures. The significance of BRT function has also been estimated in determining the best agreements between experimental and theoretical results. BRT theory calculates the electronic thermal conductivity when the dominant scatters are impurities as well as the effect of electrons on the thermal conductivity of unconventional superconductors.

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## **Topological Condensed Matter and Quantum Materials**

## Anomalous Hall and Nernst effects in equiatomic Heusler alloy CoMnCrGa: A first principles study

Hrishikesh Sinha<sup>1,\*</sup>, Bheemalingam Chittari<sup>2</sup> and <u>P. Rambabu<sup>1</sup></u>

1 Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, C. G. - 495009.

2 Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India.

\*Contact: sinhahrishikesh03@gmail.com

#### Category: Poster

*Keywords:* Berry Cuvrature, Anomalous Hall effect, Anomalous Nernst Effect, Magneto-optic Kerr effect

The Density functional theory (DFT) simulations are performed on ferromagnetic Heusler alloy CoMnCrGa[1] to study electronic, magnetic and topological features. The compound is found to be stable mechanically and dynamically. The spin-orbit coupling (SOC) induced Berry Curvature driven Anomalous (Hall, Nernst) effect are thoroughly investigated. The maximum Anomalous Hall Conductivity (AHC) and the Anomalous Nernst Conductivity (ANC) values are determined within the range of  $\pm 300$ meV around Fermi level  $E_F$  respectively. Also, the variation of ANC with temperature and chemical potential is investigated. The Curie temperature ( $T_C$ ) using mean field approximation through magnetic Heisenberg exchange interactions. These properties may suggest the CoMnCrGa compound to be a suitable candidate for practical applications.

#### **References:**

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## **Artificial Intelligence and Machine learnings in Physics**

## **Restricted Boltzmann Machine approach to solve Quantum Many-Body**

## problems

<u>Barishan Das</u><sup>1</sup>, Nirmal Ganguli <sup>1</sup>

1 Indian Institute of Science Education and Research Bhopal \*Contact: barishan20@iiserb.ac.in

#### Category: Poster

Keywords: machine learning, RBMs, quantum many body problems, Boltzmann machines

In this work, we present a neural network-based approach based on the Metropolis-Hastings algorithm and Restricted Boltzmann Machines (RBMs) for solving the one-dimensional (1D) Bose-Hubbard model. We optimize the ground state energy of the quantum system repeatedly by utilizing the Adam optimizer with a suitable learning rate. The RBM is trained via Contrastive Divergence, which allows for the efficient computation of the ground state energy of the quantum many-body system. For our purpose, we have used a popular deep learning library PyTorch, which allows for greater flexibility and interoperability with high-performance computing settings. Throughout our simulations we achieve convergence of the ground state energy to a steady value after several iterations, showcasing the stability of this strategy for quantum systems.

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#### **Other emerging areas**

## Influence of water/Ethanol mixture on Layer- by- Layer electrostatic self -assembled multilayer ultrathin film of cationic dye Safranin O and a negatively charged polymer Poly-Acrylic Acid: A spectroscopic and atomic force microscopic study

<u>Alapan Pal<sup>1</sup></u><sup>\*</sup>, Pabitra Kumar Paul<sup>1</sup>

1 Department of Physics, Jadavpur University, Jadavpur, Kolkata 700032, India \*Contact: palalapan@gmail.com

#### Category: Oral

Keywords: Layer-by-layer, self-assembled, H-aggregation, water/ethanol mixture.

Positively charged and highly fluorescent Phenazine dye Safranin O(abbreviated as SO) binds electrostatically with negatively charged polymer Poly-Acrylic acid(abbreviated as PAA) to form Layer- by-layer self-assembled(abbreviated as LbL) ultrathin film on quartz substrate. UV-vis absorption spectroscopy and steady state fluorescent spectroscopy establish formation of both H-type and J-type aggregates on PAA/SO LbL film at higher concentration of SO. It is found that under the influence of water/Ethanol mixture significant spectral changes of dye aqueous solution as well as LbL film occurs. The significant changes in UV-vis and fluorescence emission spectra of SO dye aqueous solution under the influence of different concentrations of Ethanol in water/Ethanol mixture is attributed to increase in solvent polarity surrounding the microenvironment of dye molecules as alcohols are categorized as protic solvents [1]. Fourier transform infrared spectroscopy (abbreviated as FTIR) has been employed to understand nature of electrostatic interaction between cationic SO and anionic PAA and influence of water/Ethanol mixture in LbL film. Atomic force microscopy (abberviated as AFM) has revealed surface morphology and roughness profile of PAA/SO LbL film as well as it establishes formation of aggregated structures in LbL film at higher SO concentration. surface profile of PAA/SO LbL films formed at different concentrations of SO and influence of water/Ethanol mixture on this LbL film has been monitored using Phase contrast microscopy which further revealed formation of aggregated structures in LbL film under the influence of Ethanol. The optical absorption band of SO and the corresponding transition between different electronic states in solvent medium water as well as in Ethanol have been theoretically generated by Density function theory(abbreviated as DFT) and these theoretical results are compared with experimental data.

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## **Topological condensed matter & quantum materials**

# Topological Phases And Edge States In An Exactly Solvable 1D Quantum $\Gamma$ Matrix Model

<u>Akhil Pravin Furtado</u><sup>1</sup>, Dr Kusum Dhochak<sup>2, \*</sup>

<sup>1,2</sup> Department of Physics, Indian Institute of Technology Palakkad

\*Contact: <sup>1</sup>222303002@smail.iitpkd.ac.in / akhil.furtado@gmail,com ; <sup>2</sup> kdhochak@smail.iitpkd.ac.in

#### (Unpublished work)

#### Category: Poster

*Keywords:* Topology, Γ matrices, Winding Number, Phase Transitions, Majorana Zero-energy Edge States.

We study the topological phases and phase transitions of a 1D quantum many-body model with  $\Gamma$  matrix degrees of freedom. The  $\Gamma$  matrices facilitate multiple competing couplings, thereby increasing the parameter space and resulting in a more intricate phase diagram with distinct topological phases. The model is exactly solvable with a generalized Jordan Wigner Transformation. We study the phase diagram of the model. Using certain  $Z_2$  symmetries, we characterize the topological phases with the winding number. We also confirm the presence of Majorana Zero energy Edge states by diagonalizing the real space Hamiltonian. Additionally, we examine the critical behaviour with the universality classes of the various phase transitions.

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## **Two Dimensional (2D) Materials**

## Strain-modulated electronic properties of graphene and MoS<sub>2</sub>-based heterostructures

Shivani Kumawat<sup>1</sup>, Chandan Kumar Vishwakarma<sup>1</sup>, M. Zeeshan<sup>1</sup>, B. K. Mani<sup>2\*</sup> and Sunil Kumar<sup>3</sup>

Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India
 Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India
 Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India
 \*Contact: bkmani@physics.iitd.ac.in

#### Category: Poster

Keywords: Heterostructures, Transition Metal Dichalcogenides (TMDs), Schottky barrier height.

Graphene (G) is known as a 'Wonder Material' which offers a plethora of unique electronic and optical properties [1]. Owing to their semiconducting nature, Transition Metal Dichalcogenides (TMDs) provide the advantages of an extremely large surface-to-volume ratio and high compatibility over conventional Si-based materials [2]. The integration of graphene and TMDs can lead to heterostructures with strong potential for technological applications, including photodetection, field-effect transistors, and biosensing. The application of uniaxial strain in these heterostructures is reported to enhance the functional properties and electronic structures of these materials. The present work aims to explore this.

In the present work, using first-principles calculations we investigate the structural, electronic, and optical properties of vertically stacked Graphene and  $MoS_2$  (M) based heterostructures: GM, GMG, MGM. Our simulations predict an opening of small band gaps of 8.6, 11.4, and 5.1 meV in GM bilayer, GMG trilayer, and MGM trilayer, respectively. The static dielectric constants obtained for G, M, GM, GMG, and MGM are 6.65, 4.11, 5.83, 8.14, and 8.41 respectively. From our simulations, we observed an improvement in the optical properties of MGM heterostructure. The absorption is observed to increase in the far IR regions, compared to individual monolayers. We also examine the effect of strain on electronic properties and Schottky barrier height of these heterostructures. We find that the band gap is enhanced more rapidly for tensile strain as compared to the compressive strain. The findings from our simulations could be important for technological applications such as optical sensors, modulators, photodetectors [3], etc.

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#### Soft condensed matter

## Surface Pressure Induced Nanoarchitectonics of Photoisomers of Alkylated Azo-benzene Molecules

Priyanka Priyadarshani Samal<sup>\*</sup>, Alpana Nayak

<sup>1</sup>Department of Physics, Indian Institute of Technology Patna, India \*Contact: Priyanka\_2121ph26@iitp.ac.in

#### Category: Poster/Oral

Keywords: Azo molecule, Self-assembly, Photo-switching, Atomic Force Microscopy

This paragraph starts the text section of the abstract.

Molecules containing the azogroup possess intriguing potential for a spectrum of optoelectronic applications owing to their inherent photo-switchable attributes. In this work, the self-assembly of photoisomers of alkylated azobenzene molecules at the air-water interface is studied, focusing on the trans-to-cis photoisomerization process investigated through UV-vis spectroscopy. The trans isomers initially exhibited peaks at 330 nm and 420 nm, with a calculated 52% conversion to cis upon UV irradiation. In Langmuir film experiments, the cis film was found to have a larger area per molecule (0.65 nm<sup>2</sup>) and higher elastic modulus (46 mN/m) than the trans film (0.56 nm<sup>2</sup>, 43 mN/m), indicating increased rigidity and efficiency in reducing surface pressure. Additionally, the cis film demonstrated a significantly higher surface potential and dipole moment compared to the trans film, attributed to its bent structure that allows for better alignment at the interface. Overall, the results reveal the impact of molecular structure on film properties and suggest potential applications in reversible control of monolayer characteristics at the air-water interface. Photo-switching of the Langmuir monolayer was also demonstrated by compressing the trans film to a target area and allowing it to relax before alternating UV and visible light irradiation cycles. Conducted at initial pressures of 5, 10, and 15 mN/m, results showed that surface pressure ( $\pi$ ) increased with UV light exposure, though the rise diminished at higher pressures, likely due to reduced photoisomerization effectiveness in closely packed monolayers. Visible light irradiation reverted the films to their initial state, highlighting the potential for reversible control of monolayer properties. This research is crucial for developing photo-responsive molecules for applications in pharmacology and targeted drug delivery.

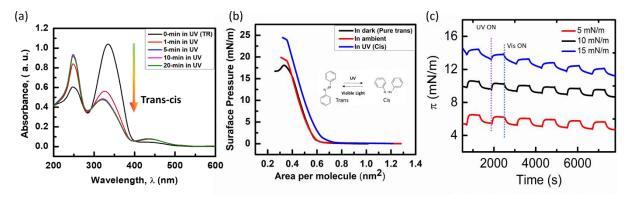


Figure 1: (a) UV-visible absorption spectroscopy (b)  $\pi$ - A isotherm of the molecule under different light irradiation conditions. (c) Photo-switching of Langmuir monolayer at constant areas with different initial surface pressures.

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## Enhancing the performance of topological photonic devices through artificial intelligence

Abhishek Kumar<sup>1,2</sup>

<sup>1</sup>International Centre for Materials Science (ICMS) <sup>2</sup>Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru abhishekkumar@jncasr.ac.in

Artificial intelligence (AI) is the most important new methodology in scientific research providing innovative, low-cost solutions for complex problems across various disciplines. In photonics, AI is particularly valuable, as it enables exploration beyond physical intuition and allows to explore the parameter space more efficiently to design and optimize the photonic devices with enhanced functionalities. Recently, topological photonic has emerged as promising candidate for developing on-chip photonic devices due to negligible scattering and bending losses. In this talk, I will show how AI based tools can be used to optimize and design the topological photonic devices with remarkable performance for high-speed on chip communication for 6G communication.

## Berry curvature induced Anomalous Hall and Nernst effects in nearly half-metal CoFeVGe: A first principles study

Abhipsha Pattnaik<sup>1,\*</sup>, Bheemalingam Chittari<sup>2</sup>, P. Rambabu<sup>1</sup> <sup>1</sup>Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur, C. G. -495009. <sup>2</sup>Department of Physical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur 741246, West Bengal, India. \*Contact: anipattnaik.123@gmail.com

#### Category: Poster

Keywords: Berry Curvature, Anomalous Hall effect, Anomalous Nernst Effect, Magneto-optic Kerr effect

Heusler alloys were discovered in the early 20<sup>th</sup> century by Fritz Heusler. These fascinating class of materials are found to have remarkable applications in the field of spintronics, thermoelectricity, topological materials, magnetic tunnel junctions, spin filtering devices, superconductivity, magneto-caloric effect, shape memory alloys etc.

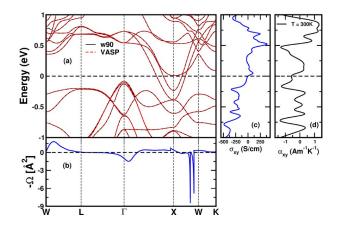


Fig. 1: (a) The band structure of CoFeVGe compound with the inclusion of spin-orbit coupling, (b) The Berry curvature of CoFeVGe along the high symmetry point path, and the Anomalous (Hall, Nernst) conductivities  $\sigma_{xy}$ ,  $\alpha_{xy}$  are respectively shown in (c) and (d). The wannier interpolated and VASP band structures are shown in solid black and dashed red lines respectively in (a).

The Density functional theory (DFT) simulations are performed on nearly half-metallic ferromagnetic Heusler alloy CoFeVGe to study electronic, magnetic and topological features. The compound is found to be stable mechanically and dynamically. The spin-orbit coupling (SOC) induced Berry Curvature driven Anomalous (Hall, Nernst) effect are thoroughly investigated. The maximum Anomalous Hall Conductivity (AHC) and the Anomalous Nernst Conductivity (ANC) values are found to be -340.2 S/m and -1.26Am<sup>-1</sup>K<sup>-1</sup> at 300K within the range of ±300meV around Fermi level  $E_F$  respectively. Also, the variation of ANC with temperature and chemical potential is investigated. The Curie temperature ( $T_C$ ) using mean field approximation through magnetic Heisenberg exchange interactions is found to be 489.3 <sup>o</sup>K. The magneto-optical Kerr effect is studied and the maximum value of polar Kerr angle ( $\theta_k$ ) is obtained as 0.19<sup>o</sup> for CoFeVGe. These properties may suggest the CoFeVGe compound to be a suitable candidate for practical applications.

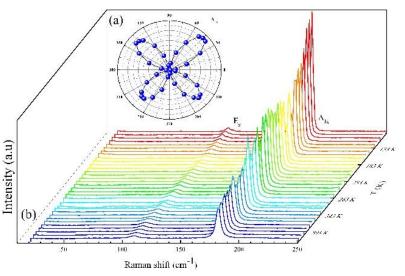
P40

#### Polarization and Temperature Dependent Raman Scattering in Lightly doped 2D Van der Waal SnSe<sub>2</sub> Crystal

Aarti Lakhara<sup>1</sup>, P. A. Bhobe<sup>1\*</sup> <sup>1</sup>Department of Physics, Indian Institute of Technology Indore, Indore, India \* Email ID- pbhobe@iiti.ac.in

Keywords: Dilute magnetic semiconductor, Raman scattering, Thermal conductivity, 2D material.

Dilute magnetic semiconductors (DMS) have garnered significant interest for their potential applications in spintronics. Recently, researchers have focused heavily on 2D DMSs due to their ability to electronically control magnetism. The layered structure of 2D materials, coupled with van der Waals interactions between layers, gives rise to unique physical properties that make them particularly attractive for such applications. Moving forward. harnessing spin in 2D material-based nanoelectronic devices holds great promise in spintronics and thermoelectric as well.



In this study, we successfully synthesized first time  $SnSe_2$  single crystals with small percentage of Fe doping. Unlike pure  $SnSe_2$ , which is nonmagnetic, Fe doping introduces magnetic properties. Previous studies by *Zhou et al.* have shown that the magnetic behavior of Fe-doped  $SnSe_2$  can vary from ferromagnetic to antiferromagnetic depending on the doping concentration. *Mei et al.* reported room temperature ferromagnetism in Fe-doped SnSe crystals. We characterized the Fe-doped  $SnSe_2$  crystals using X-ray diffraction, energy-dispersive X-ray spectroscopy (EDX), and Raman spectroscopy techniques. The Fe content was determined to be 0.14 atomic % in  $SnSe_2$ . X-ray diffraction confirmed the purity of the crystal phase. Room temperature Raman spectra shows a slight red-shift in the Raman modes, thus providing evidence of incorporation of Fe ions without too much distortion of the structure. Polarization-dependent Raman scattering studies indicated that the intensity of the  $A_{1g}$  mode varied with polarization angle (Fig (a)), while the  $E_g$  mode remained unchanged. Temperature-dependent Raman spectra recorded from 93 K to 423 K revealed variations attributable to thermal expansion effects on the Sn-Se bond length. Thermal conductivity was determined using the optothermal method, and the value comes out to be 0.6807 W/mK which is comparable to state of art thermoelectric material.

Our experimental findings represent an initial step towards expanding the family of ferromagnetic 2D materials.

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#### Development of Sustainable PU-Starch Composites for Low-Temperature Food Packaging

#### Saurabh Kumar Jha, Rani Rohini \*

#### Department of Materials Engineering, IIT Jammu, Jammu-181221, India

The present study demonstrates a new method to improve Starch/Sorbitol films for low-temperature applications by blending them with polyurethane (PU). The PU was synthesized from a 50/50 ratio of castor oil and polypropylene glycol. Toluene diisocyanate (TDI) was selected for PU synthesis because it was economical natural isocyanates. The gelatinized starch-sorbitol film was blended with the synthesized polyurethane in a DMF solution, improving the limitations of starch/sorbitol films at low-temperature applications. Characterization techniques such as Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA) were used to examine the structural, thermal, and degradation properties of the blend. The results showed that the blend is suitable for lightweight and flexible packaging. This study highlighted the prospective use of the PU-starch composite in low-temperature food packaging. This research showed the development of sustainable materials with improved usability, effectively overcoming the limitations of conventional starch-based films.

## Evidence of Spin Glass behavior with Exchange Bias and Memory Effect in β-Mn off-stoichiometric Heusler Alloy

Pankaj Kumar<sup>1\*</sup> and Sanjay Singh<sup>1</sup>

<sup>1</sup>Indian Institute of Technology (BHU) Varanasi -221005

\**Email: pankajkumar.rs.mst20@iitbhu.ac.in* 

#### Category: Oral Presentation

Keywords: Spin glass state, Heusler Alloys, Exchange bias, Memory effect, Topological Hall Effect.

The limitations on the performance of conventional electronic materials are one of the main challenges of the modern technological period. An extensive research work is being done to develop the materials that might overcome these restrictions by using quantum phenomena to exhibit outstanding efficiency. Spin-glass behavior is one of the quantum phenomena that is receiving attention in the scientific community. Spin glass states are magnetically frustrated systems caused by atomic disorders and competing interactions and are usually identified by a cusp in AC susceptibility measurements under zero field cooled (ZFC) conditions<sup>1</sup>. Spin glasses freeze at a temperature  $T_f$ , and under field-cooled (FC) conditions, their susceptibility becomes independent of temperature below  $T_f$ . As a result, a significant splitting between FC and zero-field-cooled (ZFC) conditions is usually observed. The key indicator of a spin glass transition is frequency-dependent AC susceptibility, where the transition temperature shifts when we increase field oscillation frequency<sup>1</sup>. Heusler compounds usually exhibit non-collinear and non-coplanar magnetic structures, leading to exotic phenomena like spin glass states, Anomalous Hall effect (AHE), Spin, and Topological Hall effect (THE)<sup>1-3</sup>. The THE has emerged to be an excellent electrical tool for identifying non-coplanar, non-collinear magnetic structures such as skyrmions<sup>3</sup>. Heusler alloys with a  $\beta$ -Mn structure, which has magnetic frustration and strong spin fluctuations, have been found to show spin-glass behavior, AHE, and THE<sup>1-3</sup>. The oral presentation will cover our recent findings of the exotic magnetic phases, with exchange bias, memory effects, and their spin-glass properties in beta-Mn Heusler alloys, focusing on some fascinating phenomena like aging, memory effect, exchange bias, rejuvenation, and their possibility or potential to have efficient materials in the spintronics field.

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#### **Topological Properties in a Curved Space-Time Su-Schrieffer-Heeger Model**

Priyanuj Rajbongshi<sup>1</sup> and Ranjan Modak<sup>1</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517619, India

email: ph24d004@iittp.ac.in

Category: Poster

keywords: Su-Schrieffer-Heeger, topology, spacetime, symmetry, curvature.

The Su-Schrieffer-Heeger (SSH) model, a prime example of a one-dimensional topologically nontrivial insulator, has been extensively studied in flat space-time. However, the impact of curvature and gravitational effects on the topological properties of such systems remains an open question. In recent times, a lot of studies have been conducted to understand the low dimensional quantum material in curved spacetime by constructing synthetic gravitational event horizons. Here, we investigate the Curved Spacetime (CST) version of the SSH model by introducing a position-dependent hopping parameter, which includes the warping degree of spacetime in the Hamiltonian. We then observe the energy eigenvalues and probability densities, which are different from the flat spacetime counterpart, we also calculate the local topological marker for the lattice sites which indicates the CST version is also topologically nontrivial, thus calculating various other topologically invariant quantities such as winding number. We also observe the symmetries, such as whether the CST version of the SSH model belongs to the BDI symmetry class or not and how the traditional flat spacetime symmetries react to the nontrivial curvature. Our study will open the door to a whole novel class of curvature-adjustable topological quantum materials with its potential application and usage in a wide range of areas, including quantum computation and communication.

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<sup>&</sup>lt;sup>1</sup> Corentin Morice, Dmitry Chernyavsky, Jasper van Wezel, Jeroen van den Brink, and Ali Moghaddam, "Quantum dynamics in 1d lattice models with synthetic horizons," SciPost Physics Core **5** (2022), 10.21468/scipostphyscore.5.3.042.

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# Investigation of Optical and Electrical properties of CVD grown $MoS_{2(1-x)}Se_{2x}$

Kamini Bharti<sup>1</sup>, Debamalya Banerjee<sup>1,\*</sup> Sudipta Khamrui<sup>1</sup>, Preetam Banerjee<sup>1</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur, 721302, India.

\*Contact: debamalya@phy.iitkgp.ac.in

#### **Category: Poster**

*Keywords:* MoS<sub>2(1-x)</sub>Se<sub>(2x)</sub>, Chemical Vapor Deposition, Electrical Properties, Optical Properties.

The concept of alloy engineering has emerged as a viable technique toward tuning the band gap in twodimensional transition-metal dichalcogenides (TMDCs). TMDC materials through a chemical vapour deposition route has opened up realistic possibilities to fabricate multifunctional devices. Here, we developed Field-Effect Transistors (FETs) on SiO<sub>2</sub>/Si with channel material  $MoS_{2(1-x)}Se_{(2x)}$ . This alloyed MoS<sub>2</sub> by selenium is synthesized via Chemical Vapor Deposition (CVD) method. Optical characterization, including Raman spectroscopy and photoluminescence (PL) measurements, provides insights into the modification of the electronic bandgap. Raman spectra show distinct shifts in peak positions and intensities corresponding to the varying Se concentrations, while PL spectra exhibit changes in emission intensity and wavelength, reflecting the tuneable nature of the optical bandgap. Temperature dependent properties of the FET is also studied which reveals the semiconducting nature of the alloyed system.  $MoS_{2(1-x)}Se_{(2x)}$  exhibits a three-order rise in FET current upon exposure to light. This makes it a prominent candidate for transistor and opto-electronic applications. These results show that  $MoS_{2(1-x)}Se_{(2x)}$  produced by CVD is a versatile material for customised applications in electronics and photonics, as alloying facilitates to attain desired electrical and optical properties. This work provides a comprehensive understanding of the effects of alloying on the properties of MoS2 and establishes a foundation for the development of novel materials for 2D semiconductor technology.

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## Impact of thickness on the properties of vanadium oxide (V<sub>2</sub>O<sub>x</sub>) and performance of V<sub>2</sub>O<sub>x</sub>/c-Si(n) based solar cells

**<u>Rahul</u>**, and Patima Agarwal<sup>1,2,\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India

<sup>2</sup>School of Energy Science and Engineering, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India

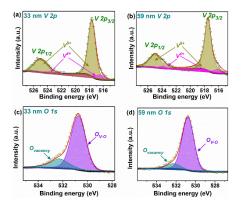
\*Contact: pratima@iitg.ac.in

#### Category: Oral

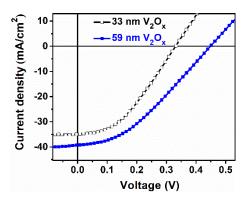
Keywords: Vanadium oxide, Carrier selective layer, dopant-free, heterojunction solar cell.

Carrier selective layers (CSLs) are fundamental and essential component of a solar cell. CSLs are of two kinds, e.g. hole selective layer (HSL) and electron selective layer (ESL). CSL help separation of photo-generated e-h pair and ensure that electrons and holes are collected to their respective electrodes. The state-of-the-art solar cell technology i.e. heterojunction with thin intrinsic layer (HIT) based solar cell ( $\eta > 26$  %), uses heavily doped (p/n a-Si:H) layers as carrier selective layers. Combination of i-a-Si:H and p/n a-Si:H layers demonstrate excellent carrier selectivity and passivation. But the better performance of HIT based solar cell comes at a cost, these are fabricated by costly techniques, e.g., PECVD and uses toxic and flammable gases, e.g., H<sub>2</sub>, B<sub>2</sub>H<sub>6</sub>, and PH<sub>3</sub> etc. for doping. Recently, various materials such as dopant-free transition metal oxides (TMOs) are used as CSLs because of their easy fabrication and cost effectiveness. Vanadium oxide (V<sub>2</sub>O<sub>x</sub>) is one of the TMOs which is utilized as a hole selective layer owing to its high optical band gap and high work function.

This work presents the fabrication of  $V_2O_x$  films on corning glass of four different thicknesses (21, 33, 59, and 107 nm) using the thermal evaporation technique at room temperature. The effect of thickness is observed on the optical and electrical properties of  $V_2O_x$  films. XRD studies show all the films are amorphous in nature. In the visible spectrum, all the films exhibit good transmission (>80%), which is crucial for using  $V_2O_x$  as an HSL in heterojunction solar cells. All the films are smooth, uniform and of device quality, as shown by AFM and FESEM images. The dark conductivity of  $V_2O_x$  films increases with increase in thickness. To investigate the impact of  $V_2O_x$  thickness on solar cell performance, solar cells are fabricated for  $V_2O_x$  films deposited at 100°C and thicknesses of 33 nm and 59 nm. The solar cell having  $V_2O_x$  thickness of 59 nm shown an improvement in η from 4.51% to 6.35% as compared to solar cell having V<sub>2</sub>O<sub>x</sub> thickness of 33 nm (Figure 2). To understand the cause of improvement in  $\eta$ , XPS studies are done (Figure 1). With an increase in thickness from 33 nm to 59 nm, there is a corresponding rise in the  $V^{5+}$  oxidation state and the number of oxygen atoms bonded with vanadium atoms. Since the work function of  $V_2O_x$  depends upon the high density of  $V^{5+}$  oxidation state and low density of oxygen vacancies, the rise in V<sub>oc</sub> is related to increase in work function of V<sub>2</sub>O<sub>x</sub>. Additionally, in spite of higher thickness, which increases the probability of parasitic absorption in TMO, increase in  $J_{sc}$  is observed. Further studies are in progress to better understand the impact of  $V_2O_x$  thickness on the  $V_2O_x/c-Si(n)$ solar cells.



**Figure 1.** XPS spectra of V '2p' and O '1s' for 33 nm and 59 nm  $V_2O_x$  films.



**Figure 2.** J-V characteristics of solar cells having  $V_2O_x$  thickness of 33 nm and 59 nm.

#### **Topological condensed matter & quantum materials**

## Influence of Ni<sup>2+</sup> Substitution on Microwave X-Band Radiation Losses in Y-Type Hexaferrites

Imlinola Jamir<sup>\*1</sup>, J.P. Borah<sup>1</sup>

<sup>1</sup>Department of Physics, National Institute of Technology Nagaland, Chumukedima PO: Dimapur-797103, Nagaland, India \*Contact: nolajamir27@gmail.com

Category: Oral

Keywords: Strontium hexaferrrite, microwave absorber, nanoparticle.

**Abstract:** Y-type strontium hexaferrite is attractive material for various applications, such as high frequency antennas and RF devices, because of its interesting magnetic properties. Ni substituted strontium hexaferrite with varying concentration of nickel were prepared using chemical co-precipitation methods for tuning its structural and magnetic properties. The structural properties were characterized by X-Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and the morphology and size distribution of the particles have been studied using high resolution field emission scanning electron microscopy (FESEM). Thermogravimetric analysis (TGA) was performed to find the stability of the sample by comparing the weight changes at a given temperature. Magnetic properties were determined using a vibrating sample magnetometer (VSM). The study on the radiation losses X band were performed by means of vector network analyzer (VNA) and indicated that the samples show reflection loss of -29.63(99.9% loss) at frequency 9.05 GHz and the results show that both the complex dielectric constant and dielectric loss decrease as measuring frequency increases. The low reflection loss makes these Y-type hexaferrites a potential candidate for high-frequency absorbers in the microwave region.

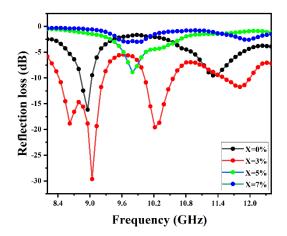


Figure 1: Measured reflection loss of strontium hexaferrite (x=0%, 3%, 5%, 7%).

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## **Two-dimensional (2D) materials**

## Pinning of borophene on Au (111)

<u>**U. Rajput**</u><sup>1</sup>, M. F. Akhtar<sup>2</sup>, V. Walve<sup>1</sup>, I. Mulani<sup>1</sup>, G. Vyas<sup>1</sup>, S. Bhowmick<sup>2</sup>, P. Kumar<sup>3</sup>,

A. Deshpande<sup>1\*</sup>

1Department of Physics, Indian Institute of Science Education and Research, Pune, India 2 Department of Material Science and Engineering, Indian Institute of Technology, Kanpur, India 3 Global Innovative Centre for Advanced Nanomaterials (GICAN), University of Newcastle, University Drive, Callaghan NSW 2308, Australia

\*Contact: aparna.d@iiserpune.ac.in

The discovery of graphene ignited extensive research in the field of van der Waals materials, revealing properties significantly different from their bulk counterparts [1]. This breakthrough also inspired exploration of two-dimensional (2D) non-van der Waals materials, including boron. The electron deficiency in boron leads to multiple allotropes, though the crystalline structures of many remain unknown, making boron a material of high scientific interest. Significant progress has been made in synthesizing various 2D boron polymorphs using different methods. These polymorphs include notable phases such as  $\alpha$ -borophene,  $\beta$ 12-borophene,  $\chi_3$ -borophene, striped borophene, and B<sub>36</sub> clusters [2]. Each phase exhibits unique structural and electronic properties that are predicted to have significant applications in batteries, sensors, hydrogen storage, catalysis, and superconductivity.

Here we will be going to demonstrate the pinning of freestanding borophene on Au (111) surface [3]. Atomic-scale characterization using Scanning Tunneling Microscopy (STM), spectroscopy (STS), and theoretical calculations indicate that the LPE borophene phase adsorbed on an Au (111) substrate is  $\beta_{12}$ . The interaction strength of borophene flakes is sufficient to perturb the herringbone reconstruction of Au (111), suggesting strong binding of the  $\beta_{12}$  phase with the substrate. We observed boron clusters along with  $\beta_{12}$  phase after one more coating cycle. This can be a valuable feature for designing borophene templates in multiple applications.

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## Electrical conductivity and dielectric characteristics of lithium aluminum germano silicate glass ceramics doped with titanium oxide

Suresh Suragani<sup>1</sup>, Ch. Tirupataiah<sup>1,\*</sup> and Kotcharla Hanumantha Rao<sup>1</sup> <sup>1</sup>Vignan's Foundation for Science, Technology and Research, Guntur-Andra Pradesh-522213, India. \*Contact: chereddyt@gmail.com

Keywords: Electrical properties, Conductivity, Dielectric properties, relaxation, electric modulus

Lithium aluminum germano silicate glass ceramic samples (LAGS) doped with titanium ions are prepared by using the melt quenching technique. The prepared samples are examined by AC conductivity and electric modulus formalisms in the frequency and temperature ranges of 4 Hz to 8 MHz and 303 K-523 K, respectively. The experimental AC conductivity data was fitted with Jonscher's power law to verify the suitability of several charge transport processes in these prepared samples [1]. The DC conductivity( $\sigma$ ), activation energy (E<sub>a</sub>), frequency exponent parameter (s), and cross-over frequency ( $\omega_H$ ) are all calculated with the aid of AC conductivity. Enthalpy to dissociate the cations from the original site to a charge compensating center (H<sub>f</sub>) and enthalpy of migration (H<sub>m</sub>) were also estimated. Correlated barrier hopping (CBH) is a rather good model for characterizing the primary AC conduction mechanism, according to the values obtained by the index s. To describe the DC conductivity data of the current oxide glass-ceramics at high temperatures, Greaves' modified version of Mott's VRH model is appropriate [2]. Moreover, the prepared samples' Cole-Cole diagrams and the real dielectric constant ( $\varepsilon'$ ), loss factor ( $\varepsilon''$ ), and loss tangent (tan  $\delta$ ) data are examined and briefly explained [3]. Due to mobile lithium ions and an increase in NBOs, the value of AC and DC conductivity increases with TiO<sub>2</sub> concentration from 1 to 5 mol%.

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## **Two-dimensional (2D) materials**

## **Optical Properties and Stability of 2D MnPS<sub>3</sub>**

Nikhil Singh<sup>1</sup>, Vaibhav Walve<sup>1</sup>, Subhrajit Dalai<sup>1</sup>, Aparna Deshpande<sup>1\*</sup>

1 Department of Physics, Indian Institute of Science Education and Research Pune, India \*Contact: aparna.d@iiserpune.ac.in

Category: Poster

Keywords: 2D materials, optical properties, spectroscopy

The discovery of 2D materials marked a significant advancement in physics and material science and opened a new and exciting field of two – dimensional materials. Since then, extensive work has been done in this field inspired by the exotic properties that two – dimensional materials possess. Over the years different classes of these two – dimensional materials such as transition metal dichalcogenides (TMDCs) have gained attention[1]. One such class of materials are the 2D van der Waals Transition Metal Phosphorous Trichalcogenides MPX<sub>3</sub> (M = Mn, Fe, Co, Ni and X = S or Se)[2]. One of the interesting properties of this class of materials is the presence of Antiferromagnetic ordering and tunable bandgaps making them good candidates for device applications. However, oxidation and degradation of these novel materials in ambient conditions has often been an obstacle to scaling them to practical applications.

Here we demonstrate the thickness dependent optical properties of  $MnPS_3$  using Atomic Force Microscopy, Raman and Optical Spectroscopy and also study its degradation in ambient conditions. Magneto – optical studies have shown strong correlations between magnetic ordering and optical properties. In the monolayer regime, photoinduced degradation has been suspected as a possible effect potentially making its application as optical devices unviable[3].

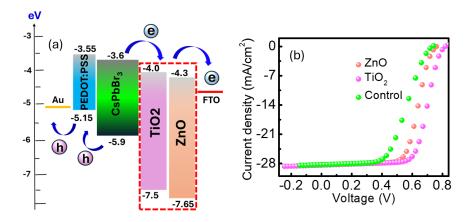
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#### Exploring the Synergistic Photophysical Properties of CsPbBr<sub>3</sub> Nanocrystals with ZnO and TiO<sub>2</sub> Nanoparticles for Advanced Optoelectronic Devices

Priyanka Dubey<sup>1</sup>, Manas Kumar Sarangi<sup>1, \*</sup> 1 Affiliation Indian Institute of Technology Patna, Bihar, India, 801106 \*Contact: mksarangi@iitp.ac.in

Keywords: Perovskite nanocrystal, Electron transport layer, Hole transport layer, Power conversion efficiency.

The efficiency of optoelectronic devices based on lead halide perovskite nanocrystals (PNCs) is greatly influenced by the rapid and efficient interfacial charge transfer (CT), which significantly boosts energy conversion. This study delves into the CT process in CsPbBr<sub>3</sub> PNCs when paired with ZnO and TiO<sub>2</sub> nanoparticles (NPs), both of which serve as excellent electron acceptors due to their optimal energy level alignment with the PNCs. Through a combination of steady-state and time-resolved spectroscopic techniques, along with current sensing atomic force microscopy, we observe smooth electron transfer (ET) from the P-NCs to both ZnO and TiO<sub>2</sub>. To further highlight the impact of ET on the performance of PNC-based photovoltaic devices, we simulate three device configurations: FTO/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (control), FTO/ZnO/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (with ZnO), and FTO/TiO<sub>2</sub>/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (with TiO<sub>2</sub>). The results reveal a remarkable enhancement in device performance—efficiency, current density, open circuit voltage, and fill factor—when ZnO and TiO<sub>2</sub> are incorporated, surpassing the control device. However, TiO<sub>2</sub> stands out with its superior ET rate, improved electrical conductivity, and overall better device performance, owing to its more favorable energy level alignment with the PNCs. This study underscores the critical role of optimizing interlayer charge transfer to maximize the performance of perovskite-based photovoltaic devices.



**Figure 1:** (a) Energy band alignment of the photovoltaic device and (b) the corresponding current-voltage curve for control device, device with ZnO and TiO<sub>2</sub>.

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## **Two-dimensional (2D) materials**

## Understanding of physical and electronic properties of ZrTe<sub>2</sub>

Pranjal Panwar<sup>1</sup>, Vaibhav Walve<sup>, 1</sup> and Aparna Deshpande<sup>1\*</sup>

1 Department of Physics, Indian Institute of Science Education and Research, Pune

\*Contact: aparna.d@iiserpune.ac.in

#### Category: Poster

#### Keywords: TMDCs, 2D Material

Transition metal dichalcogenides (TMDCs) have attracted significant attention due to their wide range of properties, from insulating to metallic behaviors. These properties arise from the unique electronic structure of TMDCs, particularly the presence of non-bonding d orbitals. TMDCs possess direct band gaps, strong spinorbit coupling, and excellent electronic, mechanical, and optical properties, making them promising for both practical applications and fundamental research [2].

Among TMDCs, ZrTe<sub>2</sub> stands out due to its intriguing physical and electronic characteristics. While ZrS<sub>2</sub> and ZrSe<sub>2</sub> are semiconductors, ZrTe<sub>2</sub> is a semimetal with a distinctive band structure [3]. It exhibits phenomena such as thermoelectric effects, charge density waves (CDW), and superconductivity, especially when doped or intercalated with different dopants. Additionally, ZrTe<sub>2</sub>'s band gap and electronic properties can be tuned by substituting different chalcogen elements.

In this work, we explore the physical and electronic properties of ZrTe<sub>2</sub> under ambient conditions. We also investigate its oxidation behavior and how its properties evolve in the presence of air. These findings provide new insights into the tunability of ZrTe<sub>2</sub>'s properties, shedding light on its potential for applications in electronics and materials science.

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#### Tuning the structure of telechelic rod assemblies: gelation and scaffolding

Om Priya Mishra<sup>a</sup> and Chamkor Singh<sup>a</sup>

<sup>a</sup> Department of Physics, Central University of Punjab, Bathinda, 151401 E-mail: (<u>ompriyamishra345@gmail.com</u>)

Keywords: Gelation, Packing fraction, Phase separation, Static structure factor

**Abstract :** The self-assembly of telechelic rod-like molecules has attracted considerable attention due to their potential utility in gelation and scaffolding applications. We simulate the structure of semiflexible telechelic polymer suspension where the end monomers on the polymer represent attractive groups, in an attempt to make a regular structure. We vary the end group monomer size and the packing fraction at a given constant temperature, the viscosity of the surrounding medium, the bending rigidity of the rods, and the strength of the end group attractions. Although we are unable to assemble a regular structure, we observe gelation and phase separation of the end groups. This we characterize using the static structure factor calculations, and we find that the suspension is more prone to gelation at a reduced packing fraction.

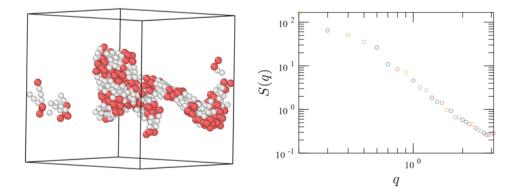


Fig. 1: A phase separated suspension of telechelic rods and corresponding static structure factor.

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#### Study on XPS and mechanical properties of Na<sub>2</sub>O-CdO-GeO<sub>2</sub>-SiO<sub>2</sub> glasses doped with Al<sub>2</sub>O<sub>3</sub>

Kotcharla Hanumantha Rao<sup>1</sup>, Ch. Tirupataiah<sup>1,\*</sup> and Suresh Suragani<sup>1</sup> <sup>1</sup>Vignan's Foundation for Science, Technology and Research, Guntur-Andra Pradesh-522213, India. \*Contact: chereddyt@gmail.com

Keywords: Melt Qunching, XRD, Spectroscopy, Mechanical properties, Glass,

25Na<sub>2</sub>O-5CdO-(15-x) GeO<sub>2</sub>-55SiO<sub>2</sub>: Al<sub>2</sub>O<sub>3</sub> (x=0,2,4,6,8 and10 mol%) glasses were prepared by melt quenching technique. Their amorphous nature was verified by XRD. The elemental content was identified by energy dispersive spectroscopy (EDS). The binding energies of existing components were analyzed by X-ray photoelectron spectroscopy (XPS), and the percentages of bridging oxygen and non-bridging oxygen were also calculated. The XPS spectra showed a higher amount of NBOs, which causes the network to depolymerize [1]. Makishima and Mackenzie's (MM) model was used to calculate mechanical parameters like Young's modulus (E), bulk modulus (K), shear modulus (S), longitudinal modulus (L), Poisson's ratio ( $\sigma$ ), fractal bond connectivity (d), and hardness (H) [2]. These evaluated mechanical parameters were high for the A5 sample. The XPS spectra and Mechanical studies endorsed the suitability of A5 sample for semiconducting applications.

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## Two-dimensional (2D) materials

# Predicting edge-localized monovacancy defects in zigzag graphene nanoribbons from Floquet quasienergy spectrum

Gulshan Kumar, Shashikant Kumar, Ajay Kumar, Prakash Parida\*

\*Contact: pparida@iitp.ac.in

Department of Physics, Indian Institute of Technology Patna, Bihta, Patna, Bihar 801106, India

#### Category: Poster

Keywords: Graphene nanoribbon, Floquet-Bloch formalism, Monovacancy defects, tr-ARPES

In this work, we prescribe a theoretical framework aiming at predicting the position of monovacancy defects at the edges of zigzag graphene nanoribbons (ZGNRs) using Floquet-Bloch formalism [1], which can be experimentally observed through time- and angle-resolved photoemission spectroscopy (tr-ARPES) [2]. Our methodology involves an in-depth investigation of the Floquet quasienergy band spectrum influenced by light with varying polarization across a range of frequencies. Particularly under the influence of circularly polarized light with a frequency comparable to the bandwidth of the system, our findings suggest a promising approach for locating monovacancy defects at either edge, a challenge that proves intricate to predict from the ARPES spectrum of ZGNRs with monovacancy defects. This has been achieved by analyzing the orientation of the Floquet edge state and the appearance of new Dirac points in the vicinity of the Fermi level. The real-world applications of these captivating characteristics underscore the importance and pertinence of our theoretical framework, paving the way for additional exploration and practical use. Our approach, employing the Floquet formalism, is not limited to monovacancy-type defects; rather, it can be expanded to encompass various types of vacancy defects.

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### Theme: Other emerging areas

## First Principles Study of Structural, Electronic and Optical properties of Quaternary Heusler LiTiRhSi Compound

Bhoopendra Kumar Dewangan<sup>1,2\*</sup>, Sapan Mohan Saini<sup>1</sup>

<sup>1</sup>Department of Physics, National Institute of Technology Raipur, Raipur (C.G.) India – 492010. <sup>2</sup>Department of Physics, Government ML Shukla PG College, Seepat, Bilaspur (C.G.), India – 495555.

\*Contact: bkdewangan.phd2021.phy@nitrr.ac.in

#### Category: Poster

Keywords: Band structure, optical properties, density functional theory, quaternary Heusler compound.

#### Abstract:

Quaternary Heusler compounds with 18-valence electrons have remarkable applications in the field of photovoltaic, spintronics and thermoelectric materials. In this study, we explored the structural, electronic and optical properties of Li based quaternary Heusler LiTiRhSi compound using a full potential linearized augmented plane-wave (FP-LAPW) method. We employed GGA-PBE approximation for the calculations of results. The electronic band structure of the studied compound shows an indirect band gap of 1.076 eV in the valence and conduction bands in the direction of  $L \rightarrow X$ , indicating that compound is semiconductor. As a function of photon energy, the optical properties like dielectric function ( $\epsilon$ ), optical conductivity  $\sigma$ , refractive index  $n(\omega)$  and reflectivity  $R(\omega)$  are calculated. These theoretical findings may provide strong support for the further experimental investigation of studied compound.

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#### Non-equilibrium theory for pump-probe spectroscopy

Shivangi<sup>1</sup>, Rajdeep Sensarma<sup>2</sup>\* 1 Tata Institute of Fundamental Research Mumbai 2 Tata Institute of Fundamental Research Mumbai \*Contact: shivangi@tifr.res.in

#### Keywords: non-equilibrium physics, pump-probe spectroscopy, Keldysh field theory

Condensed matter physics employs techniques such as thermodynamic measurements, spectroscopy, and transport methods to investigate materials. Among these, pump-probe spectroscopy stands out as a non-equilibrium technique that excites a system with a pump pulse and monitors its response with a probe pulse. This method is particularly powerful for studying strongly correlated systems, where coherent behavior and interaction effects play crucial roles. Despite its utility, interpreting pump-probe features in these systems lacks a standardized "dictionary" due to the complex interplay of interactions. While semi-classical approaches are prevalent, they often fail to capture these interactions adequately. In contrast, Keldysh field theory offers a promising framework by incorporating interaction effects, potentially unveiling interaction-specific signatures in pump-probe measurements. This research aims to develop such a theoretical framework to understand pump-probe spectroscopy in non-interacting systems, setting the stage for future studies to investigate critical features and deeper understandings of complex materials.

## **Perovskite Quantum Dots**

## Enhancing Color Gamut through Simultaneous Cation-Anion Exchange in Green Perovskite Quantum Dots

Satya Prakash Dash<sup>1</sup>, Monalisha Behera<sup>2</sup>, Jatin Dhanuka<sup>2</sup>, Sudipta Som<sup>2</sup>, Hendrik C Swart<sup>3</sup>

<sup>1</sup>Department of Physics, Odisha University of Technology and Research, Bhubaneswar- 751003, Odisha, India. <sup>2</sup>Department of Physics, Shiv Nadar University Chennai, Rajiv Gandhi Salai (OMR),

Kalavakkam – 603110, Chengalpattu (Dt), Tamil Nadu, India. <sup>3</sup>Department of Physics, University of the Free State, Bloemfontein, ZA9300, South Africa \*Corresponding author: <u>sudiptasom@snuchennai.edu.in</u>

#### Category: Poster

**Keywords:** Perovskite nanocrystal, Wide color gamut, Display, nonradiative recombination, Photoluminescence quantum yield

As liquid crystal displays (LCDs) continue to dominate the television market, there is a growing focus on enhancing display performance. Achieving vibrant and lifelike images in LCDs requires integrating features such as a wide color gamut (WCG) and high dynamic range (HDR). In this research, we explored a simple yet effective method for synthesizing  $CH_3NH_3PbBr_3$  perovskite nanocrystals. By concurrently substituting both cations and anions in  $CH_3NH_3Pb_{1-x}Sn_xBr_{3-2x}Cl_{2x}$  nanocrystals, we were able to achieve several desirable properties for commercial applications. These include tunable bandgaps, a shift in emission color from green to cyan (523 nm to 490 nm), and improved structural stability, excitonic lifetime, and color gamut [1].

CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub>, characterized by a cubic crystal structure with a space group of pm-3m and lattice parameters of a=b=c $\approx$ 5.9 Å [2], was modified by varying the x parameter from 0 to 0.4 in CH<sub>3</sub>NH<sub>3</sub>Pb<sub>1-x</sub>Sn<sub>x</sub>Br<sub>3-2x</sub>Cl<sub>2x</sub>. This alteration resulted in a color shift from green (530 nm) to blue (520 nm), attributed to an increased bandgap caused by the substitution of lead bromide (PbBr<sub>2</sub>) with tin chloride (SnCl<sub>2</sub>). While the photoluminescence quantum yield (PLQY) of the original CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub> was around 95%, it decreased to over 60% for CH<sub>3</sub>NH<sub>3</sub>PbBr<sub>3</sub> nanocrystals with a 15% SnCl<sub>2</sub> substitution, likely due to the formation of nonradiative recombination centres during the substitution [3]. Despite this reduction in PLQY, the overall stability of the nanocrystals was significantly enhanced. We successfully fabricated a warm white LED prototype with a 120% color gamut, based on the National Television System Committee (NTSC) standard, by combining CH<sub>3</sub>NH<sub>3</sub>Pb<sub>1-x</sub>Sn<sub>x</sub>Br<sub>3-2x</sub>Cl<sub>2x</sub> nanocrystals with commercial red light-emitting materials on a blue LED chip. The nanocrystals demonstrated an improved color gamut, favorable PLQY, and a narrow full width at half maximum (FWHM), underscoring their strong potential for advanced display applications.

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## Luminescence characterization of Cr<sup>3+</sup> doped aluminate phosphors for broad band near infrared light emitting applications

Monalisha Behera<sup>1</sup>, Jatin Dhanuka<sup>1</sup>, Sudipta Som<sup>1,\*</sup>, Hendrik C Swart<sup>2</sup>

<sup>1</sup>Department of Physics, Shiv Nadar University Chennai, Rajiv Gandhi Salai (OMR), Kalavakkam – 603110, Chengalpattu (Dt), Tamil Nadu, India. <sup>2</sup>Department of Physics, University of the Free State, Bloemfontein, ZA9300, South Africa \*Corresponding author: <u>sudiptasom@snuchennai.edu.in</u>

#### Category: Oral

Keywords: Near infrared, Light emitting diode, Phosphor, Broadband, Crystal field

Near-infrared (NIR) phosphor-converted light-emitting diodes (pc-LEDs) are crucial for defense and security devices, with their effectiveness largely depending on the performance of the NIR phosphor. The development of chromium-doped luminescent materials is vital for a wide range of emerging applications, including agriculture, the food industry, and noninvasive health monitoring. The importance of chromiumactivated luminescent materials in optics and security drives the rapid development of new materials and their applications [1].

In this study, a series of  $Cr^{3+}$ -activated aluminate-based phosphors were synthesized using a solid-state reaction method. Structural and spectral analyses were conducted using X-ray Diffraction (XRD), Diffuse Reflectance Spectroscopy (DRS), and Photoluminescence (PL). XRD data revealed that the synthesized phosphor has a hexagonal crystal structure with space group P-6m2, lattice parameters a=b=5.58 Å, and c=22.22 Å. The PL excitation spectrum comprises two bands at 400-540 nm and 550-750 nm, corresponding to the  ${}^{4}A_{2} \rightarrow {}^{4}T_{1}$  and  ${}^{4}T_{2}$  transitions of  $Cr^{3+}$ , respectively [2]. The DR spectrum showed two prominent absorption bands in the same spectral range as the excitation bands.

The emissions of  $Cr^{3+}$  ions are highly dependent on the crystal-field environment of the host lattices. In this host,  $Cr^{3+}$  ions occupy low-field sites, resulting in a broad emission band from 700 to 900 nm due to the spin-allowed  ${}^{4}T_{2} \rightarrow {}^{4}A_{2}$  transition of  $Cr^{3+}$  ions [3]. Using these phosphors as luminescent converters, a super-broadband pc-LED was fabricated, producing continuous emissions from 650 to 950 nm. This work indicates that these phosphors have significant potential for applications in broadband NIR pc-LEDs with visible-to-NIR emissions

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- 2. Dongjie Liu et al., Simultaneous Broadening and Enhancement of Cr<sup>3+</sup> Photoluminescence in LiIn<sub>2</sub>SbO<sub>6</sub> by Chemical Unit Cosubstitution: Night-Vision and Near-Infrared Spectroscopy Detection Applications, *Angew. Chem., Int. Ed* **60**, 14644–14649 (2021).
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## Luminescence characterization of Cr<sup>3+</sup> doped aluminate phosphors for broad band near infrared light emitting applications

Monalisha Behera<sup>1</sup>, Jatin Dhanuka<sup>1</sup>, Sudipta Som<sup>1,\*</sup>, Hendrik C Swart<sup>2</sup>

<sup>1</sup>Department of Physics, Shiv Nadar University Chennai, Rajiv Gandhi Salai (OMR), Kalavakkam – 603110, Chengalpattu (Dt), Tamil Nadu, India. <sup>2</sup>Department of Physics, University of the Free State, Bloemfontein, ZA9300, South Africa \*Corresponding author: <u>sudiptasom@snuchennai.edu.in</u>

Category: Poster

Keywords: Near infrared, Light emitting diode, Phosphor, Broadband, Crystal field

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## (Magnetism & Superconductivity)

## Electronic structure, Z<sub>2</sub> Invariant and Fermi surface of CsV<sub>3</sub>Sb<sub>5</sub> using Density Functional Theory Simulations

 Shalika R. Bhandari,<sup>1, 2</sup> Md. Zeeshan,<sup>3</sup> <u>Vivek Gusain</u>,<sup>3</sup> Keshav Shrestha,<sup>4</sup> and D. P. Rai<sup>5, 6</sup>
 <sup>1</sup>Department of Physics, Bhairahawa Multiple Campus, Tribhuvan University, siddarthanagar-32900, Bhairahawa, Nepal
 <sup>2</sup>Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden-01609, Germany
 <sup>3</sup>Department of Physics,Indian Institute of Technology, Hauz Khas, New Delhi-110016, India
 <sup>4</sup>Department of Chemistry and Physics, West Texas A and M University, Canyon, Texas 79016, USA
 <sup>5</sup>Department of Physics, Mizoram University, Aizawl 796004, India
 <sup>6</sup>Physical Sciences Research Center(PSRC), Department of Physics, Pachhunga University College, Aizawl 796001, India
 *Contact: phz228539@iitd.ac.in*

#### Category: Poster

Keywords: Kagome metals, Z2 invariant, Fermi surface, Charge density wave

This work presents the electronic structure, phonon dispersion,  $Z_2$  invariant and the Fermi surface of the kagome type  $CsV_3Sb_5$  compound by using the density functional theory calculations. The calculated phonon dispersion of  $CsV_3Sb_5$  on pristine state at ambient pressure shows the negative phonon frequencies around M and L-points in the first Brillouin Zone, which is consistent with the literature [1]. The L-point soft mode suggests the presence of a  $2 \times 2 \times 2$  reconstruction of disordered phase and the M-point soft mode is associated with the breathing phonon of V atoms. We report the Fermi surface reconstruction which is responsible for the Charge Density Wave (CDW) formation. We have also studied the pressure effect on phonon dispersion for both the pristine and the distorted phases ranging from 1GPa to 6GPa pressure. The complete suppression of the CDW Phase takes place at and above the 4GPa pressure, which agrees well with the previous experimental data [2]. We have also calculated the Fermi Surface and  $Z_2$  invariant for the above system. Our findings are key to understand the phenomenon like unconventional superconductivity, non-trivial topology and CDW formation in Kagome type CsV<sub>3</sub>Sb<sub>5</sub>.

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- 2. Z Zhang, *et al.*, "Pressure-induced reemergence of superconductivity in the topological kagome metal CsV<sub>3</sub>Sb<sub>5</sub>.", *Physical Review B*, 103, 224513 (2021).

#### Magnetic interaction in Sr<sub>0.7</sub>La<sub>0.3</sub>Fe<sub>11.75</sub>Co<sub>0.25</sub>O<sub>19</sub> - CoFe<sub>2</sub>O<sub>4</sub> composite system: Observation, evidence, and influence

Sushree Nibedita Rout<sup>a</sup>, Manoranjan Kar<sup>a\*</sup> <sup>a</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna-801106, India \*Corresponding author: mano@iitp.ac.in

**Keywords:** Hard – Soft composite; Vegard's law; Exchange interaction; Thamm-Hesse plot; Magnetization reversal

#### Abstract

(100-x) Sr<sub>0.7</sub>La<sub>0.3</sub>Fe<sub>11.75</sub>Co<sub>0.25</sub>O<sub>19</sub>-(x) CoFe<sub>2</sub>O<sub>4</sub> composites were synthesized by the one pot sol-gel autocombustion method. The individual phase purity, morphology, and magnetic hysteresis loop of the composite magnet were analyzed by X-ray powder diffraction, field emission scanning electron microscopy, and vibrating sample magnetometer, respectively. The apparent observation of room temperature hysteresis loop indicates the existence of interfacial exchange interaction. Nevertheless, magnetic parameters nearly follow Vegard's law. The nature of magnetic interaction and its dependency on the amount of each phase were analyzed by employing the Thamm-Hesse plot. The critical size of the soft phase did not corroborate with the results of  $\Delta M vs H$  plot. However, this synthesis method is found to be successful in obtaining single-step magnetization reversal in hard-soft composite magnets. The deviation from ideal non-interacting Stoner-Wohlfarth particles puts the single hard phase into the limelight.

### Surfactant-Dependent Morphology, Optical, and Thermoelectric Properties of Hydrothermally Synthesized SnSe Nanoparticles with EDTA, PVP and CTAB

Yogita Gendre, K. S. Ojha and Chinmaya Mahapatra Department of Physics National Institute of Technology Raipur, Raipur (C. G.), India

Keywords: Hydrothermal method, capping agent, optical properties and thermoelectric properties.

#### Abstract:

Transition metal chalcogenides (TMCs), composed of transition metals and chalcogens (e.g., oxygen, sulphur, selenium), are known for their unique physical, chemical, and electronic properties. These make them valuable in applications such as thermoelectric, optoelectronic, and catalysis. Tin selenide (SnSe) is a particularly promising semiconductor due to its lower toxicity, eco-friendliness, and high thermoelectric efficiency. This study examines the effect of surfactants on the morphology and thermoelectric properties of SnSe nanoparticles synthesized via a simple and cost-effective hydrothermal method with EDTA, PVP, and CTAB surfactants. The crystal structure, composition, and optical properties of the used surfactants capped SnSe nanoparticles were analysed using various techniques including XRD confirmed an orthorhombic structure, FESEM showed plate-like morphology, and EDX validated atomic composition. FTIR spectroscopy was used for vibrational analysis, while UV-Vis and PL spectroscopy determined the band gap and emission spectra. Moreover, the thermal conductivity and electrical conductivity were measured, and the thermoelectric figure of merits (ZT value) were calculated for each surfactant-capped SnSe nanoparticles.

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## Metal-Insulator transition driven by strong electron correlation and spin orbit interaction in NaIrO<sub>3</sub>

Singdha Sagarika Behera and Priyadarshini Parid\*

Department of Physics, School of Applied Sciences, KIIT University, Bhubaneswar, 751024, Odisha, India \*Contact: priyadarshini.paridafpy@kiit.ac.in

Keywords: Post perovskite, pentavalent cation, iridates, spin-orbit interaction, coulomb interaction

#### Abstract:

The ternary metal oxides containing 5d transition metal especially Ir, which adopt perovskite structure has sparked interest in both applied and basis science communities due to unique phase state formed by strong spin-orbit and coulomb interaction [1]. In this work, we investigated the structural, electronic and magnetic properties of NaIrO<sub>3</sub>, which is a pentavalent post perovskite compound. We employ GGA+PBE approximation with full relativistic pseudopotentials to perform spin orbit interactions within Quantum espresso package. The structural parameters of NaIrO<sub>3</sub> is optimized using variable cell relaxation method and fitted with the Birch-Murnaghan equation. The ground state magnetic behavior is found to be non-magnetic using the minimum energy principle. The electronic properties are compared with and without considering the strong electron correlation (U) and the spin-orbit coupling (SOC). The electronic band structure diagram shows that the  $e_g$  states of Ir atoms split into the lower and upper Hubbard bands near the Fermi level. This makes the compound insulating in nature at a particular value of U and with SOC, which agrees with earlier reported works [1,2].

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## Up-conversion luminescence of K<sup>+</sup>/Na<sup>+</sup> co-doped CaMoO<sub>4</sub>: Er<sup>3+</sup>/ Yb<sup>3+</sup> nanophosphor for temperature sensing application

Shriya Sinha<sup>1\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology (Indian School of Mines), Dhanbad, Jharkhand, India

\*<u>Email: shriyaism90@gmail.com</u>

The K<sup>+</sup>/Na<sup>+</sup> ion enhanced up-conversion emission of CaMoO<sub>4</sub>  $Er^{3+}/Yb^{3+}$  nanophosphor was synthesized through hydrothermal method. The crystal structure, phase purity and morphology of the phosphor were characterized by Xray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Transmission electron microscope (TEM). The incorporation of K<sup>+</sup>/Na<sup>+</sup> ions into CaMoO<sub>4</sub>: $Er^{3+}/Yb^{3+}$  has shown significant enhancement in the green (525 nm and 550 nm) and red (665 nm) emission bands under 980 nm laser excitation. The materials were further investigated to understand the dependence of excitation power density on temperature sensing and optical heating behavior using the fluorescence intensity ratio technique from the two thermally coupled energy levels (<sup>2</sup>H<sub>11/2</sub> and <sup>4</sup>S<sub>3/2</sub>) of  $Er^{3+}$  ions. The obtained result indicates that the present material is suitable for optical thermometry as well as for making infrared to visible up-converting devices.

Keywords: Rare Earths, Upconversion Luminescence, Temperature sensing, Thermal effect

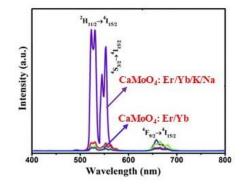


Fig. 1. Up-conversion enhancement in CaMoO<sub>4</sub> Er<sup>3+</sup>/Yb<sup>3+</sup>/K<sup>+</sup>/Na<sup>+</sup> nanophosphor

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### Extraction of Gate Field Dependent Values of Carrier Mobility in the Channel Region of an OFET

<u>Samayun Saikh</u><sup>\*</sup>, Ayash Kanto Mukherjee Indian Institute of Technology Patna, Bihta, Bihar, 801103, INDIA \*Email ID: samayun\_2021ph35@iitp.ac.in

Keywords: Organic Field Effect Transistor, Mobility, Contact resistance, Channel Resistance.

#### Abstract

Accurately determining charge carrier mobility is crucial in Organic Field Effect Transistors (OFETs) since it directly influences the development of new materials, device designs, and fabrication methods. High contact resistance ( $R_C$ ) at the metal-organic semiconductor interface can introduce errors in mobility extraction. This poster presents an equivalent circuit based analysis to refine the measurement of channel mobility ( $\mu_{ch}$ ), total  $R_C$ , and channel resistance ( $R_{ch}$ ) of an OFET. The OFET in question depicts bottom-gate-bottom-contact architecture. The process for determination combines conventional four-probe and three-probe measurement techniques to yield more precise mobility values in the channel region. Following the extraction of total  $R_C$  and  $R_{ch}$ , the values of  $\mu_{ch}$  are obtained. The extracted values of  $\mu_{ch}$  is on the order of  $10^{-2}$  cm<sup>2</sup>/Vs and exhibit an increasing trend with gate voltage ( $V_G$ ). Concurrently,  $R_C$  and  $R_{ch}$ , are found to be in the range of a few tens of M\Omega. Both the resistances show a decreasing trend with increase in  $V_G$  for a constant drain current 0.3  $\mu$ A.

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## **Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)**

## Development of Titanium oxide based Photodetector for High Performance UV Sensing

<u>Rupa Jeena<sup>1</sup>\*</u>, Pankaj Chetry<sup>2</sup>, Elizabeth George<sup>3</sup>, and Pradeep Sarin<sup>1</sup>

1 Department of Physics, IIT Bombay, Powai, Mumbai 400076, India 2 IIT Bombay Monash Research Academy, IIT Bombay, Powai, Mumbai 400076, India 3 School of Physical and Chemical Sciences, Queen Mary University of London, London, UK \*Contact: rupajeena@iitb.ac.in

#### Category: Poster

Keywords: Titanium dioxide, Photodetector, Thin film, UV Sensors.

Titanium dioxide  $(TiO_2)$ , with its wide bandgap, high stability, unique optical properties, and excellent electronic characteristics, has garnered significant attention as a promising material for ultraviolet (UV) photodetectors [1], [2]. The present work focuses on the fabrication, characterization, and performance evaluation of TiO<sub>2</sub>-based UV photodetectors, with emphasis on the response of the device to UV light.

TiO<sub>2</sub> thin films were deposited on quartz substrates using a thermal oxidation technique, ensuring high-quality crystalline growth. Structural, phase, and morphological characterizations were carried out using X-ray diffraction (XRD), Laser Raman spectroscopy (LRS), and scanning electron microscopy (SEM) to analyze the structure of the film, phase composition, and surface morphology. The optical properties of the films were investigated using UV-visible spectroscopy, confirming the wide bandgap nature of TiO<sub>2</sub>, which is crucial for efficient UV detection.

The electrical performance of the device was studied through current-voltage (I-V) measurements, both in dark and under UV illumination. The photo detectors demonstrated a significant photocurrent enhancement when exposed to UV light emitted from a UV LED, indicating strong UV absorption and charge carrier generation. The device exhibited a fast response time with reliable repeatability. Furthermore, it showed excellent stability and sensitivity, making them ideal candidates for applications such as environmental monitoring, UV sensing, and optical communication systems.

The simplicity of the fabrication process, combined with the strong UV response observed in the detector prototype, suggests that TiO<sub>2</sub>-based UV photodetectors have great potential for future optoelectronic devices designed specifically to detect UV radiation with high sensitivity and precision.

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#### Intermediate field-induced phase of the honeycomb magnet BaCo<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>

Prashanta K. Mukharjee<sup>1</sup>\*, Bin Shen<sup>1</sup>, Sebastian Erdmann<sup>1</sup>, Anton Jesche<sup>1</sup>, Julian Kaiser<sup>1</sup>, Priya R. Baral<sup>2</sup>, Oksana Zaharko<sup>2</sup>, Philipp Gegenwart<sup>1</sup>, and Alexander A. Tsirlin<sup>3</sup>

 <sup>1</sup>Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany
 <sup>2</sup>Laboratory for Neutron Scattering and Imaging (LNS), Paul Scherrer Institute (PSI), CH-5232, Villigen, Switzerland
 <sup>3</sup>Felix Bloch Institute for Solid-State Physics, University of Leipzig, 04103 Leipzig, Germany

\*pkmukharjee92@gmail.com

#### Abstract:

The Kitaev quantum spin liquid is an exotic state of matter where Majorana excitations can be realized. In pursuit of this, recent 3d-based Co<sup>2+</sup> materials, such as Na<sub>3</sub>Co<sub>2</sub>SbO<sub>6</sub>, Na<sub>2</sub>Co<sub>2</sub>ReO<sub>6</sub>, and BaCo<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>, have garnered attention due to their potential for exhibiting promising field-induced quantum spin liquid behaviour [1,2].

In our study, we explore the thermodynamic properties and field-induced behavior in one of these materials. Using magnetometry, calorimetry, high-resolution capacitive dilatometry, and single-crystal neutron diffraction, we investigate the temperature-field phase diagram of the anisotropic honeycomb magnet BaCo<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub>. Our measurements reveal four distinct ordered states under in-plane magnetic fields. Of particular interest is a narrow region between 0.51 and 0.54 T, which separates the up-up-down order from the fully polarized state and coincides with the field range where spin-liquid behavior has been previously reported. However, we show that magnetic Bragg peaks persist in this intermediate phase, ruling out its spin-liquid nature. Intriguingly, the nonmonotonic evolution of nuclear Bragg peaks suggests lattice involvement, a phenomenon also observed in other regions of the phase diagram, where significant changes in sample length occur upon entering magnetically ordered states. These findings highlight the significant role that lattice effects play in the behavior of BaCo<sub>2</sub>(AsO<sub>4</sub>)<sub>2</sub> [3].

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## **Theme: Nano and functional materials**

## Tunable Plasmonic Properties and Terahertz Conductivity of PLD-grown MoO<sub>2</sub> Films and Nanostructures

Manish Kumar, Krushna R. Mavani<sup>\*</sup>

Department of Physics, Indian Institute of Technology (IIT) Indore, Simrol, Khandwa Road, Madhya Pradesh-453552, India \*Corresponding author: <u>krushna@iiti.ac.in</u>

### Category: Poster

Keywords: Surface plasmon, Pulsed laser deposition, Raman spectroscopy, Terahertz spectroscopy, Oxides.

Molybdenum dioxide (MoO<sub>2</sub>) films were deposited on quartz substrates using the pulsed laser deposition (PLD) technique. The deposition was performed while the plume was directed at two different angles with the substrate surface: i) normal incidence  $(0^\circ)$ , and ii) a glancing angle  $(85^\circ)$  for a fixed duration of time. The deposition at a glancing angle led to the formation of columnar and porous  $MoO_2$  nanostructures with an amorphous nature, while growth at normal incidence produced a crystalline MoO<sub>2</sub> film, as confirmed by X-ray diffraction (XRD). Room temperature Raman spectroscopy showed that both the crystalline MoO<sub>2</sub> film and the nanostructures are in the monoclinic phase. Terahertz time-domain spectroscopy (THz-TDS) revealed an increase in transmission and a corresponding decrease in optical conductivity for the  $MoO_2$ nanostructures grown at a glancing angle as compared to the crystalline film. Furthermore, UV-Vis spectroscopy shows a broad absorption peak in the visible region, which corresponds to the surface plasmon resonance (SPR) effect [1], as shown in Figure 1. The absorption peak shifts to longer wavelengths in the crystalline  $MoO_2$  film due to the increased absorbance by bulk plasmons, while the  $MoO_2$  nanostructure shows higher absorbance intensity at lower wavelength. These plasmonic properties of  $MoO_2$  make it a suitable candidate as a substrate for Surface Enhanced Raman Spectroscopy (SERS). The efficiency of MoO<sub>2</sub> as an SERS substrate is similar to that of traditional noble metals such as gold (Au) and silver (Ag), making it an alternative for cost-effective plasmonic applications. Moreover, we show that the plasmon wavelength can be tuned by varying deposition conditions.

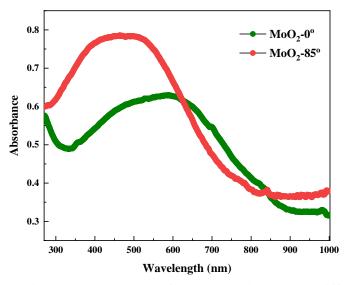


Figure 1: UV-Vis absorbance spectra of MoO<sub>2</sub> deposition at two different angles

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## Structural, morphological and electrochemical properties of Sr doped Lanthanum manganites nanofiber

Piyali Biswas and Manoranjan Kar\*

Department of Physics, Indian Institute of Technology Patna, Bihta, Patna, 801106, India \* Corresponding author: mano@iitp.ac.in.

Keywords: Electrospinning, Nanofiber, Manganites, Supercapacitor,

## Abstract:

In recent era the modern technology needs portable energy sources. Supercapacitor is knocking the technology door to replace the batteries due its several advantages. However the low cycle performance hindering it for application. As it is mentioned that the electrode in supercapacitors play significant role on its performance. Hence, there are several electrode materials, however perovskite based electrodes are drawn considerable interest due its advantages over to other materials. Hence, in this report manganite based perovskite materials are chosen. ABO<sub>3</sub>-type perovskite oxides' symmetry or structural stability is mostly determined by the size of the "A" and "B" cations, which also affects the materials' other properties[1]. Enhancing the perovskite's properties is mostly dependent on the cations' valence states, sizes and specific surface area. Here strontium modified La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> nanofiber has been prepared using electrospinning technique. Rietveld refinement of XRD patterns reveal that the rhombohedral perovskite crystal structure with space group R-3c[2]. Morphology has been studied from FESEM micrograph, calculated nanofiber diameter is about 342 nm Cyclic voltammetry (CV) are used to measure the electrochemical characteristics. The electrochemical test was performed at different scan rates 10, 30, 50, 100 and 200 mV/s 1M KOH electrolyte. The sample shows faradic behavior in the wide range potential window (-0.2-0.6V). The calculated specific capacitance was found to be 148F/g at 10 mV/s. The current findings indicate that Sr-doped LaMnO<sub>3</sub> is a material with great potential to be used as supercapacitor electrode.

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## **Optical and Photoelectrical Properties of pseudo-binary Se95(AgX)5 thin films**

Anil Kumar and Neeraj Mehta<sup>\*</sup> Department of Physics, Banaras Hindu University, Varanasi-221005, India \*Contact: dr\_neeraj\_mehta@yahoo.co.in

Keywords: Thin films, Optical materials, refractive index, Photoconductivity, Transmittance

This study explores the impact of incorporating the silver-halide salt AgX (where X = Cl, Br, and I) on the optical, electrical, and photo-electrical properties of pseudo-binary chalcogenide glass-ceramic thin films, achieving the addition of the silver halide salt AgX (X = Cl, Br, and I) at the expense of selenium content. The optical characteristics of as-prepared thin films (TFs) have been investigated using experimental transmission spectra. These spectra provide valuable insights into the behaviour of TFs in terms of light absorption, reflection, and transmission. The research reveals that varying silver halide salts affect the dispersion parameters and energy gap of these thin films. The transmission spectra,  $T(\lambda)$ , were recorded for normal incidence across the spectral range of 500 to 2500 nm. By analysing the spectral variations in the dispersion parameters, we determined the optical band gap (E\_g^opt) and Urbach tail (Ee) values. Optical bandgap decreased by 0.1 eV in the case of the silver chloride sample whereas in cases of silver bromide and silver iodide, the bandgap didn't change significantly. Urbach energy increased largely after the incorporation of silver halide salt. Our results provide evidence of an indirect optical transition in the samples, as indicated by the transition power factor (m). Employing a straightforward analysis method proposed by Swanepoel, we achieved precise measurements of the refractive index n. Additionally, the real component ( $\varepsilon$ ) and imaginary components ( $\varepsilon$ ") of the dielectric constant, as well as the high-frequency value  $(\varepsilon \infty)$ , have been determined. Notably, the infinite dielectric constant ( $\varepsilon \infty$ ) of the parent selenium TF ( $\varepsilon \infty = 2.45$ ) increases significantly after doping with AgCl  $(\varepsilon \infty = 3.33)$ , AgBr ( $\varepsilon \infty = 3.27$ ), and AgI ( $\varepsilon \infty = 4.18$ ). The optical absorption mechanism observed in these films aligns with allowed direct transitions, with the optical band gap ranging between 1.77 and 1.89 eV. The dispersion parameters were calculated using both the Wemple-DiDomenico and Solomon dispersion models. Additionally, we explored how the relaxation time ( $\tau$ ), dissipation factor (tan  $\delta$ ), electrical/optical conductivities, and surface/volume energy loss functions depend on the energy (hv) of photons. The study also delves into the nonlinear properties of the samples, considering their susceptibility and nonlinear refractive index.

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#### **Magnetism and Superconductivity**

#### A Review on Magnetic Properties of FePtX (X=Co, Cu, Mn) Ternary Alloys

Nishanta Deka<sup>1</sup>, S.K. Srivastava<sup>1\*</sup>

<sup>1</sup>Department of Physics, Central Institute of Technology Kokrajhar, Kokrajhar–783370, India <sup>\*</sup>Contact: \*<u>sk.srivastava@cit.ac.in</u>

#### **Category: Poster**

## Keywords: Magnetic recording, perpendicular magnetic anisotropy, L1<sub>0</sub> ordered FePt, annealing.

The advent of magnetic recording technology in the 20<sup>th</sup> century has contributed significantly in the advancements of present days electronic and spintronic devices. The emergence of perpendicular magnetic recording to compensate the drawback of low density longitudinal recording searches for novel magnetic materials with high magnetocrystalline anisotropy(MCA), high saturation magnetization(Ms) and high coercivity(Hc) etc. Since then materials with high perpendicular magnetic anisotropy(PMA) becomes an incessant demand of researchers for ultra-high density magnetic recording and L1<sub>0</sub> ordered FePt is one of the most explored potential candidates for this purpose. FePt alloy thin films at room temperature possesses disordered face-centred cubic(FCC) structure which upon annealing at elevated temperature(above 500°C) transforms to L1<sub>0</sub> ordered FePt face centred tetragonal(FCT) phase and helps to promote PMA under proper tuning conditions. Efforts have been made to reduce the structural ordering temperature as it thermally in stabilizes the grains and reduces MCA and hence coercivity. One of the efficient ways of doing it is doping of a third element with FePt by varying its % concentration. In this work, a detailed review on FePtX (X= Co, Cu, Mn) ternary alloy thin films with an emphasis to understand the role of substrates, in-situ annealing and post annealing on structural, morphology, and magnetic properties will be highlighted.

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## Nano and Functional materials

## Manipulating Magnetic Interactions: Unleash The Potential of Terfenol-D/CrN Thin Film Heterostructures

Mayur P. Sangole<sup>1,2</sup>, Kirandeep Singh<sup>\*1,2</sup>

1 Advanced Nanomaterials and Devices Group, Physical and Material Chemistry Division, CSIR - National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411 008, India 2 Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201 002, India \*Contact: kp.singh@ncl.res.in

Category: Poster

Keywords: Sputtering; Heterostructure; Thin Films; Exchange bias; Spintronics; Magnetism

A silicon-compatible thin film heterostructure comprised of Terfenol-D ( $Tb_{0.3}Dy_{0.7}Fe_2$ ) and Chromium Nitride (CrN) was grown by DC magnetron sputtering to examine the exchange bias effect. The influence of the bottom layer's crystal orientation, i.e., CrN, on the exchange bias effect, was investigated by recording the Isothermal magnetization loops (M-H) at room temperature. A substantial shifting of the hysteresis loop from the origin was observed with the antiferromagnetic (AFM) CrN layer in the Terfenol-D/CrN heterostructure. In the present study, we also showed that the exchange bias effect in this bilayer heterostructure can be tuned by varying the thickness of both layers.

The crystallinity of CrN, Terfenol-D, and magnetron sputtered thin film heterostructure was examined by a Grazing Incidence X-ray diffractometer (GI-XRD). We have found that processing parameters such as deposition parameters and buffer layers used before the deposition of CrN greatly influence the crystal orientation of the complete heterostructure. We have employed cross-section FE-SEM to examine the interface quality between Terfenol-D and CrN. The other complementary techniques, such as X-ray Photoelectron Spectroscopy (XPS), were used to evaluate the chemical states and to check the interface quality. The XPS and FE-SEM results indicate that the interface was interdiffusion-free.

The exchange-coupled Terfenol-D/CrN heterostructure grown at 550°C and having thicknesses below 100 nm exhibited a large exchange coupling field of nearly 148 Oe. This work's findings indicate that Terfenol-D/CrN thin-film heterostructure grown over a P-(100) Silicon substrate could be used for futuristic spintronic devices.

## Nano and Functional materials

# Unraveling the Nonlinear Optical Response of CsPbBr<sub>3</sub> Nanocrystals with Layered Materials

## Naresh Chandra Maurya, K.V. Adarsh\*

Indian Institute of Science Education and Research (IISER) Bhopal, Bhopal-462066, India Author email address <u>-adarsh@iiserb.ac.in</u>

Category: Oral/ Poster

Keywords: Nanocrystals, layered materials, nonlinear, excited state absorption, charge transfer,

Integration of Lead halide perovskite nanocrystals (LHPN) with low dimensional material shows an enormous tendency in optoelectronic devices, as in solar cells and photocatalysts processing [1-2], while a comprehensive study of the third-order nonlinear optical (NLO) response is yet to be established [3]. Here, using the Z-scan technique, we report NLO response in the CsPbBr<sub>3</sub> nanocrystals with layered material, specifically graphene Oxide (GO) and reduced graphene Oxide (rGO). Our results demonstrate a remarkably pronounced excited-state absorption (ESA) phenomenon in CsPbBr<sub>3</sub>/layered materials compared to pristine materials (CsPbBr3 and rGO) under excitation at 532 nm in the nanosecond regime, suggesting that these integrated materials can be employed as a passive optical limiter. The observed ESA is discussed in the framework of an efficient charge transfer between the CsPbBr<sub>3</sub> nanocrystals and layered materials. Further, the reduction in photoluminescence (PL) intensity and ultrafast transient absorption measurements corroborate our idea of charge transfer. Moreover, we also demonstrate our device's optical limiting parameter by fabricating the liquid-based optical limiter, showing benchmark performance compared to the reported optical limiting devices. Overall, our results provide a useful degree of freedom to engineer nonlinear optical absorption for hybrid system-based photonic devices.

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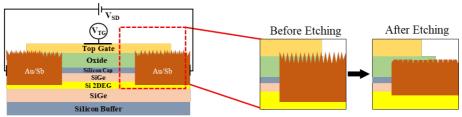
## Refining Au/Sb Contacts for Quantum Devices in Undoped Si/SiGe

Lucky Donald Lyngdoh Kynshi, Umang Soni, Chithra H Sharma, Madhu Thalakulam\* Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala 695551, India Email: madhu@iisertvm.ac.in

#### Category: Poster

Keywords: Si/SiGe heterostructure, Au/Sb Ohmic contact, Magneto transport

In our study, we addresses the challenges of creating an effective ohmic contact for undoped Si/SiGe substrates, which are essential for exploring quantum transport phenomena in mesoscopic devices like gated quantum dot and the subsequent realization of Quantum dot based spin-qubit system [1]. Typically, ohmic contacts are established by introducing dopants to overcome the Schottky barrier at the metal-semiconductor interface. While the Au/Sb alloy is commonly used as an ohmic contact in modulation-doped Si/SiGe, its application to undoped Si/SiGe is problematic due to the formation of alloy spikes after annealing [2]. These spikes penetrate the oxide layer, causing leakage currents and complicating the overlap of the ohmic region with the accumulation gate. The precise mechanisms underlying these issues and the final characteristics of the annealed region still need to be better understood.



In our work, we developed a refined Au/Sb ohmic contact process for undoped Si/SiGe substrates, addressing the spike formation issue by employing gold and silicon etching techniques. Our approach successfully minimized alloy spikes, resulting in fabricated devices that exhibited no leakage current between the top gate and the ohmic contact. The surface morphology of the annealed region revealed the presence of craters and Au-Si island precipitation, attributable to the eutectic interaction between gold and silicon. The surface also has gold concentrated in the island precipitation, suggesting an efficient Au-Si reaction. Electrical characterization of the annealed region has linear IV properties at low temperatures, and magnetotransport measurements of a Hall bar device revealed a turn-on voltage of 1V, with consistent linearity in both two-probe and four-probe measurements. The carrier concentration and Hall mobility of the device varied linearly with the top gate, with a mobility of  $10^5$  Cm<sup>2</sup>/Vs, and a power law relation  $\mu \propto n^{\alpha}$  yielded an 'a' value of 1.16, indicating that mobility is primarily limited by remote impurities. A comparison of Hall mobility and field-effect mobility in devices using phosphorus ion implantation demonstrated similar results, validating the effectiveness of our Au/Sb alloy method.

Our work successfully establishes Au/Sb as an ohmic contact for undoped Si/SiGe, with comprehensive characterization of the annealed alloy contact. This study provides a crucial foundation for further integration into mesoscopic devices.

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## Lead Free Perovskite La-YFeO<sub>3</sub>/PVDF-HFP Composite for Efficient Triboelectric Energy Harvester

<u>Sumana Lakshman<sup>1</sup></u>, Manisha Kundu<sup>1</sup>, Navonil Bose<sup>1,\*</sup>, Sukhen Das<sup>1</sup> <sup>1</sup>Department of Physics, Jadavpur University, Kolkata- 700032, West Bengal, India \* Corresponding Author: navonil05@gmail.com

*Keywords*: Triboelectric energy harvester, Lead free perovskite, High electroactive  $\beta$  phase, Porous PVDF-HFP membrane.

#### Abstract:

In recent years triboelectric energy harvesters (TEH) have drawn intensive attention due to its high output voltage, low cost, wide range of material choice, and its application as self-powered sensor<sup>[1]</sup>, health care monitoring<sup>[1]</sup>, e-skin<sup>[1]</sup> and others. In this work, a flexible TEH device is fabricated using lead free perovskite-polymer ferroelectric composite film (La-YFeO<sub>3</sub>/PVDF-HFP) as the tribonegative layer and aluminium tape as the tribopositive layer. The La doped YFeO<sub>3</sub> perovskite filler is synthesized by sol-gel technique. The structural and morphological properties of the synthesized perovskite filler is investigated by using X-Ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and field emission scanning microscopy (FESEM) techniques, which confirms the successful synthesis of the filler. The La-YFeO<sub>3</sub>/PVDF-HFP composite film is prepared by phase inversion method (PI)<sup>[2]</sup> in a water coagulation bath. The filler is added in different concentration of 1,2,3,4 wt% in PVDF-HFP matrix and the composite films are characterized by XRD, FTIR, and FESEM techniques. The XRD and FTIR results of the composite films suggest that with increase in filler wt% the electroactive β phase fraction of PVDF-HFP is enhanced. The maximum β phase of 78.9% is obtained for 3 wt% La-YFeO<sub>3</sub>/PVDF-HFP composite film (YP3). The FESEM image shows that the surface of YP3 composite film is highly porous and pores are in sub-micron range (280nm-400nm). The maximum triboelectric output voltage of ~1250 V and highest power density of 13.16 W.m<sup>-2</sup> are obtained across the theoretically infinite resistance 80 M $\Omega$  for the TEH device fabricated with YP3 film,. This device can charge 1µf capacitor up to 19 V in just 60 sec and lights commercial LEDs.

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## A first Principle study of LaMnO3 and LaB6 for colossal magneto resistive effect

<u>Tinku Kumar<sup>1\*</sup></u>, Ashok Kumar Jha and Shankar Kumar<sup>1</sup> <sup>1</sup>Patna university, Patna \*Corresponding author email <u>-tinkujaymatadi@gmail.com</u>

Keywords: magnetoresistance, CMR, correlated system

#### Abstract

Perovskite Manganites are being widely investigated both experimentally and theoretically as they have potential applications related to the colossal magnetoresistance (CMR) effect [1,2]. In addition to this these materials also offers testing ground for theories related to strongly correlated systems.

Undoped LaMnO<sub>3</sub> shows orbital ordering and John-Teller distortion and soon LaMnO<sub>3</sub> is doped it starts showing CMR effect.

In this study, an effort has been made to understand the optimized structure of  $LaMnO_3$  and  $LaB_6$  and derive density of states. Both undoped and doped perovskite Manganite have been studied to understand the factors contributing towards onset of CMR effect.

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## Origin of peculiar exchange bias phenomena in a hole doped rare-earth double perovskite series

Kazi Parvez Islam,<sup>1</sup> Suryakanta Mishra,<sup>1,2</sup> Debraj Choudhury<sup>1\*</sup>

<sup>1</sup> Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur - 721302, India.

<sup>2</sup> New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O., Bangalore - 560064,

India.

\*Corresponding Author: Dr. Debraj Choudhury, debraj@phy.iitkgp.ac.in

Keywords: Magnetic anisotropy, Inverse Exchange bias, Double Perovskite, Spin-glass, Antisite disorder.

Developing and understanding the materials that show significant Exchange Bias (EB) are at the forefront of current magnetism research and are of immense scientific and technological importance. Nevertheless, it is crucial to interpret the results with caution, as the presence of non-saturated minor loop like phenomena can obscure the true physics of the EB materials. In pursuit of this objective, we have successfully synthesised a rare-earth double perovskite system  $RE_{2-x}Sr_xCOMnO_{6-\delta}$  ( $0 \le x \le 1$ ) and investigated their diverse magnetic characteristics, with particular emphasis on EB. At x = 0.75, we observed the highest EB field of ~ 4.1 kOe at 8 K temperature when subjected to a cooling field of 6 T and sweep field of 7 T. However, upon subtracting the contribution of minor loop phenomena, we observed the presence of inverse EB (IEB) masquerading as normal EB (NEB) at x = 0.75 and two other nearest compositions. The IEB for x = 0.75 is found to be robust even at a high cooling field of 6 T, while for the other two nearest compositions, we see conversion of IEB to NEB with increasing cooling field. These peculiar phenomena can be attributed to the competition between ferro-antiferro (causing NEB) and ferro-glass (causing IEB) type interfaces. Furthermore, the entire series demonstrates complex physics, showcasing intriguing phenomena such as re-entrant double glassy states and behaviour resembling non-Griffiths-like phases.

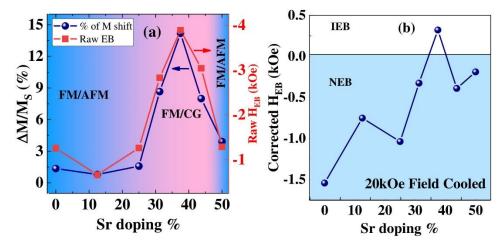


Fig. 1. (a) Variation of EB (2T field cooled) and vertical magnetization shift with hole doping as seen from the raw M(H) data at 8 K. Blue (Red) shade indicates FM/AFM (FM/Cluster-Glass) type interfaces; (b) Variation of *minor loop corrected* EB (2T field cooled) with hole doping at 8 K. 37.5% (x = 0.75) shows inverse EB.

- Suryakanta Mishra, <u>Kazi Parvez Islam</u>, Debraj Choudhury; Extrinsic origin of spontaneous exchangebias and negative magnetization: A case study on SmCrO<sub>3</sub> and DyCrO<sub>3</sub>, Journal of Magnetism and Magnetic Materials, Volume 603, 172220 (2024). https://doi.org/10.1016/j.jmmm.2024.172220
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## Theme : Magnetism & Superconductivity

## Search for rare-earth free permanent magnet in Fe<sub>2</sub>MnSn Heusler alloy

Junaid Jami<sup>1,\*</sup>, Rohit Pathak<sup>2</sup> and Amrita Bhattacharya<sup>1</sup>

1. AbCMS Lab, Department of Metallurgical Engineering and Materials Science, IIT Bombay

2. Materials Theory, Department of Physics and Astronomy, Uppsala University

\*Contact: Junaid.jami777@gmail.com

#### Category: Poster

Keywords: Permanent magnets, DFT, Magnetic anisotropy, Heusler alloy

In this work, we have tried engineering out-of-plane anisotropy in Fe<sub>2</sub>MnSn Heusler alloy by doping light interstitial atoms like B, C, H, O and N and have calculated the magnetic properties of the 12.5 at% doped samples which show an uniaxial anisotropy. The negative formation enthalpy of the doped alloys, confirms the structural stability of the defective structures. At 12.5 at% doping- B, C, O and N doped Fe<sub>2</sub>MnSn showed a flip in MAE from in-plane to out-of-plane, while H-doped compound shows an in-plane MAE for all doping concentrations and has a value of -0.75 meV at the 12.5 at%. The N-doped and H-doped compounds showed an enhanced magnetic moment of 6.77  $\mu$ B/f.u. and 6.64  $\mu$ B/f.u. respectively, which has increased in comparison to the undoped compound (6.45  $\mu$ B/f.u.). The SP of all the doped compounds has increased substantially with respect to the pristine compound (SP = 6%), with the highest value of 40% observed in nitrogen doped compound. For our doped alloys, we have studied the different exchange interactions between the magnetic atoms viz. Fe1-Fe1, Fe2-Fe2, Fe1-Fe2, Mn-Mn, Mn-Fe1 and Mn-Fe2. It should be noted that the T<sub>C</sub> in all these compounds has increased in comparison to undoped Fe<sub>2</sub>MnSn (729 K) and the largest increase in T<sub>C</sub> can be seen in C (999.8 K) and B (986 K).

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## Comprehensive Study of Dielectric Properties, AC Conduction and Resistive Switching Behavior in the Binary Se<sub>80</sub>Te<sub>20</sub> System through Incorporation of Transition Metals (Fe, Co, Ni, Cu)

<u>Nisha Kumari</u>, Vishnu Saraswat and Neeraj Mehta<sup>\*</sup> 1 Department of Physics, Banaras Hindu University, Varanasi, India \*Contact: dr\_neeraj\_mehta@yahoo.co.in

Keywords: Glass-ceramic, NSPT and CBH models, Electrical properties, Resistive Switching

Transition metals have been chosen as chemical modifiers for the binary Se<sub>80</sub>Te<sub>20</sub> (ST) system to create the ternary  $Se_{80-x}Te_{20}TM_x$  (STTM) system (where TM = Fe, Co, Ni, Cu, and x = 2). Exploring dielectric behavior, thermally activated AC conduction, and resistive switching provides valuable insights into the conduction mechanisms of chalcogenide materials. This system has been investigated for dielectric behavior over a wide range of frequencies (0.1 kHz to 500 kHz) and temperatures (303 K to 338 K). The detailed analysis reveals that the inclusion of transition metals in the parent system significantly alters the dielectric constant ( $\epsilon'$ ), dielectric loss ( $\epsilon''$ ), AC conductivity ( $\sigma_{ac}$ ), and activation energy  $(\Delta E_{ac})$ . Additionally, our findings revealed that the prepared transition metal chalcogenides (TMChGs) exhibited the Meyer-Neldel rule (MNR). When we analyzed the obtained results using relevant transport models, we found that the decreasing power-law exponent (s) with increasing temperature supports the Correlated Barrier Hopping (CBH) model for ST and STTM (where TM = Co, Ni, Cu), as they display a specific pattern of variation. Conversely, STTM (where TM = Fe) primarily demonstrates non-overlapping small polaron tunneling (NSPT), as indicated by the increasing nature of s with temperatures. Moreover, the incorporation of transition metals leads to a significant modification in the resistive switching properties. This investigation examined the current-voltage characteristics and direct current electrical conductivity of prepared thin pellet samples.

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## Interface driven switching of spin Hall magnetoresistance in ferromagnetic/high spinorbit coupled oxide heterostructure

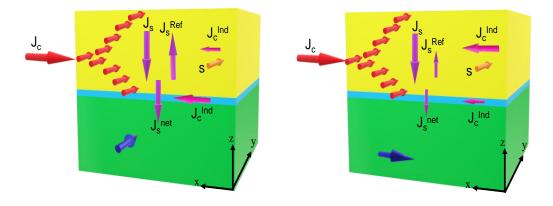
Jayaprakash Sahoo<sup>\*,1</sup> Megha Vagadia,<sup>2</sup> Shivam Sharma,<sup>3</sup> René Hübner,<sup>4</sup> Ankit kumar,<sup>1</sup> Ganesh Sahastrabuddhe,<sup>1</sup> Abir De Sarkar,<sup>4</sup> & D.S. Rana<sup>1</sup>

<sup>1</sup>Department of Physics, Indian Institute of Science Education and Research Bhopal, Madhya Pradesh 462066, India

<sup>2</sup>Department of Physics, Saurashtra University Rajkot, Gujarat 360005, India <sup>3</sup>Department of Physics, Institute of Nano-science and Technology, Mohali, Punjab, 140306, India <sup>4</sup>Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany \* jayaprakash19@iiserb.ac.in

Keywords: Magnetism, Interface, spin hall magnetoresistance, spin-orbit coupling.

#### Abstract:



Spin Hall magnetoresistance (SMR) arises due to the interplay between the spin current in the high spin-orbit coupled (SOC) material and the magnetization of the ferromagnetic material which is always positive regardless of the spin Hall conductivity of high SOC material. We are reporting the switching of SMR from negative to positive in the SrRuO<sub>3</sub>/CaIrO<sub>3</sub> heterostructure as the consequence of the spin-to-charge interconversion at the interface as well as in the bulk that is dependent on the thickness of the CaIrO<sub>3</sub> layer. In this SrRuO<sub>3</sub>/CaIrO<sub>3</sub> heterostructure, dimensionality control of CaIrO<sub>3</sub> can influence the interfacial coupling so also SMR. Our results show that when the interfacial spin-to-charge conversion effect dominates negative SMR comes into play and when the bulk effect dominates, we are getting positive SMR behavior in our superlattices. This outcome offers important new perspectives on how the competition between interfacial SOC and bulk SOC might be used to tune SMR behavior. Comprehending this concept and how it affects SMR may be vital to maximizing the performance of spintronic devices, where exact control over spin current manipulation is critical.

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## Josephson junctions with ferromagnet-heavy metal barriers

Debashree Nayak<sup>1</sup>, Kartik Senapati<sup>1</sup>

1 School of Physical Sciences, National Institute of Science Education and Research (NISER) Bhubaneswar, An OCC of Homi Bhabha National Institute, Jatni, 752050, Odisha, India \*Contact: debashree.nayak@niser.ac.in

## Category: Poster

Keyword: Superconductivity, Josephson Junction

Creating and manipulating spin polarized supercurrent has been a central theme of superconducting spintronics. When spin-singlet Cooper pairs are passed through a magnetically inhomogeneous structure, triplet Cooper pairs are generated by a process of spin mixing followed by spin rotation. Recently it has been shown theoretically that spin-orbit coupling offers an alternative approach for generating the triplet Cooper pairs. A nonequilibrium spin density appears in a current carrying heavy metal due to the Rashba and Dresselhaus spinorbit couplings[1][2]. The relative angle between this spin density and the magnetization of a proximal ferromagnetic layer is believed to facilitate spin rotation of the  $s_z=0$  triplet Cooper pairs into the long range triplet pairs. We are trying to observe this effect experimentally in nanoscale vertical Josephson junctions with a composite Pt/Ni/Pt barrier between the superconducting Nb electrodes.

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## **Renewable Energy (Conversion & Storage)**

## Carbon Dot-PVDF-HFP Nanocomposites for Flexible Piezoelectric and Triboelectric Nanogenerators

Ajay Kumar<sup>1</sup>, Navonil Bose<sup>2,\*</sup> and Mousumi Basu<sup>1</sup>

<sup>1</sup> Department of Physics, IIEST Shibpur, Howrah 711103, West Bengal, India

<sup>2</sup> Department of Physics, Jadavpur University, Kolkata- 700032, West Bengal, India

\*Corresponding Author: <u>navonil05@gmail.com</u>

#### Category: Oral/Poster

Keywords: Carbon dot / PVDF-HFP composite,  $\beta$  phase, Nanogenerators

Flexible, portable, wearable energy harvesters have wide range of applications in wearable electronics <sup>[1]</sup>, healthcare monitoring<sup>[1]</sup> and self-powered sensors<sup>[1]</sup>. Especially self-powered sensors with wireless data transmisson capacity have profound applications in IOT, machine learning and artificial intelligence. Typically polyvinylidene fluoride (PVDF), its copolymers (PVDF-HFP, PVDF-TrFE) and their composites are used for fabrication of such flexible energy harvesters due to fair piezoelectric, triboelectric and pyroelectric responses of this ferroelectric polymer. Chemical inertness and high durability are also two factors for choosing this polymer. The PVDF have five phases ( $\alpha$ ,  $\beta$ ,  $\gamma$ ,  $\delta$  and  $\varepsilon$ ) in which  $\beta$  and  $\gamma$  is the most suitable phases for electroactive response. Different nanofillers are added in PVDF to enhance the electroactive phases<sup>[2]</sup>. Here, for the development of high  $\beta$  phase of PVDF bio-derived carbon dots(C-dots) are used.

Here, we report the development of piezoelectric nanogenerator (PNG) and triboelectric nanogenerator (TNG) devices by using flexible, self-standing C-dot /PVDF-HFP composite films. The bio-derived C-dots are characterized by XRD, HRTEM and Raman spectroscopy techniques. The HRTEM result shows spherical and well dispersed C-dots with size in the 2-8 nm range. C-dot/PVDF-HFP composite films with different concentrations of C-dot are fabricated by solution casting (SC) technique. The structural and morphological properties of the composite films are investigated by using XRD, FTIR and SEM techniques. The PNG device has been fabricated by using electrode/ composite film/electrode stack structure, whereas the composite film is used as tribo-negative layer for fabricating the TNG device. The study reveals that the output performance of TNG device consisting of PVDF-HFP/C-dot composite film, and it should also be mentioned that the corresponding open circuit voltage is 140V and 40V for TNG and PNG devices respectively.

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## Multifaceted Characterization of Zinc-Doped Chalcogenide Glasses: Unveiling the Impact on Thermal, Mechanical, Electrical and and Radiation Shielding Properties

Vishnu Saraswat and Neeraj Mehta\*

Material Science Lab, Department of Physics, Banaras Hindu University, Varanasi (221005), India \*Contact: dr\_neeraj\_mehta@outlook.co.in

#### Keywords: DSC, Dielectric, Micro-Hardness, Radiation Shielding, Resistive Switching

This comprehensive study investigates the glass-to-crystal phase transformation in a novel chalcogenide glass system, Se-Te-Sn-Zn (STSZ). The researchers synthesized a series of STSZ glasses with varying Zn concentrations ( $Se_{78-x}Te_{20}Sn_2Zn_x$ , where x = 0, 2, 4, and 6) and conducted detailed thermal, structural, and electrical characterization.

The thermal analysis using Differential Scanning Calorimetry (DSC) reveals a significant increase in the crystallization rate upon adding Zn to the parent Se-Te-Sn glass. As the Zn content increases, the average heat of atomization and overall mean bond energy decrease, corresponding to a reduction in the cohesive energy of the samples. An inverse relationship is observed between the thermal stability parameter and the enthalpy released during the glass-to-crystalline phase transformation. The researchers also performed micro-indentation tests to evaluate the hardness and other mechanical properties, such as the modulus of elasticity, minimal micro-void formation energy, glass fragility index, and micro-void volume. The covalent nature of

the glassy system was examined, and the fracture toughness and crack patterns were reported. Additionally, the dielectric behavior and a.c. conduction, governed by the correlated barrier hopping (CBH) mechanism, were significantly affected by Zn concentration. The resistive switching behavior was modified by Zn incorporation, explained by the chemically ordered network (CON) model and SeyZny cluster cross-linking.

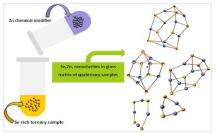


Figure 1 - optimized structures of  $Se_yZn_y$  nano-clusters embedded in quaternary STSZ glasses at cross-

Additionally, the potential of STSZ glasses as effective shielding materials for high-energy radiation (X-rays and gamma rays) was also assessed using the Phy-X/PSD program. Key shielding parameters such as linear and mass attenuation coefficients, half-value layer, and mean free path were determined, with STSZ glasses out-

performing conventional glasses. Zn substitution for Se further improved mechanical parameters like bulk modulus and Poisson's ratio.

This comprehensive study offers valuable insights into the thermal, electrical, and radiation shielding properties of STSZ chalcogenide glasses, positioning them as promising candidates for advanced technological applications.

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## Interferometry Based Ascorbic Acid Sensor Using Zno-Sno<sub>2</sub> Nanocomposite Coated Plastic Optical Fiber

## Sudipta Kumari Panigrahy\*, Sukanta Kumar Tripathy

Centre of Excellence for Nanoscience and Technology for Development of Sensor, Department of Physics, Berhampur University, Bhanja Bihar, Berhampur, Odisha, 760007

\*Corresponding author: skp.rs.phy@buodisha.edu.in

Category: Oral

Keywords: Interferometry, Ascorbic acid, Flattened fiber

## ABSTRACT

The detection of ascorbic acid has become crucial as deficiency of ascorbic acid (AA) in human blood serum can cause critical health issues like scurvy, parkinson's disease, rheumatoid arthritis etc. In the present work the ZnO-SnO<sub>2</sub> nanocomposite was synthesized using chemical method. The structural and optical characterization of the synthesized nano composite was done using X-ray diffraction (XRD), Scanning electron microscopy (SEM), UV absorption spectroscopy (UV) and Photoluminescence spectroscopy (PL). For the desired sensing application, an interferometry-based flattened fiber optic biosensor is proposed for the detection of AA. For this, the middle portion of the PMMA fiber is flattened using our home-made arrangements. The middle-flattened portion of the fiber was then coated with ZnO-SnO<sub>2</sub> nanocomposite. The Limit of Detection (LOD) and sensitivity of the sensor for the flattened configuration were found to be 0.3 mg/dl and 4.25 nW/(mg/dl) respectively. The LOD of the proposed sensor is less than the normal range of AA in blood i.e. 0.4 mg/dl to 2 mg/dl, hence the proposed configuration can be deemed to a low-cost fiber optic method for the detection of ascorbic acid.

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## Theme: Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)

## Impact of Different Antireflection coatings on Silicon solar cells

Anterdipan Singh<sup>1</sup> and Pratima Agarwal<sup>2,\*</sup>

1 Department of Physics, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India

2 School of Energy Science and Engineering, Indian Institute of Technology Guwahati, Guwahati, Assam 781039, India \*Contact: pratima@iitg.ac.in

#### Category: Oral

*Keywords:* Antireflection Coating (ARC), Single layer ARC(SLARC), Double layer ARC(DLARC) This article presents a simulation study on the impact of widely used Single and Double-layer Anti-reflection coating (DLARC) for Silicon solar cells (SSC). Anti-reflection performance for different ARC designs is evaluated using the average reflectance ( $R_{avg}$ ) value in the 400nm-860nm wavelength range. ZnO, ZnS, SnO<sub>2</sub>, were chosen for SLARC design because of their refractive index being close to Ideal values. MgF<sub>2</sub>-ZnS, SiO<sub>2</sub>-ZnS, SiO<sub>2</sub>-TiO<sub>2</sub>, and MgF<sub>2</sub>-TiO<sub>2</sub> designs were chosen for fabricating the DLARC. However, DLARCs were found to be superior to SLARCs in terms of anti-reflection performance. The calculated  $R_{avg}$  for the DLARCs reflect the superiority of DLARCs over SLARCs. SiO<sub>2</sub>-TiO<sub>2</sub> DLARC has the least  $R_{avg}$  (1.46%) values compared to other DLARCs, followed by MgF<sub>2</sub>-TiO<sub>2</sub>( $R_{avg}$  =1.69%), MgF<sub>2</sub>-ZnS ( $R_{avg}$  =1.76%), and SiO<sub>2</sub>-ZnS ( $R_{avg}$ =1.97%). Later the impact of the different DLARCs on the silicon solar cells are evaluated using TCAD sentaurus. The changes in performance parameters, External quantum efficiency etc, are also investigated for further understanding of the underlying physics. The reflection spectra of different DLARC have been given in fig 1, alongside the performance parameters of the SSC having SiO<sub>2</sub>-TiO<sub>2</sub> DLARC and ZNO SLARC

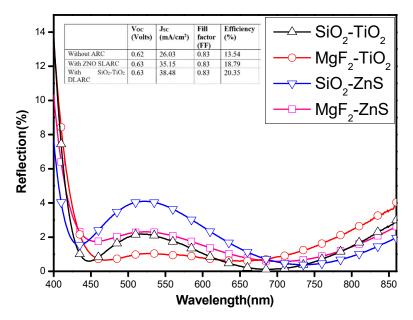


Fig 1- Simulated Reflection spectra for different DLARCs on the silicon substrate using TCAD sentaurus.

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## **Soft Condensed Matter**

## **Controlling the Nanoarchitecture of Discotic Liquid Crystal for Electronic Device Applications**

Himangshu Paul\*, Alpana Nayak

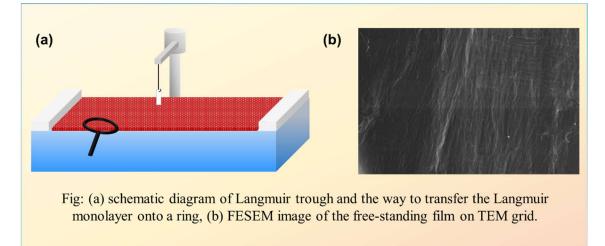
Indian Institute of Technology Patna, India, 801106 \*Contact: himangshu\_2221ph22@iitp.ac.in

## Category: Poster

Keywords: Discotic Liquid Crystal, Nanoarchitectonics, Self-Assembly, Free-Standing Film

Discotic liquid crystal (DLC), composed of disk-shaped molecules, exhibit unique self-assembly properties that enable the formation of highly ordered structures, making them suitable for various deivce applications. This research focuses on the characterization and optimization of discotic liquid crystal (DLC) thin films for electronic device applications. The study investigates the stability of DLC monolayers at the air-water interface by analyzing the variation of area per molecule over time under fixed surface pressure conditions. The area relaxation behavior indicates that a more pronounced change in area suggests a less stable monolayer, while minimal changes indicate a robust arrangement of molecules. Additionally, the impact of temperature on the DLC monolayer is examined through surface pressure versus area per molecule isotherms, revealing that the limiting area per molecule increases with temperature, indicating greater molecular spacing due to enhanced thermal motion. The elastic modulus of the monolayer decreases with rising temperatures, suggesting a reduction in rigidity as thermal energy disrupts intermolecular interactions. To create free-standing films, the Langmuir monolayer is compressed and transferred onto various substrates, demonstrating the strong intermolecular interactions that allow for stable film formation. Overall, this research aims to advance the understanding of DLC nanoarchitecture and its implications for enhancing the performance of electronic devices, establishing DLCs as key materials in the development of innovative, high-efficiency organic electronics.

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## Theme: Magnetism & Superconductivity

## Ion-implantation-induced Structural & Magnetic Modifications in Cr/SmCo<sub>5</sub>/Pt/Co<sub>20</sub>Fe<sub>60</sub>B<sub>20</sub> Multilayer Thin Films

Gourav Sharma<sup>1,\*</sup>, Sambhunath Bera<sup>1</sup>, Harshvardhan Tyagi<sup>2</sup>, Raj kumar<sup>3</sup>

<sup>1</sup>Center for Advanced Materials & Devices, BML Munjal University, Gurugram, Haryana, 122413, India <sup>2</sup>Amity Centre for Spintronic Materials, Amity University, Noida, UP 201313, India <sup>3</sup>Inter University Accelerator Centre, New Delhi, 110067, India

\*Contact: gourav.sharma.22pd@bmu.edu.in

#### Category: Poster

Keywords: Exchange Spring magnets, ion implantation, X-ray Reflectivity, Magnetic Anisotropy

Magnetic and structural properties of Si-substrate/Cr/SmCo<sub>5</sub>/Pt/Co<sub>20</sub>Fe<sub>60</sub>B<sub>20</sub> multilayer thin films have been investigated before and after low energy gaseous ion implantation. SmCo./CoFeB bilayer film shows exchange spring magnetic behavior. Interface quality plays an important role in the performance of this bilayer system. We have incorporated a very thin Pt layer in between SmCo<sub>5</sub> & Co<sub>20</sub>Fe<sub>60</sub>B<sub>20</sub> layers to reduce interdiffusion. Two multilayer samples have been irradiated with 45 keV He<sup>+</sup> ions & 15 keV Ne<sup>+</sup> ions respectively at a fluence of  $3 \times 10^{16}$  ions/cm<sup>2</sup> to study the ion implantation induced changes of structural and magnetic properties. The internal structure of the multilayer samples before and after irradiation has been very minutely characterized by the X-ray reflectivity (XRR) study. Theoretical simulation was carried out to extract the information of individual layer thickness, electron density, and surface & interface roughness of the multilayer samples and its modifications due to jon implantation. XRR analysis reveals that there are significant changes in the internal structure of both the samples after ion implantation. VSM study of the pristine sample shows magnetic anisotropy with in-plane easy axis and out-of-plane hard axis. Azimuthal in-plane MOKE measurement of pristine sample shows two-fold uniaxial anisotropy. This uniaxial anisotropy reduces after He<sup>+</sup> ion irradiation whereas four-fold anisotropy arises after Ne<sup>+</sup> ion irradiation. This change of the magnetic properties is due to the ion implanted induced structural modifications of the multilayer samples.

## Bhaskara Law: A New Paradigm for Understanding Energy Phenomena Beyond Thermodynamics

Mathan babu bhaskaran Head,R&D,DRBMLAB LIMTED Mathanbabu.b@bmlab.in

Keywords: Energy, Thermodynamics, Bhaskara Law, Fundamental Forces, Curie Effect

## Abstract :

The principles of thermodynamics have long served as the foundation for understanding energy transformations and the behavior of physical systems. However, these laws primarily focus on how the four fundamental forces—gravitational, electromagnetic, weak, and strong nuclear—interact within a single, observable property of matter: heat. While this framework is effective for describing macroscopic energy transfer processes, it inherently limits our comprehension of the underlying mechanics that govern energy creation and destruction.Bhaskara Law introduces a groundbreaking approach to energy science by expanding our understanding beyond the thermodynamic domain. It posits that energy is not merely conserved or converted but also undergoes a continuous cycle of creation and annihilation, a phenomenon that thermodynamics does not account for. This new theory provides a unified perspective on energy phenomena that occur at both microscopic and macroscopic levels. Unlike classical thermodynamics, which views energy transformations as linear processes governed by entropy, Bhaskara Law reveals complex, nonlinear interactions between energy states.

A key distinction of Bhaskara Law is its ability to explain energy behaviors in systems that defy classical thermodynamic predictions, such as the Curie effect. It offers insights into how energy can appear and dissipate in unconventional forms, paving the way for new technologies in renewable energy. By decoupling energy analysis from the sole dependence on heat and entropy, Bhaskara Law bridges gaps left by thermodynamic laws, allowing us to explore energy creation and destruction as complementary processes rather than isolated events. This presentation will discuss how Bhaskara Law provides a broader framework for understanding energy interactions across various scientific domains. It will explore how this law redefines our perception of energy boundaries, extends the understanding of complex systems, and opens new avenues for research in condensed matter physics. With its capacity to transcend thermodynamics, Bhaskara Law offers a fundamental shift in energy science, laying the groundwork for novel experimental methods and practical applications.

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# Designing Hybrid Quantum Devices Using Photon-Photon Coupling for Quantum Technologies.

## Rakesh Kumar Nayak, Abhishek Maurya, Meghana Mishra, Rajeev Singh, Biswanath Bhoi\*.

Nano-Magnetism and Quantum Technology Laboratory, Department of Physics, Indian Institute of Technology (BHU), Varanasi, 221005, Uttar Pradesh ,India.

Email of Presenting Author: rakeshkumarnayak.rs.phy22@itbhu.ac.in

\*Email of corresponding author: <u>biswanath.phy@iitbhu.ac.in</u>

Category: Poster

Keywords: Photon-Photon Coupling, Level Attraction, Level Repulsion .

In recent decades, research in quantum information science has increasingly focused on controlling and manipulating electromagnetic waves, uncovering intriguing phenomena such as photon-photon coupling and leading to significant advancements across various quantum technology fields. Photon-photon coupled hybrid systems hold substantial promise for improving quantum processing technologies [1]. This study investigates the crucial role of managing photon mode interactions, including different anti-crossings, to develop information processing devices with optimal tunability and scalability.

A framework is introduced that facilitates photon-photon coupling with the ability to switch between level repulsion (LR) and level attraction (LA). These advancements have enabled the realization of quantum gates and quantum hybrid devices paving the way for more robust and scalable quantum communication networks and quantum computing systems.

We carried out numerical simulations, illustrate these switching features in two distinct photon-photon mode, demonstrating how dynamic adjustments between LR and LA can improve the performance and versatility of quantum devices [2]. The findings highlight the importance of precise control over photon-photon interactions for creating scalable and adaptable quantum technologies, paving the way for progress in quantum computing, communication, and sensing applications.

Furthermore, the study examines the characteristic features of these photon mode interactions through a quantum mechanical model. This model allows for fine-tuning of parameters and enables the observation of interactions at room temperature. The results emphasize the potential of these hybrid systems to develop versatile and scalable quantum devices, which are crucial for the progress of quantum technology.

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## Exploring Charge Transfer and Energy Levels in TCPP<sup>2+</sup> Complexes: Insightfrom HOMO-LUMO Analysis

Anju<sup>\*</sup> and L.K. Saini

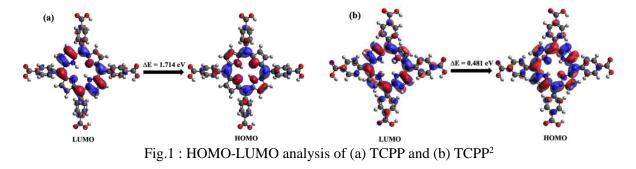
<sup>1</sup> Department of Physics, Sardar Vallabhbhai National Institute of Technology, Surat, - 395007, India \*Contact: anjur7883@gmail.com

## Keywords: DFT, TCPP, HOMO-LUMO, optoelectronic

This research is based on applying Density Functional Theory calculations to examine the optoelectronic potential of protonated porphyrin 5, 10, 15, and 20-tetrakis(4-carboxyphenyl) porphyrin (TCPP<sup>2+</sup>). Our computational study investigates the inherent energy states and charge transfer properties of TCPP<sup>2+</sup>. The electronic characteristics are determined using HOMO-LUMO and energy bandgap ( $\Delta E$ ) analysis. We focus on how the protonated and its pure equivalent, TCPP, exhibit distinct charge transfer behaviours.

On comparison of the multiple global chemical reactive descriptors (GCRD), such as maximal charge transfer,  $\Delta N$ max, an important outcome is revealed[1-2]. A greater  $\Delta N_{max}$  value indicates that protonated TCPP is more reactive than pure TCPP. Because of its inherent property, protonated TCPP shows more reactivity than pure TCPP. The rate of charge transfer increases in protonated TCPP while it decreases in pure TCPP. According to our findings, protonated TCPP exhibits higher reactivity and charge transfer, which makes it a viable option for a variety of optoelectronic uses, including optical switches, sensors, and power regulators.

These recently identified properties of protonated TCPP offer enormous potential for the use of customized porphyrins in innovative devices with precisely calibrated optoelectronic capabilities. They also provide a thorough understanding of the intricate interactions between cationic porphyrin and pure porphyrin structures.



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## Multiferroics & Heterostructures

## Insights into the origin of multiferroicity and large in-plane piezoelectricity in AlXY (X = S, Se; Y = Cl, Br, I) monolayers

Nilakantha Tripathy, Abir De Sarkar\*

Institute of Nano Science and Technology, Quantum Materials and Devices Unit, Knowledge City, Sector 81, Manauli, Mohali, Punjab 140306, India \*Email: abir@inst.ac.in, abirdesarkar@gmail.com

Category: Poster

Keywords: 2D materials, Multiferroics, Ferroelectricity, Ferroelasticity

#### Abstract

Understanding the interplay of properties in two-dimensional (2D) multiferroic materials is of paramount importance for crafting the blueprint of cutting-edge functional devices in the next generation. In the present study, we report a family of stable multiferroics AlXY (X = S, Se; Y =Cl, Br, I) with the coexistence of ferroelectricity and ferroelasticity, using DFT calculations. The AIXY monolayers (MLs) exhibit large in-plane ferroelectric polarization ( $P_v$ ) ranging from 148 to 177 pC/m with a moderate switching barrier of 0.102 to 0.192 eV/atom. The polarization in these MLs owes its origin to the repositioning of Al atoms, actuated by soft B<sub>2u</sub> phonon mode in the paraelectric (PE) phase (Pmmn). These MLs exhibit robust ferroelasticity with a large reversible strain of 38-45.1% and moderate switching barriers of 0.175 to 0.213 eV/atom. The ferroelectric (FE) and ferroelastic (FA) phases differ in the electric polarization direction by 90° rotation. Besides a strong anisotropy in mechanical properties, in-plane piezoelectricity, and carrier mobilities is observed in the AlXY MLs. Moreover, FA switching provides a highly effective way for finely tuning these anisotropic properties of AlXY MLs. Complementing these findings, we devised an empirical predictive model built on descriptors derived from linear regression analysis, linking atomic polarizability, Bader charge, lattice constant (b), layer thickness (h), bandgap, and effective mass of electron in order to estimate polarization (P<sub>y</sub>) and in-plane piezoelectric constants  $(d_{22}, d_{21})$  of AlXY MLs, which is in excellent agreement ( $R^2 = 0.95$  to 0.98) with results obtained from DFT.

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## Nano and Functional materials

## Exploring the Structural, Morphological, and Optical Properties of Hydrothermally Synthesized ZnO Nanorods

M. Nageswara Rao<sup>1</sup>, B. Naveen Kumar Reddy<sup>2,\*</sup> and R. Nagaraju<sup>3</sup>

1,2Department of Physics, School of Applied Science and Humanities, Vignan's Foundation for Science Technology and Research, Vadlamudi, Guntur-522 213, Andhra Pradesh, India

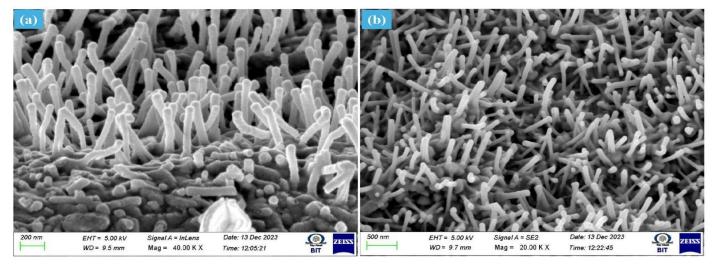
3 Department of Chemistry, School of Applied Science and Humanities, Vignan's Foundation for Science Technology and Research, Vadlamudi, Guntur-522 213, Andhra Pradesh, India

\* Contact:bussireddynaveen@gmail.com

#### Category: Poster

Keywords: ZnO nanorods, XRD, FE-SEM, Hydrothermal method.

**Abstract**: In this study, zinc oxide (ZnO) nanorods were grown on a silicon substrate through a hydrothermal method. A ZnO thin film, employed as a seed layer, was initially prepared using the sol-gel process. The nanorods were synthesized on this seed layer at 90 °C over duration of 6 hours. Various characterization techniques, including X-ray Diffraction (XRD), Field-Emission Scanning Electron Microscopy (FE-SEM), and UV-visible spectroscopy, were used to examine the structural, morphological, and optical properties of the ZnO nanorods. XRD analysis confirmed that the nanorods were oriented vertically along the c-axis [1]. FE-SEM imaging showed a uniform distribution of nanorods, with average lengths and diameters measured at 395.2 nm and 98.4 nm, respectively [2]. Energy-dispersive X-ray spectroscopy (EDX) analysis verified the presence of only zinc and oxygen without detectable impurities. The UV-visible absorption spectrum further revealed the band gap of the synthesized nanorods. These well-aligned ZnO nanorods hold promise for applications in solar cells, gas sensors, and biosensors.



**Fig. 1 (a-b)** Cross-sectional FESEM images of ZnO nanorods. (a) 200 nm, (b) 500 nm. References:

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## Electro-Optical And Thermal Characterization Of Copper Tartrate Crystals Grown In Silica Gel

Ms.Lakshmichhaya R.Patil<sup>1\*</sup>, Dr.S.J.Shitole<sup>2</sup>

1 PhD Student of Department of Physics R.C.Patel Arts,Science & Commerce College,Shirpur-4254051<sup>1</sup> 2 Principal,,Smt.H.R.Patel Mahila College,Shirpur-425405<sup>2</sup> \*laxmlpatil123.lp@gmail.com

Keywords: Silica gel, Chemical reaction, TGA, DSC

## Abstract:

Copper Tartrate crystals were grown by Gel Growth technique by single diffusion.Silica gel of Optimum specific gravity was set with tartaric acid at optimum pH and aging period.Band gap of copper tartrate crystal is determined using Ultraviolet-Visible Spectroscopy .Blue Color of Copper tartrate crystal and transparency is confirmed using Photoluminescence spectroscopy.Dimensions of crystals are found from Powder X-Ray Diffraction data.

## Table 1: Optimum Conditions For Crystal Growth of $CuC_4H_4O_6$

Sr No	Specific parameter	Optimum value
1	Specific gravity of Silica gel	1.04 g/cc
2	pH of gel medium	4.00
3	Concentration of inner reactant'tartaric acid'	1M
4	Concentration of outer reactant 'Copper Chloride'	1M
5	Gel setting time	24 Hr -36 Hr
6	Growth period	$1^1_2$ month
7	Diffusion method	Single diffusion
8	Gel Aging	4 days after Gel Setting

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## DEVICES

## Resistively detected electron spin resonance and g factor in few-layered exfoliated MoS<sub>2</sub> devices

<u>Chithra H. Sharma<sup>1,2\*</sup></u>, Appanna Parvangada Pemmaiah<sup>2</sup>, Lars Tiemann<sup>2</sup>, Kai Rossnagel<sup>1</sup>, Jens Martin<sup>3</sup>, Robert H. Blick<sup>2,4</sup>

<sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany.

<sup>2</sup>Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Luruper Chaussee 149, Hamburg 22761 Germany. <sup>3</sup>Leibniz Institut für Kristallzüchtung, 12489 Berlin, Germany

<sup>4</sup>Material Science and Engineering, University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA.

\*Contact: Sharma@physik.uni-kiel.de

Category: Oral

Keywords: Electron-spin-resonance, MoS<sub>2</sub>, g factor, Transport, Transition-metal-dichalcogenides

Electron spin resonance (ESR) is a powerful technique to investigate the behavior of electron spins and extract information such as g factor, spin-relaxation times and spin-orbit interaction strength. While using resistively detected ESR (RD-ESR), manipulation of the electron spins in a device environment can be studied. [1,2] This is an important tool for the development of spintroic devices, qubits etc.

 $MoS_2$  has recently evolved as a material with great potential for hosting quantum devices and spintronic applications. Hence, the demonstration of RD-ESR and the determination and improved physical understanding of the *g* factor is of great importance. Nevertheless, its application has been limited so far by highly resistive contacts to  $MoS_2$ . Here, we exploit n-doped few-layered  $MoS_2$  devices with tin (Sn) contacts demonstrating ohmic behavior at low temperatures. By means of RD-ESR, we determine the *g* factor in multi-layered  $MoS_2$  and observe that the *g* factor value is independent of the charge carrier density within the limit of our measurements.

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## Nano and Functional materials

## Charge Confinement at Hetero-Semiconductor Junction and Enhancement of Electronics Properties

Biswanath Das<sup>1</sup>, Kumari Neha<sup>1</sup>, Sabyasachi Saha<sup>2</sup> and P.V. satyam<sup>1</sup>\* <sup>1</sup>School of Basic Sciences, IIT Bhubaneswar, Argul, Jatni, 752050 <sup>2</sup>Defence Metallurgical Research Laboratory (DMRL), Hydrabad, Telangana, 500058 \*Contact: satyam@iitbbs.ac.in

Category: Poster

*Keywords:* Silicon Carbide (SiC), X-Ray Reflectivity (XRR), Differential Phase Contrast (DPC), Density Functional Theory (DFT).

Germanium (99.999%) thin epitaxial layer have been deposited on 4H-SiC using Molecular Beam Epitaxy at Ultra High Vacuum (10<sup>-10</sup> mbar) with substrate at a temperature 500°C. Cross-sectional HRTEM and High-Resolution STEM images show the single crystal growth of Ge have been done on SiC and it also reveals that the growth is layer-plus-island (SK-Growth). In order to understand the interface of Ge-SiC, we conducted a first principles calculation of the heterostructure using the VASP (Vienna Ab initio Simulation Package) software package. The crystal structure of 4H-SiC (0001) and Ge (111) have been used to create a heterostructure with the smallest possible lattice mismatch. The Partial Density of States (PDOS) provides information about the variation in bandgap and the lowering of excitation states resulting from the passivation of surface dangling bond states. Additionally, the bader charge density analysis has been conducted, and it has been determined that there is charge confinement at the interface. Here, electrons from Germanium have been transferred to the interface, resulting in the formation of an interface dipole. This dipole can affect the bandstructure and reduce the bandgap. Electron density fluctuations near the interface were identified through X-Ray Reflectivity (XRR) measurements of the sample. In addition, Differential Phase Contrast (DPC) imaging was employed to analyze the development of the electric field at the interface. This analysis plainly demonstrates that the periodicity of the SiC crystal has been disrupted at the interface, and there is a region that is highly sensitive to the electric field. Electron Energy Loss Spectroscopy was employed to quantify the charge at the interface. This confinement of charge at the interface improves the electronic properties of the interface and is beneficial for the application of devices.

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## Nano and functional materials

# O<sub>2</sub>-assisted phase transition from mixed oxide phases of Mo to stable MoO<sub>3</sub> phase

<u>Athira C<sup>1</sup></u>, <sup>\*</sup> Subhashis Gangopadhyay

1 Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031, India<sup>1,2</sup> \*Contact: subha@pilani.bits-pilani.ac.in

#### Category: Oral

Keywords: Nanostructures, TMO, phase transition, thermal oxidation.

Nanostructured transition metal oxides (TMO), known for their unique electronic, magnetic, and optical properties at the nanoscale, have emerged as leaders in revolutionizing electronic applications [1]. At the nanoscale, these compounds undergo significant structural changes with widescale morphologies, resulting in the emergence of novel electromagnetic phenomena, which are not present in their bulk counterparts [2]. Among various TMOs, molybdenum oxides (MoOx) are one of the most appealing metal oxides because of their unique structural properties. Versatile applications of  $MoO_3$ and  $MoO_2$  span across several domains, encompassing electrochemical supercapacitors, lithium-ion batteries, electrocatalysis, sensors, and field emission devices [3]. Mo oxides usually appear in a mixed oxide phase which can undergo different phase transitions under specific growth conditions. In this work we aim to address a major challenge of the selective growth of a single oxide phase with an enhanced crystallinity of different oxide nanostructures. High purity MoO<sub>3</sub> films are deposited on quartz substrates, using a vacuum assisted thermal evaporation technique ( $\sim 10^{-5}$  mbar). Afterwards, thermal oxidation in controlled ambient is performed at various temperatures to obtain a selective oxide phase. Structural, morphological, chemical, and electrical properties of these oxide layers are investigated using various surface characterization techniques such as XRD, SEM, Raman spectroscopy, and XPS. XRD results show high crystalline quality of the oxide films. Orthorhombic MoO<sub>3</sub> phase is usually observed for oxidation temperatures up to 500°C. FESEM imaging depicts two distinct nanostructured morphologies such as large, faceted clusters of elongated shape and homogeneous distribution of small granular islands. At a certain growth condition, asymmetric growth of 1D nanorods are also formed. Oxidation states of these nanostructures are carefully analyzed with the help of XPS to obtain an oxide film with a single oxide phase.

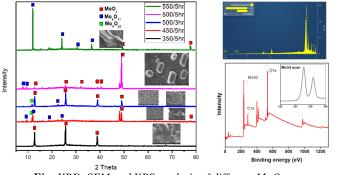


Fig: XRD, SEM and XPS analysis of different MoO<sub>x</sub> nanostructures

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## **MAGNETISM & SUPERCONDUCTIVITY**

## Evidence for multigap superconductivity in the Dirac semimetal PdTe

<u>Amit Vashist<sup>1</sup></u>, Bibek Ranjan Satapathy<sup>1</sup>, Harsha Silotia<sup>1</sup>, Yogesh Singh<sup>2</sup>, and S. Chakraverty<sup>1</sup>

<sup>1</sup>Quantum Materials and Devices Unit, Institute of Nano Science and Technology, Sector-81, Punjab, 140306, India. <sup>2</sup>Department of Physical Sciences, Indian Institute of Science Education and Research Mohali, Sector 81, S. A. S. Nagar, Manauli, PO: 140306, India

\*Contact: amitvashist42@gmail.com

#### Category: Oral

Keywords: Dirac semimetal, Unconventional superconductor, dHvA oscillation

PdTe is a type-II superconductor and has recently been identified as a Dirac semimetal, which has generated significant research interest as a potential candidate for unconventional superconductivity based on ARPES measurement [1]. There are conflicting reports on whether it is a strongly or weakly coupled superconductor, depending on the quality of the crystals. The ARPES measurements also claimed it as a bulk nodal gap superconductor, which is in contrast to the recent thermal measurements, where it has been shown to be a multigap superconductor [2]. We use electrical transport and magnetization measurements to investigate the superconducting and Fermi surface properties of PdTe. The anisotropy in the upper critical magnetic field has been observed depending on the direction of applied magnetic field. The magnetic field vs temperature (H - T) phase diagram extracted using resistivity data shows an upward curvature similar to several multigap superconductors. Magnetization measurements show the presence of de Haas-Van Alphen (dHvA) oscillation. The Fourier transform of quantum oscillations revealed the presence of two Fermi pockets. Moreover, Landau fan diagram for a small Fermi pocket confirms the presence of non-trivial Beery phase  $\pi$ , consistent with the Dirac nature of PdTe.

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## Revolutionizing Encapsulation: The Role of Barium-Linked Carrageenan Gel for encapsulation of flavour, fragrance and probiotics.

Aman Shukla\*, Priyank purohit Graphic Era Hill University, School of Pharmacy, Dehradun Uttarakhand,248001. Contact: amanlesnar12@gmail.com

*Keywords:* Barium-linked carrageenan, Encapsulation technology, Controlled release, Hydrophobicity, Probiotics, encapsulation

#### Abstract

Among polyelectrolyte complex gels, barium-linked carrageenan gel serves as a reference material in encapsulation technology due to its ability to offer improved and smart elucidation of encapsulated compounds in the food, pharmaceutical and cosmetic industries. Protection of active agents like flavours, aroma, and probiotics from heat, oxidation, and degradation. Carrageenan gel properties are enhanced when it is blended with barium ions as crosslinking is enhanced and hydrophobicity increases thus making it very effective in encapsulating water insoluble compounds. This helps in retaining the volatile flavours and fragrances for a longer time hence facilitating steady releasing of the same thereby increasing the longevity of the food and cosmetic products. In pharmaceuticals, barium-connected carrageenan helps with the control of release agents in drugs and helps the probiotics survive their passage through the digestive system. The gel matrix reaches enhanced level for gradual and proportional release of the encapsulated compounds to improve the health. This review shows how barium enhances carrageenan's properties of encapsulation by enhancing stability while providing an opportunity to control the rate of release. With further review, barium linked with carrageenan shall revolutionise encapsulation technology and promote the performance of products on other industries. Due to its flexibility, it can be used in almost every formulation and has enormous development possibilities in the future.

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## Modification, functionalization, detection and analysis of physiochemical alteration in polymer iota-carrageenan by replacing monovalent ion

Shashank Kailkhura\*, Priyank Purohit Graphic Era Hill University, School of Pharmacy, Dehradun Uttarakhand, 248001. Contact: kailkhurashashank@gmail.com

*Keywords:* reverse gelling, infrared spectroscopy, mass spectroscopy, X-ray diffraction, molecular interactions.

Polymers are the macro molecules many small monomer combine together to form long chain known as polymer. Iota-carrageenan is polymer which is obtained from red-seaweed seeking attention of researcher working on polymer due to there various novel material properties. When functionalize polymer iota-carrageenan we replace ions (Ca,Na,NH<sub>4</sub>,Ba,) observe various changes in different physiochemical properties of polymer iota-carrageenan these changes in the physiochemical properties shows valuable result for nano formulation, targeting drug delivery system,ionic solvent,drug carrier,conformation changes in the polymer, and reverse gelling properties. Here in this article we also provide information by performing various experiment in controlled condition to exchange ion, alteration of the pysiochemical properties of polymer iota-carrageenan,detection that the ion is linked with the help of modern analytical techniques (IR,MASS,XRD) with the help of IR analytical techniques we also understand the molecular interaction of carrageenan with ions (inter-molecular and intra-molecular).

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## **Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)**

## Analytical Model for Plasmonic Waves and Charge Density in Ternary AlScN/AlN/GaN Heterostructures

Neha Pande<sup>1,2</sup>, Kavita T. Upadhyay<sup>2,3</sup> and Manju K. Chattopadhyay<sup>4\*</sup>

1 School of Instrumentation Devi Ahilya University, Indore, Madhya Pradesh, India 2 Department of Electronics and Telecommunication Engineering, Institute of Engineering and Technology, Devi Ahilya University, Indore, Madhya Pradesh, India

3 Department of Electronics and Communication Engineering, IPS Academy, Institute of Engineering and Science, Indore, Madhya Pradesh, India

4 School of Instrumentation Devi Ahilya University, Indore, Madhya Pradesh, India

\*Contact: mkorwal@yahoo.com

## Category: Oral

Keywords: high electron mobility transistors (HEMT), Terahertz, plasmon frequency, polarization.

Over time, THz-related technologies have seen extensive application across various domains, encompassing THz mixers, frequency multipliers, imaging systems, transceivers, and sensors [1-3]. We present an analysis of the plasmon frequency and 2DEG of ScAlN/AlN/GaN high electron mobility transistors (HEMTs). We investigate the influence of HEMT parameters on the plasmon frequency and the sheet charge density of the 2DEG. Notably, the ScAlN/AlN/GaN heterostructure induces plasmon oscillations in the Terahertz (THz) range, surpassing frequencies observed in other semiconductor compounds. Furthermore, our study reveals substantial sensitivity in tuning these frequencies, particularly through adjustments in applied gate voltage. We optimize structural parameters to identify conditions that maximize the plasmon frequency for a given doping concentration. The potential applications of the interaction between radiation and plasmons span various fields, including developing detectors, mixers, and THz wave generators.

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## Structural, Electrical and Dielectric properties of Co-doped Zn spinel ferrite

<u>Laxmikant Banaj</u>, Sadhana Agrawal<sup>\*</sup> Department of Physics, National Institute of technology, Raipur \*Contact: sagrawal.phy@nitrr.ac.in

Keywords: spinel ferrite, dielectric, solution combustion method, AC conductivity

## Abstract

A series of Co-doped Zn spinel ferrite (Zn<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub>: xCo, x = 0.0, 0.2, 0.4 and 0.6 mol %) samples were prepared by using the solution combustion method. The XRD pattern analysis confirms that all the prepared samples have a cubic crystal structure with an Fd-3m space group (227). The most prominent peak is (311) and the average crystallite size of the sample has been found to be 40.00 nm. SEM images reveal irregular, rock-like grains, while the EDX spectrum verifies the presence of all essential elements in the prepared samples. The FTIR spectra of the prepared sample revealed two band close to 560 cm<sup>-1</sup> and 434 cm<sup>-1</sup> may be related to tetrahedral and octahedral sites. The dielectric constant and the dielectric loss decrease with higher frequency region. The impedance and electric modulus analyses identified a temperature-dependent relaxation mechanism. AC conductivity increases at higher temperatures and frequencies, while the activation energy decreases with increasing frequency.

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## Studies of the Structural, Electrical and Magnetic Characteristics of KCuCr(PO4)<sub>2</sub> Compound

Shalini Mishra\*, Netram Kaurav \*Contact: imshalini09@gmail.com

## Keywords: XRD, Dielectric Properties and Magnetic Properties

KCuCr(PO<sub>4</sub>)<sub>2</sub> is a compound of considerable interest because of its intriguing magnetic properties resulting from geometric frustration. The compound has an intricate lattice structure in which copper (Cu<sup>2+</sup>) and chromium (Cr<sup>2+</sup>) ions engage via a network of phosphate (PO<sub>4</sub>) groups. This configuration results in conflicting magnetic interactions, producing a frustrated magnetic system that resists traditional ordering. We have synthesized the single-phase polycrystalline material KCuCr(PO<sub>4</sub>)<sub>2</sub> using a solid-state technique. We used the lab source 1.54 Å (Cu-K $\alpha$ ) x-ray diffraction method to check the progress of the synthesis and the structural properties of KCuCr(PO<sub>4</sub>)<sub>2</sub>. This showed that the crystal structure is monoclinic. The Maxwell-Wagner model elucidates the frequency-dependent characteristics of the dielectric constant. Nyquist plots indicate the existence of both grain and grain boundary phenomena. Jonscher's Power Law examines the frequency dependence of conductivity, which adheres to the massive overlapping polaron tunnelling concept. The activation energy, determined via the Arrhenius equation, is roughly equivalent to the energy required for electron hopping. Impedance and conductivity tests show that the sample has a negative temperature coefficient of resistance (NTCR), which means that it behaves like a semiconductor at higher temperature. Magnetic measurements indicate that the material exhibits antiferromagnetic behaviour with a Néel temperature T<sub>N</sub> of 17 K.

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## Influence of PEG and EDTA on Morphological, Optical, vibrational, and Photocatalytic Properties of CdS Nanostructures

Labhesh Baid\* and K. S. Ojha Department of Physics, National Institute of Technology Raipur, Raipur (C.G.), India \*Corresponding Author Email address: labheshbaid777@gmail.com

Keywords: CdS, Spherical and flower-like particle, PEG, EDTA, Photoluminescence, Photocatalyst

### Abstract

CdS nanostructures with spherical and star-flower morphologies were synthesized via a single-step hydrothermal method. XRD analysis revealed a mixed cubic-hexagonal phase with a crystalline size of 6 nm for EDTA-capped CdS and a pure hexagonal phase with a crystalline size of 10 nm for PEG-capped CdS. HRSEM confirmed the formation of star-flower and spherical morphologies composed of tiny nanocrystals. EDAX analysis verified the purity and desired composition of the materials, while FTIR confirmed the successful encapsulation by EDTA and PEG. Raman spectroscopy was employed to analyze the vibrational properties, while UV-Vis spectroscopy revealed a red shift in the band gap compared to bulk CdS. Photoluminescence (PL) spectra exhibited visible light emission in the yellow-orange range, highlighting the potential of these nanostructures for optoelectronic applications. Moreover, the flower-like CdS showed improved photocatalytic activity for MB dye degradation under sunlight.

## DFT Calculations for Spin-Orbit Coupling in Magnetic Materials

Sayan Kumar Das<sup>1</sup>, and Sumita Singh<sup>1\*</sup> Department of Physics, Patna University, Bihar, India \*Corresponding author: sumita-phy@patnauniversity.ac.in

Keywords: Spin-Orbit Coupling, DFT, anisotropy, MAE, magnetic materials

#### Abstract

Investigation of SOC in magnetic materials is grounded in the basic concepts of quantum mechanics and the physics of solids. SOC arises due to the interaction of electron spin with its orbital motion around the host nucleus and leads to significant changes in the electronic structure along with the magnetic properties of materials. The effect becomes particularly relevant for systems in which the relativistic contributions cannot be neglected, such as the class of heavy transition metals and rare-earth elements.

The major computational framework for the investigation of SOC in magnetic materials is provided by DFT. Based on the well-known Hohenberg-Kohn theorems and the Kohn-Sham equations, DFT is a practical way to study the electronic structure of many-body systems. The incorporation of SOC into the DFT computations introduces the capability of accurately predicting and analyzing the effect of SOC on different material properties, including but not limited to magnetic anisotropy and the magnetocrystalline anisotropy energy, MAE.

Advanced computer codes such as Quantum ESPRESSO and WIEN2k are the major computational methodologies involved in carrying out DFT calculations with SOC. Such tools simulate the electronic structure and magnetic properties within high-performance computing systems, facilitating the computationally intensive processes involved.

The empirical validation of the DFT predictions is attained through techniques such as X-ray absorption spectroscopy, electron paramagnetic resonance, and X-ray magnetic circular dichroism. These provide empirical evidence to support the accuracy and reliability of computational models. Advances in state-of-the-art current density functional theory, high-throughput computational methodology, and machine learning further enhance the exploration of spin-orbit coupling in magnetic materials. These contributions will lead to new materials with tailor-made properties for their applications in optoelectronics, spintronics, and many other new technologies.

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# 2-D MXene Enhanced the dielectric and ferroelectric properties of PVDF-CCTO composites

Amar Dev<sup>1</sup>, P. Kour<sup>2</sup> and Manoranjan Kar<sup>1\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna 801103, India <sup>2</sup>Department of Physics, Birla Institute of Technology, Mesra, Patna Campus, Patna-800014, India \*Corresponding author Email: mano@iitp.ac.in,

#### Abstract:

Modern machinery's energy storage devices, transistors, actuators, and other crucial electronic parts frequently use polymer-based dielectrics. PVDF has a higher dielectric constant than other polymers, it is the most promising fluorine-containing polymer for various electronic devices. CCTO is a complex oxide with a very high dielectric constant and a cubic perovskite structure that does not phase transition over a broad temperature range. MXene-enhanced PVDF-CCTO composites significantly improve dielectric properties due to the combination of MXene's high conductivity, large surface area, and strong polarization abilities, together with the high permittivity of CCTO. CCTO has been synthesized by sol-gel method, and Acid treatment has been done to etch the MXene to remove max phase. The drop-casting method has been employed to synthesize PVDF- CCTO-MXene composite film. XRD Pattern confirm the pure phase synthesis of CCTO. Surface morphology of the composite film and power has been studied through SEM. Ferroelectric and dielectric properties have been increased with increasing MXene wt%. These composites show promise for various electronic, energy storage, and sensor-based applications.

Keywords: MXene, Ferroelectric, Polymer composites, Rietveld refinement

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# Unveiling electronic and magnetic properties at the interface of (CaNbO<sub>3</sub>)/(Ca<sub>2</sub>VMoO<sub>6</sub>) Perovskite Oxide Heterostructure using DFT+U

Aiswarya Priyambada<sup>1</sup>, Priyadarshini Parida<sup>1\*</sup>

<sup>1</sup>Department of Physics, School of Applied Sciences, KIIT University, Bhubaneswar 751024, Odisha, India \*Contact: priyadarshini.paridafpy@kiit.ac.in<sup>\*</sup>

Keywords: Interface study, double perovskite heterostructure, DFT, C-type AFM, Electronic band structure.

Transition metal (TM) based oxides have been the center of attraction due to their rich physical properties such as electrical transport, magnetism, optical response, superconductivity, thermal conductivity, etc., which make them a perfect candidate for study of electron correlations. These rich behaviors in the bulk transition metal oxides arise due to the interaction between the charge, orbital, and spin degrees of freedom of strongly correlated d-electrons [1]. In this work, we have investigated structural electronic and magnetic properties at the interface of 4d-3d-4d TM based (CaNbO<sub>3</sub>)/(Ca<sub>2</sub>VMoO<sub>6</sub>) perovskite heterostructure within density functional approach as incorporated within Quantum ESPRESSO. The optimized structural parameters such as lattice parameters, bond lengths, and bond angles of the heterostructure are taken from variable-cell relaxation (VC) method. The individual constituents of this heterostructure show G-type antiferromagnetic and ferromagnetic behavior respectively [2, 3] however, at the interface region magnetic behavior found to be C-type antiferromagnet. Unlike magnetic properties, the heterostructure show conducting behavior at the interface which is also distinct from the individual bulk constituents.

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### Asia-Pacific Conference on Condensed Matter Physics 2024

# Structural, Magnetic and Mössbauer Studies of Fe<sub>2-x</sub>Co<sub>x</sub>Mo<sub>3</sub>O<sub>8</sub> Polar Magnetic Material.

Tarun Pratap Singh<sup>1</sup>, P. Rambabu<sup>1</sup>, Pradip Das<sup>1</sup>, V. Raghvendra Reddy<sup>2</sup>, G.R. Turpu<sup>1</sup>

1 Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya, Bilaspur 495009, India 2 UGC-DAE-CSR, University Campus, Khandwa Road, Indore 452001, India \*Contact: tarunpratap96@gmail.com

#### Category: Oral

*Keywords:* Multiferroics, Polar Magnet, Magnetization, <sup>57</sup>Fe-Mössbauer Spectroscopy.

Multiferroicity in condensed matter has been an active area of research to explore the physics involved in there [1]. Polar magnets form a new class of multiferroic materials and being studied intensely in recent times [2]. Here we report the structural, Mössbauer and magnetic properties of polar magnetic material Fe<sub>2-x</sub>Co<sub>x</sub>Mo<sub>3</sub>O<sub>8</sub> (x = 0,0.1,0.2). Rietveld refined RT-XRD confirms hexagonal structure (P6<sub>3</sub>mc) for Fe<sub>2-x</sub>Co<sub>x</sub>Mo<sub>3</sub>O<sub>8</sub> (x = 0,0.1,0.2). Magnetization measurements exhibit antiferromagnetic (AFM) ordering at temperature T<sub>N</sub> i.e. 60.97K, 60.05K and 60.05K for Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>, Fe<sub>1.9</sub>Co<sub>0.1</sub>Mo<sub>3</sub>O<sub>8</sub>, and Fe<sub>1.8</sub>Co<sub>0.2</sub>Mo<sub>3</sub>O<sub>8</sub>, respectively. Room temperature Mössbauer spectroscopic studies confirm the +2 oxidation state of Fe. The isomer shift  $\delta$  (mm/s) for Fe<sub>2-x</sub>Co<sub>x</sub>Mo<sub>3</sub>O<sub>8</sub> (x=0,0.1,0.2) is 0.74±0.006, 0.93±0.003 and 0.93±0.004 for site A and 0.89±0.006, 1.12±0.018, and 1.107±0.002 for site B, respectively and the quadrupole splitting  $\Delta$ E (mm/s) is 0.53±0.020, 0.70±0.005 and 0.69±0.006 for site A and 1.03±0.018, 0.90±0.03 and 0.88±0.04 for site B, respectively. The hyperfine field obtained for site A is 58.7±0.07T and for site B is 180.7±0.03T in Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>, at 5K.

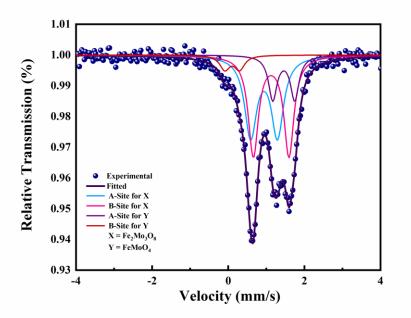


Fig:(1) Room temperature Mössbauer spectra of Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>

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# Synergistic Ferroelectric-Magnetic Properties and Conduction Mechanism in BaZr<sub>0.1</sub>Ti<sub>0.9</sub>O<sub>3</sub> – Ni<sub>0.5</sub>Co<sub>0.2</sub>Zn<sub>0.3</sub>Fe<sub>2</sub>O<sub>4</sub> Multiferroic Composites

Somnath Sahu<sup>\*</sup>, Shashi Priya Balmuchu, Pamu Dobbidi Department of Physics, Indian Institute of Technology Guwahati, Assam-781039, India. \*Corresponding author e-mail: ssahu@iitg.ac.in

#### Abstract:

The  $BaZr_{0.1}Ti_{0.9}O_3$  (BZT) -  $Ni_{0.5}Co_{0.2}Zn_{0.3}Fe_2O_4$  (NCZF) composite stands at the forefront of advanced multifunctional materials, boasting remarkable multiferroic properties. A comprehensive exploration of the ferroelectric and magnetic properties, along with the conduction mechanism in these composites, is key to unlocking the full potential of their multifunctional properties and optimizing their performance for multifunctional devices such as sensors, MERAM, etc. This investigation aims to uncover the intricate relationships between the ferroelectric, magnetic, and conduction mechanisms of (1-x)BZT-xNCZF (x = 0, 0.05, 0.10, 0.15, 0.20, 1) ceramic composites. These compositions exhibited dense microstructures with minimal oxygen vacancies, ranging from  $\sim 18\%$  to 29%. The MH curves are analyzed using the law of approach to saturation magnetization over the temperature range of 5 K to 300 K. Both saturation magnetization  $(M_s)$ and remnant magnetization  $(M_r)$  rises, while coercivity  $(H_c)$  is reduced with increasing NCZF content as well as with temperature. Bloch's spin wave theory is used to study temperature-dependent saturation magnetization, revealing deviations from Bloch's T<sup>3/2</sup> law and the modified Kobler's Bloch law in all samples. The measurements of energy storage performance reveal an improved response for the x = 0.05 composition, which exhibits a recoverable energy density of ~ 272 mJ/cm<sup>3</sup> and an efficiency of 88%. All compositions reveal a transition from ferroelectric to paraelectric phases, with the transition temperature shifting from 353 K to 403 K. Remarkably, the x = 0.20 sample displayed two distinct phase transitions: a ferroelectric-toparaelectric transition at 343 K and a ferromagnetic-to-paramagnetic transition at 423 K. The conductivity of the composites adheres to the McLachlan model, which accounts for interactions between the constituent phases. Furthermore, the conduction mechanism is described by Mott's variable-range hopping (VRH) model, suggesting that localized polarons are crucial to the microscopic electrical behavior. Thus, understanding the ferroelectric-magnetic properties and conduction mechanism provides a comprehensive view of these materials, potentially guiding the design of advanced composites for sensors, energy storage, and multifunctional devices.

# **Theme:** DEVICES (ELECTRONICS, SPINTRONICS, OPTOELECTRONICS, SENSORS & ACTUATORS)

## Nucleation to Motion: Skyrmions in Pd/Fe Multilayers

Tamali Mukherjee<sup>1\*</sup>, Banasree Sadhukhan<sup>2</sup>, and V Satya Narayana Murthy<sup>1</sup>

<sup>1</sup>Birla Institute of Technology and Science, Pilani, Hyderabad Campus, India <sup>2</sup>SRM Institute of Science and Technology, Chennai, India

\*Contact: p20220034@hyderabad.bits-pilani.ac.in

#### Category: Poster

Keywords: Magnetic skyrmions, Spintronics, Micromagnetic simulation, PdFe bilayer.

Skyrmions are small swirling topological defects in ferromagnetic materials that show promising features to be used as a 'bit' of information in future spintronic devices. We use a PdFe bilayer (of dimension 200 x 200 nm<sup>2</sup> and thickness 1 nm) on Ir (111) to study skyrmion formation by applying a magnetic field and electric current and its dynamics by applying an electric current pulse. From the spin-spiral initial state, the skyrmion phase in the ferromagnetic background is achieved at the threshold magnetic field of 1.7 T applied in the +z direction. With the increasing strength of the magnetic field, the number of skyrmion increases, and their diameters are reduced. Skyrmions get annihilated at 5 T of the magnetic field, and the layer becomes ferromagnetic. Instead of the magnetic field, if a nano-second current pulse is applied to induce the required spin transfer torque (STT) to change the initial spin-spiral phase, we get the final relaxed state as a skyrmion of opposite core magnetization nucleated in a spin-spiral background. The threshold current pulse to observe skyrmion formation is  $10^{11}$  A/m<sup>2</sup> applied in the +z direction. After nucleation, the skyrmion dynamics are studied by applying STT or spin-orbit torque (SOT) provided by a nano-second current pulse. A proper arrangement of skyrmions in the sample must be implemented to be convenient in the context of spintronic devices. Different desired arrangements like T-shape,  $\pi$ -shape, L-shape, and so on can be formed by modulating the magnitude and pulse width of the current density pulse applied in specific directions. The magnetization dynamics of the PdFe free layer is given by the Landau-Lifshitz-Gilbert (LLG) equation and solved by Mumax3.

$$\frac{d\overrightarrow{m}_{free}}{dt} = -\gamma \overrightarrow{m}_{free} \times \overrightarrow{H}_{eff} + \alpha \overrightarrow{m}_{free} \times \frac{d\overrightarrow{m}_{free}}{dt} + \overrightarrow{\tau}_{STT} + \overrightarrow{\tau}_{SOT}$$

The material parameters used to carry out the simulation are, saturation magnetization ( $M_s$ ) = 6.3 x 10<sup>5</sup> A/m, Gilbert constant ( $\alpha$ ) = 0.023, exchange constant ( $A_{ex}$ ) = 2.269 x 10<sup>-12</sup> J/m, interfacial DMI ( $D_{int}$ ) = 3.64 x 10<sup>-3</sup> J/m<sup>2</sup>, first order anisotropy constant ( $Ku_1$ ) = 1.4 x 10<sup>6</sup> J/m<sup>3</sup> and easy axis is taken in (0, 0, 1) direction.

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## **Devices**

## Substrate dependent study of LaVO<sub>3</sub> Thin Films for Resistive Switching Application

<u>Richa Bharti</u>, Indranil Maity, and Ajay D. Thakur Department of Physics, Indian Institute of Technology Patna

\*Contact:richa\_2321ph11@iitp.ac.in

Category: Poster

Keywords: Resistive Switching, Pulsed laser deposition, Endurance, ON-OFF ratio

#### Abstract

Lanthanum vanadate, LaVO<sub>3</sub> (LVO) films were synthesized using the Pulsed Laser Deposition (PLD) technique on various substrates, including Si, Si/SrRuO<sub>3</sub> (SSRO), FTO-coated glass, and ITO coated glass, to determine the most suitable substrate for resistive switching applications. To evaluate the performance of the LVO films, I-V measurements were performed, revealing that the films grown on SSRO exhibited better switching behavior including enhanced device-to-device stability, a higher ON-OFF ratio, and improved endurance compared to those on other substrates. Structural and morphological characterizations were performed using X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM) and Atomic force microscopy (AFM) to determine the crystallite size, surface morphology and film thickness respectively. These findings suggest that SSRO is the most promising substrate for the development of reliable LVO-based resistive switching devices.

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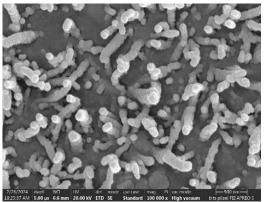
# Copper-Zinc Mixed Oxide (CZO) based nanostructured thin films for hydrophobic surface preparation

Arti Saini, Subhashis Gangopadhyay\*

Department of Physics, Birla Institute of Technology and Science, Pilani, Rajasthan, 333031, India \*Contact: subha@pilani.bits-pilani.ac.in

Keywords: Mixed metal oxide, Nanostructure, Surface morphology, Contact angle

CuO and ZnO are well-explored p-type and n-type semiconductors found in a wide range of morphologies at nanometer length scale (nanowire, nanorod, nanosheet, nanoflower, nanosphere). However, mixed oxides of Cu and Zn can be considered as new material (CZO) with significantly different electrical and chemical properties, depending on their chemical ratio. Moreover, these mixed oxides have huge potential for application in the field of gas sensing [1], self-cleaning [2], energy storage, catalyst, and many more. Within this work, we will study the formation of different CZO nanostructured surfaces during the thermal oxidation of thin metal films along with their water repellent properties for self-cleaning application. High purity Cu and Zn films were co-deposited on quartz substrates using a vacuum assisted dual (DC-RF) sputter system, keeping the base pressure below  $\sim 10^{-5}$  mbar. To obtain the mixed oxide layers, controlled thermal oxidation of the asdeposited metal films has been performed in air ambient conditions at various temperatures for different durations, using a muffle furnace (TEMPCON). Structural, morphological, chemical, wettability, optical and electrical properties of these oxide layers have been investigated using multiple surface characterization techniques such as x-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and x-ray photoemission spectroscopy (XPS), contact angle measurement system. XRD and XPS confirm the composition of both Cu and Zn within the mixed oxide films whereas the hierarchical structure of CZO is observed in FESEM imaging. Variation in surface contact angle has been observed for different hierarchical surface nanostructures. Finally, a correlation between the surface morphology, chemical composition and contact angle will also be discussed in terms of surface free energy.



CZO mixed oxide surface morphology grown after oxidation at 500°C for 1H30m

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## Exploring the Structural, Optical, Dielectric, and Magnetic Properties of Ni0.65Zn0.35Al0.8Fe1.2O4 Spinel Ferrite

Sachin Verma\*, Abhishek Maurya, Rajeev Singh and Biswanath Bhoi<sup>a</sup> Nano-Magnetism and Quantum Technology Lab, Department of Physics, I.I.T. (BHU) Varanasi, Uttar Pradesh - 221005, India. \*Email of presenting author: Sachinverma.rs.phy22@iitbhu.ac.in <sup>a</sup>Email of corresponding author: biswanath.phy@iitbhu.ac.in

Keywords: Spinel Ferrite, Solid State Reaction, Spintronics Application.

Spinel ferrites have been extensively studied over the past few decades due to their broad applications ranging from electronics and telecommunications industries to biomedical fields. The recent discovery of low magnetic damping ( $\alpha \approx 3 \times 10^{-3}$ ) in spinel ferrites, particularly Ni<sub>0.65</sub>Zn<sub>0.35</sub>Al<sub>0.8</sub>Fe<sub>1.2</sub>O<sub>4</sub> (NAFO), highlights their potential for spintronic applications. To fully harness this potential, it is essential to understand their other physical properties, which have garnered significant research interest.

In this work, a pure-phase  $Ni_{0.65}Zn_{0.35}Al_{0.8}Fe_{1.2}O_4$  bulk sample was successfully prepared using a solid-state reaction method, aimed at further research and potential integration into thin-film technologies. High-purity NiO, ZnO, Al<sub>2</sub>O<sub>3</sub>, and Fe<sub>2</sub>O<sub>3</sub> powders were mixed with a molar ratio of 0.65:0.35:0.4:0.6 with isopropyl alcohol as a medium for wet grinding over 5 hours. Post-evaporation of alcohol, the powder mixture was dried at 100°C for 24 hours, followed by calcination at 800°C for 3 hours to induce spinel phase formation. The processed powder was then re-grounded with a binder, compacted under 200 kg/cm<sup>2</sup>, and sintered at 1200°C for 3 hours, with a controlled thermal cycle to ensure a high-quality, crack-free pellet. The resulting material was analyzed using X-ray diffraction to determine its crystallographic properties, with Rietveld refinement confirming the successful formation of a pure  $Ni_{0.65}Zn_{0.35}Al_{0.8}Fe_{1.2}O_4$  spinel ferrite phase. UV-visible spectroscopy was employed to analyze the optical properties, including the band gap and refractive index. The dielectric properties, such as capacitance, dielectric constant (ɛ), dielectric loss, AC conductivity, complex impedance, and modulus of the AFO sample, were examined across different frequencies and temperatures. The magnetic measurements were performed to determine the saturation magnetization and coercivity of the material. This comprehensive analysis sheds light on the previously undiscovered traits in the material's transport phenomena and optical attributes, opening an exciting and active field of research into its other physical properties.

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## An Effective Supramolecular Mg(II)-Metallohydrogel Based Non-Volatile Memory Device With High Endurance

Arpita Roy<sup>\*</sup> and Soumya Jyoti Ray <sup>1</sup>Department of Physics, Indian Institute of Technology Patna, Bihar-801106, India \*Email:arpita\_2021ph08@iitp.ac.in

**Keywords:** Mg(II)-metallohydrogel, Resistive switching, Non volatile memory, Endurance, Neuromorphic computing

#### Abstract

Supramolecular gels are versatile materials that possess "smart" properties. They are used in various industries such as sensors, cosmetics, foods, nanoelectronics, logic gates and regenerative medicine. These gels are formed through the combination of hydrogels and supramolecular chemistry<sup>1,2</sup>. In this work, we have developed a well-organized and efficient method to rapidly synthesize a supramolecular metallohydrogel of Mg(II)-ion which is Mg@3AP. This metallohydrogel is prepared by using 3-amino-1-pentanol as a low molecular weight gelator in water at room temperature. Here, we have investigated the hierarchical microstructural features of Mg@3AP using Field-emission scanning electron microscopy. We have analysed the metallohydrogel formation approach using FT-IR spectroscopic studies. Furthermore, we have fabricated a (Mg@3AP)-based Schottky diode device in a lateral metal-semiconductor-metal geometry to explore its charge transport behavior<sup>3</sup>. Here, Mg@3AP metallogel based RRAM (Resistive random access memory) device have showed a proper bipolar resistive switching<sup>4</sup> behavior at room temperature. This RRAM device demonstrated exceptional switching endurance with over 10000 consecutive switching cycles and a high ON/OFF ratio of approximately 100. Due to its simple fabrication process, robust resistive switching behavior and enhanced stability, these structures are suited for applications in non-volatile memory design, neuromorphic computing.

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### Study of electron-phonon coupling, anisotropic phonon mediated superconductivity in boride

Subhajit Pramanick<sup>1</sup>, Sudip Chakraborty<sup>2</sup>, and A Taraphder<sup>3</sup>

<sup>1,3</sup>Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur 721302, India <sup>2</sup>Materials Theory for Energy Scavenging Lab, Harish-Chandra Research Institute, A CI of Homi Bhabha National Institute, Chhatnag Road, Jhunsi, Prayagraj 211019, India

Category: Poster

Keywords: Electron-Phonon Wannier, Anisotropic superconductivity, Migdal-Eliashberg Theory

In the field of condensed matter physics and material science, the discovery of novel superconducting materials remains a formidable challenge. Although superconductivity in binary borides has been verified through numerous experiments and computations, superconductivity in ternary borides is still relatively unexplored. In this research work, we have investigated electron-phonon coupling and anisotropic phonon-mediated superconductivity in a ternary boride using Migdal-Eliashberg theorem implemented in Electron Phonon Wannier (EPW) code [1]. Thermodynamical stability has been confirmed by negative formation energy and absence of imaginary phonon mode also confirms its dynamical stability. The composition of our material consists of Mo atoms that are confined to a particular x-y plane. This makes an opportunity to form a strong coupling between  $\sigma$ -bonding states dominated by d-orbitals of Mo atoms and in-plane vibration of Mo atoms, i.e., LA and TA modes of acoustic branch of its phonon dispersion. It leads to cooper pair formation which creates superconductivity anisotropic. Unlike MgB<sub>2</sub> [2], due to significant distance between two Mo atoms,  $\pi$ -bonding states are unable to create another gap that makes it a single-gap superconductor. However, it also remains future challenge for scientific community to study the effect of pressure or doping on its electron-phonon coupling and anisotropic superconductivity.

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# Solution-processed thin film heterostructures for interface-dominated multilevel resistive switching memory devices with reactive gas selectivity

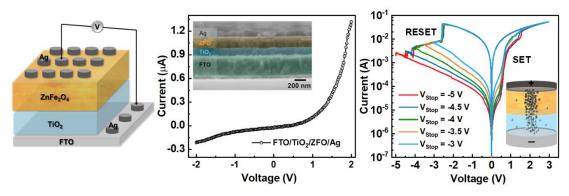
Priya Kaith, Ashok Bera\*

Department of Physics, Indian Institute of Technology Jammu, J&K, 181221, India Corresponding author e-mail: ashok.bera@iitjammu.ac.in

Category: Oral

*Keywords:* Heterostructure memory devices, multilevel resistive switching, temperature stability, and reactive gas selectivity

Abstract: World modernization and digital developments have led to ever-increasing energy and data storage demands. Two-terminal heterostructure memory devices acted as one of the promising candidates for non-volatile memory devices because of their low power consumption, scalability, and simple metal-insulator-metal structure. Integrating different functional materials with varying lattice symmetries on a nanometre scale via solution-processed synthesis while maintaining their functional tunability is an effective strategy for designing low-cost, stable, and easy-to-fabricate memory devices. [1] Herein, we explore the potential of spinel-structured copper ferrite CuFe<sub>2</sub>O<sub>4</sub> (CFO) and zinc ferrite ZnFe<sub>2</sub>O<sub>4</sub> (ZFO) films in combination with the n-type TiO<sub>2</sub> layer for improved switching performances. A simple fluorine-doped tin oxide (FTO)/CFO/Ag device exhibits bipolar resistive switching behaviour, including scattered SET and RESET voltages and endurance deterioration. By incorporating a  $TiO_2$  layer into the conventional device, we overcame these issues with the additional benefits of multilevel switching for FTO/TiO2/CFO/Ag device and increased temperature stability up to 250 °C. [2] Secondly, the solution-processed TiO<sub>2</sub>/ZFO heterointerface devices exhibit multilayer resistive switching with endurance stability for  $10^4$  cycles and a retention time of  $10^5$  s. In addition, it can maintain switching after dripping water onto the device and drying at 100 °C. On the contrary, in vacuum or inert environments, the lack of filament formation leads to negligible switching characteristics with an ON/OFF ratio of  $\sim 2$  due to the loss of a low resistance state. We varied the device's ambient environmental conditions so that the TiO<sub>2</sub>/ZFO interface allows for easy charge transport and reduces the depletion region in the presence of reducing gases. This allows for variable ON-OFF ratios and intermediate resistance states based on the gas type, providing an additional pathway for active gas sensing. Our findings open up new possibilities for combining memristors with gas sensing in multifunctional modern electronic devices.



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# Computation of Activity, Activity Coefficients and Excess Free Energy of Sub-binary Groups of Solid Ternary Alloy CuPtNi by Using MIVM Model

M. K. Jha<sup>1</sup>, G. K. Shrestha<sup>2</sup>, I. Koirala<sup>1</sup>, I.S. Jha<sup>3</sup> and V. K. Jha<sup>4\*</sup> <sup>1</sup>Central Department of Physics, TU, Kirtipur, Kathmandu, Nepal <sup>2</sup>Department of Physics, Pulchowk Engineering Campus, Pulchowk, Lalitpur, Nepal <sup>3</sup>Department of Physics, Mahendra Morang Campus, Biratnagar, Nepal <sup>4</sup>Department of Physics, St. Xavier's College, Kathmandu, Nepal <sup>\*</sup>Email id: vkjha@sxc.edu.np

#### Keywords: Solid alloy, activity coefficient, MIMV

There has not been enough research on the solid alloys of group IB and VIIIB in periodic table. We have chosen, Platinum based ternary alloy as CuNiPt for the study of thermodynamic properties in its sub-binary constituents. The precise properties of binary sub-groups of above alloy can vary based on the specific composition and processing of the alloy, including the proportions of Copper, Nickel, and Platinum, as well as any additional elements and the applied heat treatment. Thermodynamical properties like activity, activity coefficients and excess free energy for sub-groups CuNi, CuPt and NiPt of solid ternary alloy CuNiPt have been calculated by using Molecular Interaction Volume Model (MIVM) model which has been used by Dong Ping Tau in the study of solid ternary alloy C-Fe-Co [1]. The experimental data for these binary alloys CuNi, CuPt and NiPt have been obtained from the book named "Selected Values of Thermodynamic Properties of Metals and Alloy" by R. Hultgren et al. [2]. The typical thermodynamic property, activity coefficients of Ni and Pt in sub-group NiPt at 1625 K with Ni and Pt concentrations of 52%-48% respectively is around 0.55. Whereas for Cu and Ni in alloy CuNi at temperature 1823K, the activity coefficients of Cu and Ni are 1.43 when the concentration of Cu is around 55% and that of Ni is around 45%. Similarly, for Cu and Pt in alloy CuPt at temperature 1350 K, with cu concentration of 54% and Pt of 46%, the activity coefficient is found to be around 0.425.

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# Simultaneous Growth of Graphene and Carbon Nanotubes on Dielectric Surfaces via One-Step Chemical Vapor Deposition Technique

Julfikar Ali Sarkar<sup>a</sup>, Muhammed Junais Pulikkathumbayil<sup>a</sup>, Shripal Singh<sup>a</sup>, M. Aslam<sup>a,\*</sup>

<sup>a</sup>Department of Physics, Indian Institute of Technology Bombay, Mumbai, India

Presenting author: rajusarkar010101@gmail.com, \*Corresponding Author: m.aslam@iitb.ac.in

#### Category: Poster

Key Words: Graphene, Carbon Nanotubes, Dielectric Surface, Chemical Vapor Deposition (CVD) Technique

Carbon-based nanostructures, ranging from zero- to three-dimensional (0–3D) forms like quantum dots, CNTs, graphene oxide, and graphene, showcase diverse structural variations. 3D carbon architectures, achieved through stacking or compositing CNTs with graphene oxide, add volume and uniquely combine conductivity with flexibility, making them valuable in energy storage, solar cells, sensors, and capacitors.<sup>[1]</sup> Standard fabrication methods—mixing, stacking, and coating CNTs or graphene with active materials—have made versatile 3D hybrids possible.<sup>[2]</sup> However, controlling thickness, aspect ratio, and distribution remains challenging.<sup>[3]</sup> Achieving aligned CNTs on graphene, for instance, requires precise tuning of parameters like temperature, gas composition, pressure, and substrate or catalyst choice, as CNT growth (driven by carbon atom nucleation) and graphene layer formation follow different kinetic pathways.

This study introduces a one-step, copper-vapor assisted CVD method for synthesizing a 3D carbon network of multi-walled carbon nanotubes (MWCNTs) interwoven with mono- to few-layer graphene (3D CNTs/G) directly on various dielectric surfaces, such as quartz and Si/SiO<sub>2</sub>. The direct growth on dielectric surfaces enables efficient device fabrications with good quality by avoiding tricky transfer processes. The synthesis exploits copper vapor to simultaneously grow MWCNTs (average diameter ~150 nm) and graphene (average thickness ~0.92 nm) in a single step, overcoming the usual complexities of multi-step carbon hybrid formation. Microscopic and spectroscopic analyses—SEM for large-area continuous distribution, AFM for thickness, Raman spectroscopy for defect, XRD for (002) phase, and UV-visible for optical characterization—confirm the structural integrity and alignment of the CNTs with graphene layers, producing a robust 3D architecture. With its tunability and simplicity, this process holds great promise for scalable manufacturing, particularly in energy storage devices, solar cells, sensors, and other optoelectronic applications, where the flexibility, conductivity, and high surface area of the 3D CNT/graphene hybrid structure provide an ideal platform for enhanced performance and efficiency.

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# Spin-Charge Magnetoelectric coupling and Transport Response of Lanthanum based semiconducting nanocomposite

Harsh Sharma and Debajyoti Nath\*

Department of Education, National Institute of Technology Agartala, Tripura 799046, India

*E-mail address of author: harshjnv2@gmail.com (H Sharma)* \**E-mail address of corresponding author: debajyotinit@gmail.com (D Nath)* 

#### Abstract

Lanthanum based semiconducting nanocomposite materials of  $0.5LaFeO_3$  -0.5ZnO, prepared by chemical low temperature "pyrophoric reaction process"[1,2]. Structural characterization has been carried out through X-ray diffraction technique, which shows coexistence of both the phases of the sample. These composites reveal the strain mediated magnetoelectric effect with longitudinal ( $\alpha E_{33}$ ) and transverse ( $\alpha E_{31}$ ) configurations at lower frequency region under an external magnetic field [2, 3]. The complex impedance and modulus diagram illustrate the contribution of grain and grain boundaries effects towards the non-Debye type phenomena [3,4]. The relaxation frequency is changed with an application of magnetic fields ascribing the spin dependent mechanism of the electrical transport at the grain boundaries. The Nyquist diagram attributes the magnetic domain wall motion across the grain boundaries pinning center of the system [5, 6]. So, the present study is directed towards to offer some helpful ideas for developing the lead free device applications.

Keywords: Magnetoelectric coupling, Impedance, Nanocomposites and Nyquist plots

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# Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)

# Efficient Formation of Ohmic Contacts on Si/SiGe Heterostructures Using a Novel Spark Annealing Technique

Hari Krishnan S, Boney M, Lucky Donald Lyngdoh Kynshi, Madhu Thalakulam\*

Indian Institute of Science Education and Research, Thiruvananthapuram, Kerala \*Contact: madhu@iisertvm.ac.in

#### Category: Poster

Keywords: ohmic-contacts, spark-annealing, 2DEG

The development of reliable ohmic contacts is critical for the performance of semiconductor devices in Si/SiGe heterostructures, which are pivotal for quantum computing and high-speed electronics applications. In this work, we explore a novel spark annealing technique to form low-resistance ohmic contacts on Si/SiGe heterostructures using antimony (Sb) in combination with gold (Au) or silver (Ag) as the contact metals. The process involves a controlled electrical spark generated by a sharp needle, which is connected to a capacitor and a voltage source. This spark induces localized heating and annealing of the contact interface, promoting the diffusion of Sb into the Si/SiGe substrate and thereby forming a robust, low-resistance contact.

Our results demonstrate that the spark annealing technique can achieve comparable contact resistance values to traditional thermal annealing methods, with the added advantage of more uniform surface profile and localized annealing, which minimizes thermal damage to the surrounding areas of the substrate. The influence of various parameters, including spark energy, contact material composition, and annealing duration, on the electrical properties of the contacts is systematically investigated.

This approach provides a promising route for the efficient fabrication of ohmic contacts in Si/SiGe-based devices, potentially enabling advances in device performance and scalability.

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# Comprehensive Study on the Structural, Optical, Magnetic, and Dielectric Properties of Eu<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub>

Abhishek Maurya\*, Sachin Verma, Rajeev Singh, Biswanath Bhoi<sup>1</sup>

Nano-Magnetism and Quantum Technology Lab, Department of Physics, Indian Institute of Technology (BHU) Varanasi, Uttar Pradesh - 221005, India

\* Presenting author's Email: Abhishekmaurya.rs.phy22@itbhu.ac.in

<sup>1</sup> Corresponding author's Email: biswanath.phy@iitbhu.ac.in

Keywords: Garnet, solid-state reaction, spintronic

#### Abstract

Rare-earth iron garnet materials, denoted by the general formula  $R_3Fe_5O_{12}$  (RIG), constitute a diverse class of magnetic insulators that have attracted considerable attention over many decades due to their applications in microwave, magneto-optical and spintronic devices. While yttrium iron garnet (Y<sub>3</sub>Fe<sub>5</sub>O<sub>12</sub>: YIG) has been extensively studied for its low magnetic damping, high spin density, and high Curie temperature—key attributes for spintronic applications—other rare earth garnets with similar properties have not been explored as thoroughly. Therefore, a more comprehensive investigation of these rare earth iron garnets (RIGs) is needed.

Here, we present a study of the structural, optical, magnetic, and dielectric properties of pure phase  $Eu_3Fe_5O_{12}$  (EuIG) synthesized via a solid-state reaction route. X-ray diffraction (XRD) analysis provides information about the single-phase nature of the material and allows for the calculation of grain size using the Williamson–Hall (W-H) method. UV–visible spectroscopy is used to determine the optical properties of EuIG, revealing its band gap and average refractive index. Magnetic measurements were performed to assess the saturation magnetization and coercivity of the material, which indicate how easily the material can be magnetized and demagnetized. A thorough analysis of the dielectric response, including capacitance, dielectric constant ( $\epsilon$ ), dielectric loss, AC conductivity, complex impedance, and modulus as functions of frequency and temperature, is performed to understand the material's potential for microwave devices and spintronics applications.

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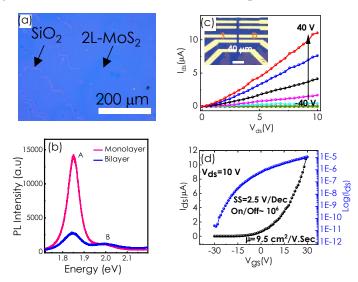
# Large area continuous bilayer MoS<sub>2</sub> film grown by chemical vapour deposition technique and their Field effect transistor performance

Umakanta Patra, Faiha Mujeeb, Abhiram K, Jai israni, Subhabrata Dhar

Indian institute of technology, Bombay, Mumbai, 400076 \*Corresponding Author: Umakanta Patra, patraumakantaiitb@gmail.com

Keywords: CVD, Bilayer, MoS<sub>2</sub>, HRTEM, Field effect transistors.

Bilayer (2L) transition metal dichalcogenides (TMD) have the ability to host interlayer excitons, where electron and hole parts are spatially separated that leads to much longer lifetime as compared to direct excitons. This property can be utilized for the development of exciton-based logic devices, which are supposed to be superior in terms of energy efficiency and optical communication compatibility as compared to their electronic counterparts. However, obtaining uniformly thick bilayer epitaxial films with large area coverage is challenging. Here, we have engineered the flow pattern of the precursors over the substrate surface to obtain large area ( $mm^2$ ) covered strictly bilayer MoS<sub>2</sub> films on SiO<sub>2</sub> by chemical vapour deposition (CVD) technique without any plasma treatment of the substrate prior to the growth. Bilayer nature of these films is confirmed by Raman, low-frequency Raman, atomic force microscopy (AFM) and photoluminescence (PL) studies. The uniformity of the film has been checked by Raman peak separation and PL intensity map. High resolution transmission electron microscopy (HRTEM) reveals that crystalline and twisted bilayer islands coexist within the layer. Back gated field-effect transistor (FET) structures fabricated on the bilayers show on/off ratio of  $10^6$  and subthreshold swings (SS) of 2.5 V/Decade. Top gated FET has been fabricated with 15 nm thick atomic layer deposited Al<sub>2</sub>O<sub>3</sub> as a gate dielectric. Device shows an excellent performance with an on/off ratio of  $10^5$ .



**Figure** (a) Optical microscopic image of the continuous bilayer  $MoS_2$  grown on a SiO<sub>2</sub>/Si substrate. (b) room temperature PL spectra (c) output characteristics, inset shows the optical image of the device (d) transfer characteristics of back gated FET based on 2L-MoS<sub>2</sub> films.

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# Photoluminescence properties of Eu<sup>3+</sup> and Dy<sup>3+</sup> doped SrCO<sub>3</sub> nanophosphors synthesized by hydrothermal method

<u>Swati Rani<sup>1,\*</sup></u>, Indranil Maity<sup>2</sup>, Anil K. Yadav<sup>1</sup>, Ajay D. Thakur<sup>2</sup> <sup>1</sup>Department of Physics, Ch. Charan Singh University Meerut, UP 250004, India <sup>2</sup>School of Basic Sciences, Indian Institute of Technology, Patna 801106, India

\*Contact: swatirani1320@gmail.com

Keywords: RE doped phosphors; strontium carbonate phosphors; hydrothermal method.

Photoluminescence materials, also known as phosphors, have versatile applications in various fields such as display devices, optical storage, in-vivo bio-imaging, color LEDs, flat panel displays, etc. Phosphors convert ultraviolet (UV) or blue light into a broad visible spectrum and, hence can be utilized to produce desired light suitable for various lighting applications. Phosphors typically consist of a host material, providing space for the luminescence mechanism, doped with activators that influence their luminescence properties. Among various host materials, strontium carbonate (SrCO<sub>3</sub>) has got lot of attention due to their excellent stability and unique optical properties as compared to other sulfide-based phosphors. Lots of research is going on towards the enhancement of luminescence properties of SrCO<sub>3</sub> by doping rare earth elements. However, the emission color, intensity, and afterglow time of RE doped SrCO<sub>3</sub> phosphors have not been explored much. In this work, we have synthesized SrCO<sub>3</sub>: Eu<sup>3+</sup>, Dy<sup>3+</sup> nanophosphors by hydrothermal method, and their structural, morphological, and luminescence properties were studied by X-ray diffraction (XRD), and Field effect scanning electron microscopy (FESEM), and photoluminescence emission (PL) spectroscopy. The X-ray diffraction (XRD) analysis indicates that the synthesized sample possesses an orthorhombic phase with the Pmcn space group. FESEM images reveal that the SrCO<sub>3</sub> nanophosphors exhibit pseudospherical shapes with an irregular morphology. Photoluminescence (PL) emission spectra, recorded at various excitation wavelengths, show emission peaks at 608 nm. This red light emission is attributed to the hypersensitive forced electric dipole transition  ${}^{5}D_{0}-{}^{7}F_{2}$  of Eu<sup>2+</sup> ions. Here, Eu<sup>3+</sup> functions as the luminescent center responsible for the red emission, while  $Dy^{3+}$  serves as a trap center to enhance the afterglow duration within the SrCO<sub>3</sub> host lattice. These red phosphors with strong absorption in the blue region are promising candidates for manufacturing flat panel displays, and LEDs.

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#### **Magnetism & Superconductivity**



# A complex magnetic study: Evidence of spin-glass transition below long-range magnetic ordering and its correlation with renormalization of phonon modes

<u>Sipun Mohanty</u><sup>1</sup> and Samrat Mukherjee<sup>1</sup> <sup>1</sup>Department of Physics, National Institute of Technology Patna, Bihar, India, 800005

#### \*Contact: mohanty.sipun143@gmail.com

### Category: Oral

*Keywords:* Double perovskite; Iridates; Spin-glass behaviour; Vogel-Fulcher law; Spin-phonon coupling.

This report presents a systematic study on complex magnetic behaviour arising due to the interplay of three active magnetic cations (Nd/Sm, Co and Ir), forming 3d-5d-4f magnetic sublattices. The B-site ordered double perovskites Nd<sub>2</sub>CoIrO<sub>6</sub> and Sm<sub>2</sub>CoIrO<sub>6</sub> were successfully prepared by conventional solid-state method. Detailed structural analysis revealed that both samples crystallized in monoclinic structure with P2<sub>1</sub>/n (No.-14) space group. Both samples show a paramagnetic-ferrimagnetic (T<sub>FiM</sub>) transition around 100 K, additionally, a low temperature transition is observed at around 10 K in the SCIO sample. The ac susceptibility analysis confirms a spin glass type transition just below the long-range ordering temperature in NCIO sample, The obtained characteristic flipping time of a single spin from both the law (Power law and Vogel-Fulcher law) and nonzero Vogel-Fulcher temperature ( $T_0 \approx 89.1$  K) further verified the existence of cluster spin-glass behaviour below the ordering temperature. The temperature evolution of phonon modes (up to 4 K) suggests that the phonon mode above the magnetic ordering temperature is mainly governed by the lattice degrees of freedom; notable renormalization of the mode frequency below the ordering temperature is due to the coupling of lattice with the underlying magnetic degrees of freedom.

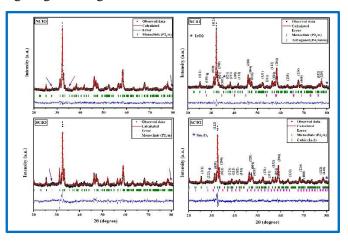


Figure 1: Rietveld refinement of room temperature XRD pattern of  $Nd_2CoIrO_6$  (NCIO) and  $Sm_2CoIrO_6$  (SCIO) sample.

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# Self-Powered Deep UV Photodetector Based on Si-doped n-( $\overline{2}01$ ) Ga<sub>2</sub>O<sub>3</sub> Grown on p-(0001) GaN/Sapphire Substrates using PLD

Ajoy Biswas, Bhabani Prasad Sahu, Amandeep Kaur, Subhabrata Dhar

Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

\* Corresponding author: Ajoy Biswas, Email id: ajoybiswas975@gmail.com

## Category: Poster

**Keywords:** *β*- Ga<sub>2</sub>O<sub>3</sub>, Epitaxial film, PLD, Photodetector, Responsivity.

Recently,  $\beta$ -phase gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) has received much attention for applications in UV-light emitting diodes and detectors due to its ultra-wide bandgap (~4.9 eV) nature [1]. The material also exhibits high thermal and chemical stability. It has been reported that intrinsic Ga<sub>2</sub>O<sub>3</sub> often shows unintentional n-type behavior, which can be attributed to the oxygen vacancies. Ga<sub>2</sub>O<sub>3</sub> can also be extrinsically doped n-type with Si and Sn [2]. However p-type doping of Ga<sub>2</sub>O<sub>3</sub> is still a challenge. GaN is another wide bandgap semiconductor which can be controllably doped p-type. There are reports of epitaxial growth of Ga<sub>2</sub>O<sub>3</sub> on GaN. It will thus be interesting to study n- Ga<sub>2</sub>O<sub>3</sub> /p-GaN heterojunctions for UV detector applications.

Here, we have deposited Si-doped Ga<sub>2</sub>O<sub>3</sub> layers on p-type Mg-doped (0001)GaN/c-sapphire substrates using pulse laser deposition (PLD) technique. It is observed that the epitaxial quality of Ga<sub>2</sub>O<sub>3</sub> film depends on the oxygen pressure inside the chamber and the substrate temperature during growth. The optimum growth conditions are obtained by analyzing the X-ray diffraction (XRD) data. It has been found that the grown Ga<sub>2</sub>O<sub>3</sub> layer has monoclinic  $\beta$ -phase with ( $\overline{2}$ 01) growth orientation. Surface morphology and roughness of the films are investigated using scanning electron microscopy (SEM) and atomic force microscopy (AFM) techniques, respectively. This devices are found to show rectifying current-voltage characteristics, which suggests the formation of p-n junctions. Photo-responsivity of this detector found to be as high as 34mA/W at 245nm wavelength of the photons. This devices are also found to respond very fast; within a few milliseconds.

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# TIPS-Pentacene Memristor: A Rewritable and Solution-Processable Platform for Organic Small-Molecule Memory Devices

Nikhitha Rajan and Ayash Kanto Mukherjee<sup>\*</sup> Department of Physics, Indian Institute of Technology Patna, Bihta 801106, India \*Contact: akm@iitp.ac.in

Keywords: Organic Memristor, Non- volatile memory, TIPS Pentacene, Resistive switching

CMOS technology is approaching its limits due to the inherent constraints of the Von Neumann architecture. Memristors, which integrate computing and storage in a single device, offer a potential solution to overcome this bottleneck, enabling faster and more efficient data processing in future computing systems. Memristors have recently attracted considerable attention due to its characteristics of in-memory computing. Among them, organic small molecule-based memristors can be a potential candidate for lightweight, flexible, and environmentally friendly memory devices. However, despite several investigations, solution-processed intrinsic small molecular memristors with lower operating voltage are still challenging. In this work, a solutionprocessed intrinsic low power memristor using the small molecule 6,13-Bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene) is developed, featuring environmental stability and a low set voltage of around 0.5V. The device also shows excellent retention (>10<sup>4</sup> s) and reliable endurance. Structural characterization, including X-ray diffraction and field-emission scanning electron microscopy (FESEM), reveals a continuous film with high grain density and crystallite size around 46 nm. The switching mechanism is identified as charge trapping/de-trapping named the trap-controlled space-charge-limited current (SCLC) model. Capacitance measurements further support the retention of high and low resistance states and non volatile nature of the device. Furthermore, all measurements were performed under ambient laboratory conditions, demonstrating improved environmental stability compared to conventional small molecular devices. In conclusion, the TIPS-Pentacene memristor presents a promising solution for the next generation of memory devices, offering a combination of low cost, scalability, and energy efficiency.

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# **Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)**

# Modeling the Temperature Rise in the Active Region of In<sub>x</sub>Ga<sub>1-x</sub>N LEDs: Implications for Design and Operation

Krishna Kumar<sup>1</sup> and Bijaya Kumar Sahoo

Department of Physics, National Institute of Technology Raipur G.E Road, Raipur -492010 (C.G) India <sup>1</sup>Corresponding author's Email ID: kkumar.phy@nitrr.ac.in ; Mo: +919575520846

#### Category: Poster

#### Abstract:

InGaN-based commercial light-emitting diodes (LEDs) face significant limitations in high-power applications due to excessive heat generation, stemming from poor thermal management. Thermal conductivity (*k*) of such materials plays a critical role in mitigating heat, and the BIP effect has been found to enhance *k*. For an  $In_xGa_{1-x}N$  alloy, the lowest thermal conductivity is observed at x = 0.5. This study presents an in-depth investigation into heat conduction within the active region of LEDs, utilizing the 2D heat flux equation to explore the temperature profile in given structure under fitted boundary conditions. The finite difference method was employed to simulate the structures, revealing that increasing Indium composition leads to a reduction in center temperature. Interestingly, while rise in temperature at the center of sample were observed with increasing boundary temperature, which varied depending on *x* and BIP effect at the same temperature. Among selected samples,  $In_{0.3}Ga_{0.7}N$  structure provides a possible way to the heat control. This research introduces a novel approach to heat management in InGaN-based devices, providing new insights for enhancing performance and reliability in high-power LED applications

Keywords: InGaN material; Built-in-polarization; Thermal conductivity; Heat flux equation; FDM.

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# Synthesis and characterization of titanate based perovskites and their applications as photocatalysts and gas sensors

Manoj A. More, Swapnil A. More, Matthew D. Femi, Gotan H. Jain, Ganesh E. Patil\* S.N.J.B's KKHA Arts, SMGL Commerce and SPHJ Science College, Chandwad. Dist. Nashik 423101 [India] \*Corresponding Author: ganeshpatil\_phy@rediffmail.com

Keywords: Nanomaterial, Hydrothermal method, Spray pyrolysis, Sol-gel method, Titanates, Perovskite, Gas sensor, Photocatalyst.

**Abstract:** The titanate based perovskite materials are the class of compounds having the general formula ATiO<sub>3</sub>. The titanate based perovskites have gained the attraction of researchers owing to their distinctive physical, chemical and optical properties which make them useful for multiple applications. Titanate based perovskite nanomaterials are recently used as photocatalysts as well as they are used in solar cells, transistors, sensors, etc. In particular, the titanate based perovskites are capable to detect various harmful gases like H<sub>2</sub>S, CO<sub>2</sub>, CO, LPG, NH<sub>3</sub>, etc. present in the atmosphere at the trace level and with high sensitivity due to their exceptional structural and electrical characteristics. This gas sensing ability of such materials is useful to fabricate the gas sensors for the application in industrial process control and environment monitoring. Similarly, the tunable optical properties of such materials make them useful in photocatalytic activities. This review provides an overview about the various methods for the synthesis, characteristic study as well as photocatalytic and gas sensing applications of the titanate based perovskite materials like FeTiO<sub>3</sub>, NiTiO<sub>3</sub>, CdTiO<sub>3</sub>, PbTiO<sub>3</sub>, CoTiO<sub>3</sub>, etc. The purpose of this review is to elaborate the advancements in the gas sensing and photocatalytic applications of the titanate based perovskite materials.

# **Theme: Nano and Functional Materials**

# Magnetoelastic and magnetodielectric coupling in the solid solution system $(1-x)Ba(Fe_{1/2}Nb_{1/2})O_3$ -xLaFeO<sub>3</sub> (x = 0.50)

Arun Kumar<sup>1\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Science Education and Research (IISER) Pune-411008, India

\*Contact: Email ID: arun.kumar@acads.iiserpune.ac.in

### Category: Poster/Oral

Keywords: Perovskites, Magnetic phase transitions, Magnetoelastic coupling and magnetodielectric coupling

Perovskite oxides with the general formula  $ABO_3$  (where A is an alkaline earth or rare-earth cation, and B is a transition metal cation) continue to be a focal point of research in condensed matter physics due to their intriguing electronic and magnetic properties [1]. The formation of solid solutions between perovskites allows for fine-tuning of material properties to meet specific technological demands, such as in microelectronic devices, ceramic capacitors, piezoelectric sensors, actuators, and memory devices [2].

In this work, we investigate the new solid solution system  $(1-x)Ba(Fe_{1/2}Nb_{1/2})O_3-xLaFeO_3$  with x = 0.50, abbreviated as BFN-0.50LF, using a combination of macroscopic and microscopic techniques to explore structure-property correlations. The system crystallizes in a cubic structure with the space group *Pm-3m*. Temperature-dependent magnetization measurements reveal successive magnetic transitions at ~175 K and ~30 K. Our analysis of temperature-dependent X-ray diffraction and dielectric data highlights two key features of the BFN-0.50LF system: (i) magnetoelastic coupling linked to the magnetic transitions, evident from changes in the unit cell volume, and (ii) magnetodielectric coupling, as indicated by anomalies across the two transitions. This study offers insights into designing environmentally friendly, lead-free perovskites with potential technological applications.

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## Exploring the magnetoelectric functionality in PMN-PT/FSMA multiferroic heterostructure for flexible MEMS applications

Diksha Arora and Davinder Kaur\*

Functional Nanomaterials Research Laboratory, Department of Physics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India \*Corresponding author: davinder.kaur@ph.iitr.ac.in, Tel.: +91-1332-285407, Fax: +91-1332-273560

*Keywords:* PMN-PT, ferromagnetic shape memory alloy, nonvolatile memory, Ni foil, flexible magnetoelectric sensor.

#### Abstract

Flexible microelectromechanical systems (MEMS) are poised to scaffold technological innovations in wearable sensing, implantable health monitoring systems and touchless human-machine interactivity. In this work, a flexible, cost-effective and room temperature sensitive Ni/FSMA/PMN-PT magnetization-graded magnetoelectric (ME) heterostructure has been reported. Flexible Ni foil with -q (piezomagnetic coefficient) and ferromagnetic shape memory alloy (FSMA; Ni-Mn-In) layer with +q provides the desired q-grading. The Ni/FSMA/PMN-PT heterostructure displays ME output of 3.7 Vcm<sup>-1</sup>Oe<sup>-1</sup>, significantly higher than Ni/PMN-PT (1 Vcm<sup>-1</sup>Oe<sup>-1</sup>). The q-grading induced bending moment impedes the asymmetry-related flexural strain and strengthens the ME interaction. The zero-bias ME output of 0.4 Vcm<sup>-1</sup>Oe<sup>-1</sup> has been ascribed to the interaction between q-grading-induced transverse magnetization and AC magnetic field. Ni/Ni-Mn-In/PMN-PT ME heterostructure displays excellent magnetic field sensing parameters: correlation coefficient, sensitivity, inaccuracy and hysteresis of 0.99916, 0.74 mV/Oe, 1.5% full-scale output (FSO) and 1.8% FSO, respectively. The reversible and repeatable nonvolatile switching of the ME coefficient obtained with positive and negative electric fields is useful for next-generation memory devices. The fabricated heterostructure shows excellent flexibility with steady performance up to 1500 bending cycles. Such Ni/FSMA/PMN-PT based ME heterostructures are propitious for multifunctional flexible magnetic field sensors and nonvolatile memory applications.

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## **Theme: Magnetism & Superconductivity**

## Review on magnetic properties of ternary alloy thin films

Dhananjoy Rajbanshi<sup>1</sup>\*, S.K. Srivastava<sup>1</sup>

<sup>1</sup>Department of Physics, Central Institute of Technology, Kokrajhar-783370, Assam, India

\*Contact:dhananjoyrajbanshi@gmail.com

#### Category: Poster

*Keywords:* Ternary alloy, perpendicular magnetic anisotropy, heat-assisted magnetic recording (HAMR)

In recent years, the observation of perpendicular magnetic anisotropy in amorphous rare earth-transition metal (RE-TM) alloys have attracted the attention of researchers for academic research and their possible uses in a range of useful systems, including random access memory, spintronics, and perpendicular magnetic recording media. Despite the amorphous nature of RE-TM alloys, these compounds exhibit different types of magnetic parameters such as perpendicular magnetic anisotropy, spin-orbit coupling, exchange coupling, magnetic compensation temperatures, etc. The research community is also very interested in the TM-TM metal alloys in addition to RE-TM metal alloys because of its many potential uses, especially in magnetic storage technology. Because of their high energy density of magnetic anisotropy, magnetocrystalline anisotropy (MCA), and thermal stability. L1<sub>0</sub> ordered alloy thin films have captured significant attention from researchers in recent years [1]. Their potential applications in high-density perpendicular magnetic recording, heat-assisted magnetic recording (HAMR) media, and magnetic random access memory make them a focal point of ongoing research and development. We are going to review the magnetic properties of FePt, FePd, CoPt, CoTb, etc. alloys thin films can be further tuned by adding third TM or RE elements to form ternary alloys[2].

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## **Nano and Functional Materials**

# Nacre-Inspired Composite Films: Enhancing Mechanical Performance through Polyvinyl Alcohol, Graphene Oxide and Biomass-derived Carbon Nanomaterials Integration

Ankush Kumar<sup>\*</sup> and Ajay D. Thakur

Department of Physics, Indian Institute of Technology Patna, Bihta, 801106, INDIA

\*Contact: ankush\_2121ph18@iitp.ac.in

#### Category: Poster

Keywords: Carbon nanomaterials, Tensile strength, Hierarchical structure, Composite films.

Researchers have long been inspired by the strength and toughness of biological structures. Nacre, also known as mother-of-pearl, possesses a brick-and-mortar structure composed of aragonite calcium carbonate and layers of organic proteins. This unique arrangement gives nacre its remarkable strength and toughness. In this study, biomass-derived carbon nanomaterials (BGCNMs) and graphene oxide (GO) were dispersed in water with varying ratios, while the amount of PVA solution was kept constant for all possible BGCNM and GO combinations. PVA was used as the matrix material to create composite films. The BGCNMs, GO, and PVA formed an interconnected network that closely mimicked the layered structure of the nacre. PVA and PVA/GO were prepared as control samples. Subsequently, composite films were synthesized with varying GO to BGCNM ratios, including 1:1, 1:2, 1:3, and 2:1. These composite films were fabricated using a solvent evaporation method. Changes in the microstructure, mechanical properties, and thermal stability of the composite films were studied. Tensile tests were conducted to evaluate their mechanical properties. As the BGCNM content increased, a significant improvement in tensile strength was observed.

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## Crystal structures, dielectric and magnetic properties in Sr doped Ba<sub>3</sub>MnSb<sub>2</sub>O<sub>9</sub> perovskites

Manish Kumar Tekam<sup>\*</sup>, Shalini Mishra, and Netram Kaurav

Department of Physics, Govt. Holkar (Model, Autonomous) Science College, Bhawarkuan, A.B. Road, Indore (M.P.)

452001

\*Contact: manishktkm@gmail.com

*Keywords:* A-site doping<sup>1</sup>, Perovskite oxides<sup>2</sup>, Crystal strucutre<sup>3</sup>, Magnetic properties<sup>4</sup>.

The effects of doping via A-site substitution on the structural, dielectric, and magnetic properties of the triple perovskite  $Ba_3MnSb_2O_9$  are investigated by substituting Sr2+ ions for Ba2+ ions. This A-site doping in parent compound Effects have been studied using X-ray diffraction, dielectric and magnetization measurements. The substitution of Strontium in A-site  $Ba_{3-x}Sr_xMnSb_2O_9$  (x = 1 and 3) leads to exchange interaction, giving rise to exotic quantum properties. The Sr-substituted  $Ba_3MnSb_2O_9$  perovskite was obtained using a conventional solid-state reaction method. Room-temperature crystal structures were determined by powder X-ray measurement, combined by Rietveld refinements of the substituted series. The parent compound  $Ba_3MnSb_2O_9$  has a monoclinic distorted structure with space group C2/c. Temperature dependent dielectric measurements reveals the existence of magnetodielectric effect in the nanomaterial. The results of magnetic susceptibility and specific heat measurements, show an antiferromagnetic transition, indicating the onset of the magnetic transition.

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# Magnetic and Dielectric Property Enhancement in M-Type Hexaferrites for Cutting-Edge THz Applications

Manjushree Maity<sup>1</sup>, Rajeev Singh, Biswanath Bhoi\*

Nano-Magnetism and Quantum Technology Lab, Department of Physics, I.I.T. (BHU) Varanasi, Uttar Pradesh - 221005, India.

<sup>t</sup>Email of presenting author: manjushreemaity.rs.phy23@itbhu.ac.in \*Email of corresponding author: biswanath.phy@iitbhu.ac.in

Keywords: M-type Hexaferrite, Ferromagnetic Resonance, Terahertz Device

Terahertz (or millimeter-wave) technologies are among the most promising and rapidly advancing fields in modern engineering, crucial for the next generation of high-speed telecommunication systems[1]. However, this progress relies on the thorough investigation and study of promising materials for use in THz devices. Due to the high demand for materials with tunable terahertz resonance lines, M-type hexaferrites (MFe<sub>12</sub>O<sub>19</sub>, M = Ba, Sr) have garnered significant research interest for their inherent ferromagnetic resonance absorption in the Sub-terahertz or terahertz band.

In this work, we synthesized two M-type hexaferrites  $SrAl_4Fe_8O_{19}$  (SAF) and  $Sr_{0.54}Ca_{0.46}Al_{6.5}Fe_{5.5}O_{19}$  (SCAF)[2] using conventional solid-state reaction method. To achieve a pure phase of SAF and SCAF, high-purity oxide powders of the constituent elements were thoroughly mixed in the appropriate molar ratios using isopropyl alcohol as a wet grinding medium, grinding for 12 hours in a mortar and pestle. After drying the mixture of respective compounds in an oven at 100°C for 24 hours, the powders were calcined at 1350°C for 24 hours to form the hexaferrite phase. The resulting powder was reground, compacted at 200 kg/cm<sup>2</sup>, and sintered at 1400°C in air for 6 hours, following a controlled heating and cooling cycle to ensure a crack-free pellet. The crystallographic structures of the pellet were analyzed using an X'pert Pro (PW 3040) X-ray diffractometer, and the Rietveld profile refinement method was employed to confirm the presence of a pure hexaferrite phase with the P63/mmc space group. A detailed investigation of the electrical properties, including capacitance, dielectric constant, dielectric loss, AC conductivity, complex impedance, and modulus, was conducted on both samples across various frequencies and temperatures using a high-performance frequency LCR meter. Furthermore, the increased coercivity for both samples, as measured from the magnetic hysteresis loops recorded with a SQUID magnetometer, indicates high-frequency ferromagnetic resonance, thus enhancing their efficiency for applications in the THz frequency range.

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# Fabrication of flexible substrate with partially embedded back-contacts for piezoelectric ZnO-based arms movement sensors

Habeebur Rahman, and Davinder Kaur\*

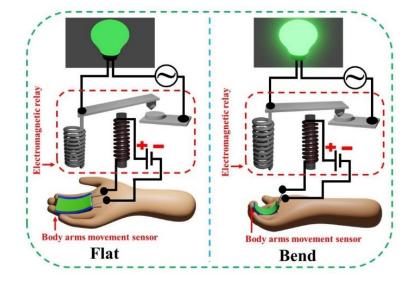
1 Functional Nanomaterials Research Laboratory (FNRL), Department of Physics and Centre for Nanotechnology, Indian Institute of Technology Roorkee, Uttarakhand, India

\*Contact: davinder.kaur@ph.iitr.ac.in

Keywords: movement sensor, embedded contacts, flexible, piezoelectricity, ZnO

This work uses a facile method to fabricate the partially embedded and firm back contact to address the contactbreaking issue in flexible electronic devices. The polyvinyl alcohol (PVA) solution in distilled water is employed to synthesize the environment-friendly bendable substrate. The partially embedded back contact using copper wire was made during the substrate development. For connection and flexibility checks, silver (Ag) and molybdenum disulfide (MoS<sub>2</sub>) were sputter-coated over the flexible substrate, and different current-voltage (I-V) measurements were performed. The results showed excellent contact between the partially embedded copper wire and the deposited thin films. For bending characterization, the I-V measurements at different angles (0° to 180°) have been carried out for both materials. It revealed the overlapping plots for all angles, suggesting an unperturbed bending response. For practical demonstration, the flexible substrate with partially embedded interdigitated electrodes (IDE) was fabricated over which a thick film of zinc oxide (ZnO) nanoplates was coated. The IV measurements in flat-bend-flat cycles revealed an enhanced current due to the piezoelectric nature of ZnO in bending states and a full recovery in flat states. Therefore, the as-fabricated device can be considered cost-effective and ready to use as a body-arms movement sensor for medical applications. This paragraph starts the text section of the abstract.





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# Emulation of Neuromorphic Learning in a Preferentially Grown Cobalt Oxide Thin Film Memristor

Indranil Maity\*, Richa Bharti, A. K. Mukherjee, and Ajay D. Thakur Department of Physics, Indian Institute of Technology Patna, Bihta 801106, India \*Contact: indranil\_1921ph16@iitp.ac.in

*Keywords:* Neuromorphic computing, Hebbian learning, Resistive switching, Spike time-dependent plasticity, Pulsed laser deposition

Neuromorphic computing is a very promising field that deals with mimicking brain-inspired cognitive tasks in an electronic device. In this context, resistive switching (RS) devices are the best choice due to extraordinary structural and functional similarities with neural synapses. This study demonstrates brain-like experiential learning/forgetting ability using a variety of synaptic adaptation rules, including short-term potentiation (STP)/depression (STD), long-term potentiation (LTP)/depression (LTD), spike-rate dependent plasticity (SRDP), and spike-time dependent plasticity. The SRDP and STDP characteristics of the device revealed the realization of asymmetric Hebbian learning in the device. The model device utilized here is a unidirectional thin film of nanocrystalline  $Co_3O_4$  fabricated on a p-Si (100) substrate using pulsed laser deposition to achieve a metal-insulator-semiconductor (MIS) type resistive switching (RS) device. In addition, we have found analog bipolar-type switching behavior with outstanding RS features in terms of endurance (10<sup>3</sup> cycles), retention (10<sup>4</sup> s), and ON-OFF ratio (~316), making it appropriate for CMOS-compatible memory systems. The conduction and RS mechanisms are explained using a tentative band diagram derived from UV-visible spectroscopic data.

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## Enhanced physical properties of BiFeO<sub>3</sub>-modified Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> thin film

## prepared by pulsed laser deposition technique for memristor devices

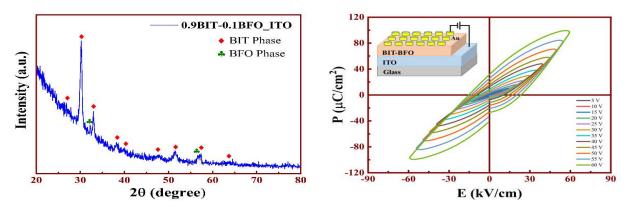
Priyanka Mitra<sup>1\*</sup> and B. Harihara Venkataraman<sup>1</sup>

1 Department of Physics, BITS-Pilani, Hyderabad Campus, Jawahar Nagar, Shameerpet, Telangana-500078, India \*Contact: p20190457@hyderabad.bits-pilani.ac.in

#### Category: Oral

Keywords: Multiferroic composite thin film, Pulsed laser deposition, GIXRD, Ferroelectric properties.

In the digital era, multiferroic materials are attractive owing to their simultaneous coupling of the ferroelectric and ferromagnetic order parameters. The urge to stimulate the magnetoelectric effect has driven researchers to utilise these materials for various applications like capacitors, sensors, spintronics, actuators and NVRAM devices. Usually, these material classifications exist in single or composite forms; however, due to the inherent characteristic limitations, single-phase materials may not be suitable for electronic applications compared to hybrid-phase. Keeping this in view, the 0.9Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> (BIT) - 0.1BiFeO<sub>3</sub> (BFO) diphasic composite thin film has been prepared using the Pulsed Laser Deposition (PLD) technique. This thin film sample was grown on the ITO-coated glass substrate using the KrF laser (248 nm). Deposition time is crucial in obtaining a highquality multiferroic composite thin film, among other deposition conditions like oxygen gas pressure, repetition frequency, and substrate temperature deposition. The as-grown hetero-structured thin film was characterized by Grazing Incident X-ray Diffraction (GIXRD), Field Emission Scanning Electron Microscopy (FeSEM), Atomic Force Microscope (AFM), X-ray Photoelectron Spectroscopy (XPS), and Electric Field-Dependent Polarization (P-E) techniques. The XRD pattern confirmed the co-existence of the diphasic composite thin film with a significant phase from the orthorhombic BIT and a minor Bragg reflection from the BFO (rhombohedral) phase. A sharp characteristic peak at  $2\theta \sim 30.08^{\circ}$  has confirmed the phase formation of a bismuth titanate associated with a low intense peak at  $2\theta \sim 32.10^{\circ}$  of the bismuth ferrite phase. The presence of all the constituent elements of BIT and BFO crystalline phases is validated by XPS analysis. The roomtemperature ferroelectric analysis exhibited a hysteresis loop with an enhanced magnitude of  $2P_r$  (~65  $\mu$ C/cm<sup>2</sup>) and  $2E_c$  (~ 38 kV/cm) than their bulk counterpart. Hence, this uniformly deposited di-phasic composite thin film configuration could be exploited as a better candidate for memory-based device applications.



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# Soft Multi-functional Materials for Sensing

Khashti Datt Pandey<sup>1</sup>\*, Indranil Maity<sup>1</sup> and Ajay D. Thakur<sup>1</sup>

Indian Institute of Technology Patna, Bihta, 801106, India

\*Contact: khashti\_2121ph05@iitp.ac.in

Category: Oral

Keywords: Soft, Multifunctional, Piezoelectric, Hydrogel

Soft multifunctional polymer materials are compact materials with multiple stimuli-sensing capabilities and structural properties, including flexibility and stretchability. These materials find applications in various areas, such as energy harvesting, robotics, and flex sensing for medical use, as well as fast wound healing, etc. In our study, we synthesized a hydrogel blend using Poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and Polyvinyl alcohol (PVA) through the freeze-thaw method. This hydrogel exhibits mechanical robustness and has a low swelling ratio. We investigated the properties of this hydrogel by varying the percentage content of the porous aluminosilicate nanofiller. Notably, the hydrogel possesses several functionalities, including an electret nature, piezoelectric behaviour, piezoresistive properties, etc. With the filler content the hydrogel stiffens, and piezo-response enhances; at 3% filler content maximum of about 0.8 V is observed on finger tapping. Due to these functionalities, along with its structural properties and non-toxicity, the PVDF-HFP/PVA blend hydrogel holds promise for applications in energy harvesting (e.g., utilizing small forces generated during physical movements of body parts that would otherwise go to waste), soft robotics, soft flex-sensing, fast wound healing, water remediation, etc.

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# Theme: Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)

# Investigation of Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> Interface Charge for the Feasibility of Charge Sheet Super Junction

Swadhin Kumar Jena<sup>1</sup>, Chiranjibi Padhee<sup>1</sup>, Akshay K<sup>2</sup> and Parlapalli Venkata Satyam<sup>1</sup>

<sup>1</sup>School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India <sup>2</sup>School of Electrical Sciences, Indian Institute of Technology Bhubaneswar, Odisha, India

Email: satyam@iitbbs.ac.in , akshay@iitbbs.ac.in, s22ph09002@iitbbs.ac.in

#### Category: Poster

Keywords: Superjunctions (SJs); MOS capacitor; C-V measurement; fixed negative charge

#### **ABSTRACT**

Superjunctions (SJs) are among the most innovative and significant concepts in the field of power devices. The technical challenges of fabricating a void-free p-pillar in super junctions (SJs) led to the proposal of a new and intriguing concept known as charge sheet super junctions (CSSJs). Here, we present the fabrication, characterization, and simulation of the Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> bi-layer interface on Si, which could potentially replace the p-pillar in SJs. We conducted an experimental study where we deposited an Al<sub>2</sub>O<sub>3</sub> layer onto the native SiO<sub>2</sub> of silicon using atomic layer deposition (ALD) and fabricated a metal oxide semiconductor (MOS) capacitor device. We studied the morphology and stoichiometry of the deposited film using field emission scanning electron microscopy (FESEM) and energy dispersive X-ray spectroscopy (EDX) techniques, respectively. We used a high-frequency capacitance-voltage (C-V) measurement technique for electrical characterization of the Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> bilayer of the deposited negative charge is present at the interface. Technology computer-aided design (TCAD) simulation was performed for the study of the interface of the Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> bilayer by creating the MOS capacitor structure. The presence of a fixed negative charge at the interface was also found in the TCAD simulation result, which complemented the experimental result. Therefore, this result indicates possible future applications in the SJs.

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#### **Theme: Magnetism and Superconductivity**

#### Exchange coupled hard/soft nanocomposite: A promising candidate for high energy product permanent magnet

<u>Subrata Ch. Sarkar</u><sup>1</sup>, S. K. Srivastava<sup>1\*</sup> <sup>1</sup>Department of Physics, Central Institute of Technology Kokrajhar, Kokrajhar-783370, India E-mail: \*<u>sk.srivastava@cit.ac.in</u>

#### Category: Poster

Keywords: Exchange coupled, hard/soft nanocomposite, exchange interaction, energy product

Permanent magnets are the fundamental component in the development of modern technology, with their applications extending to fields such as energy generation, transportation, communication, and medical imaging etc. Exchange coupled nanocomposite permanent magnets have gained significant attention in the past two decades. The interphase magnetic exchange coupling of soft ferromagnetic phase with hard ferromagnetic phase at the nanoscale leads to a single phase magnetic behavior that results in enhanced coercivity, remanence, and thus improved high-energy products when compared to the conventional permanent magnets. There is renewed interest in this class of permanent magnets because they offer the possibility of reducing the use of expensive and strategically valuable elements which are necessary for making high-performance magnets like rare earths elements Nd, Sm, Pr as well as precious metals Pt, Pd. It has been theoretically calculated that the energy product of exchange-coupled permanent magnets could reach a value of 1 MJ/m<sup>3</sup> (120 MGOe). The precise control over the thickness and grain size of the hard and soft phases is essential for effective interphase exchange coupling between them. Studies have shown that reducing the grain size to the nanoscale enhances the interphase exchange interaction, leading to improved coercivity and remanence. Additionally, the introduction of interfacial layers (spacer layer) and the use of annealing techniques have been explored to further refine the magnetic properties. This work reviews the recent progress made in rare-earth element based and non-rare earth element based exchange coupled nanocomposite permanent magnets, with an in-depth analysis of their magnetic properties and applications.

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#### Enhancing Sonocatalytic Dye Degradation using 2-D MoS<sub>2</sub> Nanosheets

Monisha Sarkar, Manisha Kundu, Navonil Bose<sup>\*</sup> and Sukhen Das Department of Physics, Jadavpur University, Kolkata 700032, India

\*Corresponding Author: navonil05@gmail.com

Keywords: 2-D MoS<sub>2</sub> nanosheets, Piezocatalysis, Dye Degradation, ROS,

The presence of emerging pollutants in industrial wastewater is a global problem and requires appropriate treatment techniques [1-2]. Herein, reusable, stable and highly efficient 2-D  $MoS_2$  nanosheets are prepared via a one-step hydrothermal process and proposed as an environment friendly piezocatalyst for treating polluted water. The morphology, composition, and optical properties of the prepared MoS<sub>2</sub> nanostructures are investigated by using different techniques including X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HR-TEM) and Raman spectroscopy. Mono to four layer structure of the MoS<sub>2</sub> nanosheets is confirmed by TEM. Moreover, the d-spacing of the nanosheets and optical band gap are found to be ~0.6 nm and 1.19 eV respectively. 2-D MoS<sub>2</sub> nanosheet shows ultrafast removal of RhB dye under ultrasound assistance. At the optimal concentration of 15 ppm RhB dye, very low catalyst dosage, a remarkable RhB dye degradation efficiency of 99% is achieved within 9 min. The remarkable piezocatalytic assisted degradation performance of MoS<sub>2</sub> nanosheets via reactive oxygen species (ROS) mechanism is attributable to its super-active edges of the 2-D stacked layer structure. Various ROS traps are used to find out the major reactive species in the sonocatalytic degradation of RhB dye. The very fast removal of the dye is attributed to the large surface area of the  $MoS_2$  which provides large number of active sites for the adsorption and piezocatalysis degradation of organic dyes under ultrasonic assistance. Consequently, these hydrothermally prepared  $MoS_2$  nanosheets can be considered as a promising catalyst for the degradation of emerging pollutants from an aqueous solution.

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## Effect of addition of Mn for Al on Structural, Magnetic Properties of Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>15-x</sub>Mn<sub>5+x</sub> (x=0, 2.5, 5) High Entropy Alloys

Priyanka Kumari, Rohit R. Shahi\*

Functional Materials Research Laboratory, Department of Physics, Central University of South Bihar Gaya, Bihar 824236, India

\*Contact: rohitrshahi@cusb.ac.in, rohitrshahi@gmail.com

Keywords: High entropy alloys, Magnetic Materials, Mechanical Alloying, Annealing

In this study, we have investigated the effect of the addition of Mn for Al in Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>15-x</sub>Mn<sub>5+x</sub> (x=0, 2.5, 5) High Entropy Alloys (HEAs). Three different  $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{10}Mn_5$ ,  $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{7.5}Mn_{7.5}$  and  $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_5Mn_{10}$  HEAs were synthesized through the mechanical alloying technique. Phase formation, microstructure and magnetic properties of as- synthesized and 700°C annealed Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>15-x</sub>Mn<sub>5-x</sub> (x=0, 2.5, 5) HEAs are investigated in detail. XRD analysis confirmed the formation of fcc phase with a minor concentration of bcc and σ phase for Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>15-x</sub>Mn<sub>5-x</sub> (x=0, 2.5, 5) HEAs. The value of saturation magnetization and coercivity is 73.14 emu/g & 18 Oe for Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>10</sub>Mn<sub>5</sub> HEA, and the value of Ms slightly decreased for Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>7.5</sub>Mn<sub>7.5</sub> and Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>5</sub>Mn<sub>10</sub> HEAs. However, no significant change was observed in the value of Hc with the increase in the content of Mn. The relative volume phase fraction of bcc phase has increased for 700°C annealed Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>15-x</sub>Mn<sub>5-x</sub> (x=0, 2.5, 5) HEAs. The value of Ms and Hc is increased significantly and found to be 105 emu/g & 49 Oe, 106 emu/g & 49 Oe and 102 emu/g & 47 Oe for 700°C annealed  $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_{10}Mn_5$ , Co<sub>35</sub>Cr<sub>5</sub>Fe<sub>10</sub>Ni<sub>30</sub>Ti<sub>5</sub>Al<sub>7.5</sub>Mn<sub>7.5</sub> and  $Co_{35}Cr_5Fe_{10}Ni_{30}Ti_5Al_5Mn_{10}$ HEAs, respectively. Our investigations provide detailed insight for phase formation and its corelation with change in magnetic properties with the addition of Mn for Al and annealing at 700°C.

#### Analysis of LiTiPtZ (Z =Al, Ga and In) quaternary Heusler alloys for optoelectronic and energy harvesting applications

Lokanksha Suktel and Sapan Mohan Saini\*

*Email: <u>smsaini.phy@nitr:ac.in</u>* <sup>a</sup> Department of physics, National Institute of Technology Raipur, Chhattisgarh, India

#### Abstract

Equiatomic quaternary Heusler's (EQHs) alloys are emerged as a potential candidate for thermoelectric materials, due to its simple crystal structure, tuneable band gaps, and excellent transport properties. Computational methods are reliable in envisaging the ground state and several other properties of materials. In this work we have inspected the physical properties (structural, electronic, mechanical, optical, dynamical) of a novel series of EQH LiTiPtZ (Z = Al, Ga, and In) alloys. These physical properties were examined by the density functional theory as implemented in wien2k code. For the treatment of exchange and corelation effect generalised gradient approximation has been employed. We have analysed the absorption coefficient and optical conductivity and found the high absorption in visible and ultra-violet region, suggesting the potential use of these alloys in optoelectronic devices. We have also studied various transport properties of LiTiPtZ (Z = Al, Ga, and In) alloys, which indorse the application of these material in eco-friendly energy harvesting. The computed elastic and mechanical parameters ensure the mechanical stability of these compounds. The outcome of this work is quite fascinating from the fundamental view, and it has an immense significance in alloys practical realizations and applications.

## Effects of CTAB, EDTA, and PVP surfactants on structural and optical properties of ZnSe nanocrystals

Priya Chandra<sup>\*</sup>and K.S. Ojha

<sup>1</sup>Department of Physics, National Institute of Technology Raipur, Chhattisgarh, India-492010 \*Contact: pchandra.phd2022.phy@nitrr.ac.in

#### Abstract:

ZnSe is a direct band gap polycrystalline semiconductor from the II-VI group, known for its significant potential in optoelectronic applications and photocatalytic activation. This study explores the influence of various surfactants - Cetyl-trimethyl-ammonium-bromide (CTAB), Ethylene-diamine-tetra-acetic-acid (EDTA), and Poly-vinyl-pyrrolidone (PVP) on the surface of ZnSe nanocrystals synthesized via a simple hydrothermal method. Comprehensive analyses of the structural, morphological, and optical properties were conducted using differnt techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), Fourier-transform infrared spectroscopy (FTIR), UV-visible spectroscopy, and photoluminescence (PL) spectroscopy. The XRD and FTIR results confirmed the successful formation of ZnSe nanocrystals, while PL spectra exhibited distinct emission in the visible region. This study highlights the role of surfactants in modulating the properties of ZnSe nanocrystals.

Keywords: Zinc selenide, hydrothermal method, EDTA, CTAB, PVP.

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## Investigation of the impact of hydrothermal reaction temperature on the structural, optical and electrical properties of the NiTiO<sub>3</sub> and its application for gas sensing

Ganesh E Patil\*, Manoj A More, S. D. Shinde and Gotan H Jain

Department of Physics, SNJB's KKHA Arts, SMGL Commerce and SPHJ Science College, Chandwad 423101 India \*Presenting Author: ganeshpatil\_phy@rediffmail.com

Keywords: Hydrothermal method, Perovskite material, Nickel titanate, Gas sensor, TEM

Abstract: In this work we are presenting the hydrothermal method to synthesize the NiTiO<sub>3</sub> perovskite nanoparticles (NPs). The effect of variation in reaction temperature on the structural, optical, electrical and gas sensing properties of NiTiO<sub>3</sub> nanoparticles was investigated. The synthesized nanoparticles at different reaction temperatures were characterized by various characterization methods like XRD, FTIR, UV-Visible Spectroscopy, FESEM, TEM, HRTEM and SAED. The results of UV-Visible analysis revealed that band gap of NiTiO<sub>3</sub> decreased from 2.90 eV to 2.56 on increase in reaction temperature from 140 °C to 200 °C. The XRD analysis showed that crystallite size decreased in the range of 21 nm to 12 nm on increase in reaction temperature. The various parameters of the material like dislocation density, microstrain and crystallinity were also calculated from XRD data. The average particle size was estimated by FESEM analysis and found to be increased on increase in reaction temperature. FTIR analysis confirmed the formation of NiTiO<sub>3</sub> sensor characteristics in terms of sensitivity, selectivity, response and recovery time was carried out. The study of gas sensing performance of NiTiO<sub>3</sub> revealed that NiTiO<sub>3</sub> synthesized at 140 °C showed maximum sensitivity to H<sub>2</sub>S gas at 250 °C.

#### **Devices (Electronics, Spintronics, Optoelectronics, Sensors & actuators)**

#### Investigation on Crystal Structure, Dielectric, and I–V Characteristics of Mg doped SnO<sub>2</sub> Compound for Application in Optoelectronics

K. K. Singha<sup>1</sup>, and S. K. Srivastava<sup>1\*</sup>

<sup>1</sup>Department of Physics, Central Institute of Technology Kokrajhar, Kokrajhar–783370, India

\*Contact: \*<u>sk.srivastava@cit.ac.in</u>

Category: Poster

Key Words: Mg doped SnO2; XRD analysis; Zero Dielectric loss; I-V characteristics

#### Abstract

The magnesium–doped tin dioxide compounds were prepared and their properties were revealed through crystal structure, Raman spectra, optical, dielectric, and I–V measurements for a possible application in optoelectronics devices. The synthesis of polycrystalline  $Sn_{1-x}Mg_xO_2$  ( $0 \le x \le 0.10$ ) compounds was achieved using the solid–state reaction technique. A tetragonal rutile–type structure has been formed for  $SnO_2$  as revealed by XRD. The results of Raman spectroscopy have confirmed that the synthesis process has produced a tetragonal rutile phase of  $SnO_2$  with Mg ions successfully integrated into the material. The UV–Vis spectrophotometer measurements of absorbance and transmittance revealed that the optical band gap of  $SnO_2$  increased with increasing magnesium doping concentration. Moreover, the transmittance value improved by 8% (from 83% to 91%) when the magnesium doping concentration was increased. The dielectric characteristics of  $SnO_2$  compounds doped with magnesium were explained using the Maxwell–Wagner model. The sample's electrical properties were determined by applying a tin metal contact and measuring the sample's I–V characteristics using a two–probe Keithley 6517b electrometer. The results revealed a linear relationship between current and voltage, indicative of Ohmic behavior.

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#### Nano and Functional materials

#### Effect of Mn Doping on the Temperature-Dependent Dielectric Relaxation Behavior and Electric Conduction Mechanisms of Bi<sub>0.85</sub>La<sub>0.15</sub>FeO<sub>3</sub> Ceramics

Mukesh Shekhar<sup>1,3</sup>, Sonu Rani<sup>2</sup>, Pawan Kumar<sup>3</sup>\*

<sup>1</sup>Department of Education, Central University of Jharkhand, Ranchi-835222, India <sup>2</sup>Department of Physics, Magadh Mahila College, Patna University, Patna-800001, India <sup>3</sup>Department of Physics, Mahatma Gandhi Central University, Bihar-845401, India \*Contact: pawankumarmgcub@gmail.com

#### Category: Oral

Keywords: Multiferroic, Dielectric Relaxation, Activation Energy, Electric Modulus

This study investigates the temperature-dependent microscopic dielectric relaxation and electric conduction processes in the polycrystalline samples of Bi<sub>0.85</sub>La<sub>0.15</sub>Fe<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> ceramics synthesized by the modified solgel method [1-3], using complex impedance, complex electric modulus, and frequency-dependent ac conductivity studies. The relaxation time and associated activation energies were calculated using the Arrhenius method. Results indicate that dielectric properties are optimal for the 5% Mn doping in Bi<sub>0.85</sub>La<sub>0.15</sub>FeO<sub>3</sub> ceramic, and the value of corresponding activation energy is maximum. The frequency-dependent dielectric constant aligns well with the modified Debye relaxation model, suggesting the presence of multiple relaxation processes. Temperature-dependent AC conductivity follows Jonscher's universal power law, with the thermally assisted SPH conduction model fitting lower co-doping concentrations. In contrast, the Overlapping Large Polaron Tunneling (OLPT) model is applicable at higher co-doping levels. The high Z' values at lower temperatures and frequencies suggest increased electric polarization and negative temperature coefficient of resistance (NTCR) behavior. Contributions from grains and grain boundaries were evaluated through Nyquist plot analysis.

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#### Nano and Functional materials

#### Synthesis and Characterization of La<sub>2</sub>BMnO<sub>6</sub> (where B = Co, Ni, Cu) for Energy Storage Applications

<u>Amod Kumar<sup>1</sup></u>, Yaswant Kashyap<sup>2</sup>, Tupan Das<sup>3</sup>, Rakesh Kumar Pandey<sup>2</sup>, Manoranjan Kar<sup>3</sup>, Pawan Kumar<sup>1</sup>,\*

<sup>1</sup>Department of Physics, Mahatma Gandhi Central University, Bihar-845401, India. <sup>2</sup>Department of Chemistry, Mahatma Gandhi Central University, Bihar-845401, India. <sup>3</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna-801103, India \*Contact: pawankumarmgcub@gmail.com

#### Category: Oral

Keywords: Double perovskites, Sol-gel, XRD, Rietveld, Supercapacitor

The technological and industrial development that has emerged in recent decades often implies excessive energy consumption, and currently, most of the energy sources used are non-renewable. This research investigates the potential of double perovskite oxides  $La_2BMnO_6$  (where B = Co, Ni, Cu) as electrode materials for energy storage applications. These materials offer promising properties due to their structural flexibility, tunable electronic structures, and high theoretical capacity. Perovskite oxides have attracted significant attention in energy storage performances because of their eccentric physical and chemical features [1]. Herein, we aim to study the electrochemical characterization of double perovskite  $La_2BMnO_6$  (where B = Co, Ni, Cu) prepared through a facile sol-gel route. The synthesized materials were characterized using various techniques, including X-ray diffraction (XRD) and electrochemical impedance spectroscopy (EIS). The Rietveld refinement of all XRD patterns was performed to evaluate changes in lattice parameters, unit cell volume, and crystal structure. The electrochemical performance of the nanocomposites of double perovskite materials (70 wt %), Graphene oxide (10 wt%), Polypyrrole (10 wt%), and the PVDF binder (10 wt %) on graphite sheet as substrate, have been evaluated through cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electron transfer rate measurements. At first, the electrochemical studies of the working electrodes have been carried out in a three-electrode setup, followed by a two-electrode setup for energy storage applications. The results demonstrate the influence of the B-site cation on the structural, electronic, and electrochemical properties of the double perovskites. The findings provide valuable insights into designing and optimizing electrode materials for advanced energy storage devices.

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#### **Nano and Functional materials**

## Impact of Aluminium Doping on the Nanocrystalline La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> as an Electrode Material for Supercapacitor Applications

<u>Aliva Panigrahi<sup>1</sup></u>, Amod Kumar<sup>1</sup>, Yaswant Kashyap<sup>2</sup>, Piyali Biswas<sup>3</sup>, Rakesh Kumar Pandey<sup>2</sup>, Manoranjan Kar<sup>3</sup>, Pawan Kumar<sup>1</sup>\*

> <sup>1</sup>Department of Physics, Mahatma Gandhi Central University, Bihar-845401, India. <sup>2</sup>Department of Chemistry, Mahatma Gandhi Central University, Bihar-845401, India. <sup>3</sup>Department of Physics, Indian Institute of Technology Patna, Bihta, Patna-801103, India \*Contact: pawankumarmgcub@gmail.com

Category: Oral

Keywords: Perovskite, XRD, Rietveld, Supercapacitor

The choice of stable and effective electrode material is crucial for the development of supercapacitor devices. Several classes of materials have proved their potential to become electrodes in supercapacitors. Among them, perovskite oxide electrodes are widely studied because of their high energy and power density. The ionic size of both cations in ABO<sub>3</sub>-type perovskite materials affects the stability or symmetry of the material, which has a significant effect on how well it works overall. However, cyclic stability has been a major setback for their wide-scale application as an electrode for supercapacitors. This can be resolved by partially substituting the cations with a suitable dopant whose ionic sizes and valency will impact the electrochemical performance of perovskites such as LaMnO<sub>3</sub> [1-3]. In the present investigation, the effect of Al and Sr doping in the nanocrystalline LaMnO<sub>3</sub> has been studied to optimize its electrochemical properties for the supercapacitor device application. The X-ray diffraction (XRD) patterns show that all the samples are essentially in the  $\alpha$ phase of Lanthanum strontium manganite, which could be indexed to  $R\overline{3}c$  (# 167) space group in hexagonal symmetry. The Rietveld refinement of all XRD patterns was carried out to access the corresponding change in the lattice parameters and unit cell volume with the replacement of La<sup>3+</sup> with  $Sr^{2+}$ , which has a greater ionic radius, and  $Mn^{3+}$  with  $Al^{3+}$ , which has a similar ionic radius. The supercapacitor devices were fabricated on the graphite sheet and characterized using a three-electrode and two-electrode electrochemical cell design. In an aqueous potassium hydroxide (KOH) electrolyte solution, experiments on cyclic voltammetry (CV), galvanostatic charge-discharge techniques (GCD), and electrochemical impedance spectroscopy (EIS) were conducted at room temperature. The electron transfer studies were performed to study the effect of doping on the electron transfer rate. These findings aid in the strategic design of optimized solid-state supercapacitors, broadening the application of Lanthanum Manganite as a stable and effective electrode material in various electrochemical energy storage systems.

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## Investigation of anisotropic superconducting properties of diagonally grown Fe*T*<sub>x</sub>Se (*T*: Fe, Cr) single crystals via electrical transport measurements

Anil K. Yadav<sup>1\*</sup>, Veg Singh Bhatt<sup>1</sup>, Ajay D. Thakur<sup>2</sup>, C. V. Tomy<sup>3</sup>

<sup>1</sup>Department of Physics, Ch. Charan Singh University Meerut, UP 250004, India <sup>2</sup>Department of Physics, Indian Institute of Technology Patna, Patna 801106, India <sup>3</sup>School of Basic Sciences, Indian Institute of Technology Bombay, Mumbai 400076, India \*Contact: anilphy@ccsuniversity.ac.in

#### *Keywords: Fe*-superconductor, Single crystals, Angular measurements, Anisotropy

Among all iron based superconductors, Fe-11 systems of compounds are simplest in structure as well in compositions. In Spite of exhibiting low transition temperature, these are good candidates to explore superconducting mechanisms in iron based superconducting compounds [1]. Here, we report on the superconducting anisotropy of diagonally grown Fe $T_x$ Se (T = Fe, Cr) single crystals [2,3], as investigated through both conventional and angular magneto-transport measurements. Conventional methods suggest isotropic behavior for these crystals while angular transport measurements reveal presence of anisotropy. Each crystal displays two symmetric dips in the angle-dependent resistivity measurements, in contrast to the optimally superconducting FeSe<sub>0.5</sub>Te<sub>0.5</sub>. A scaling approach was used for the quantitative analysis of anisotropy across all superconductors studied.

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#### Effect of Shell on Suppression of Dielectric Loss and Relaxation Behaviour of PVDF/BaTiO<sub>3</sub>@Al<sub>2</sub>O<sub>3</sub> Polymer Nanocomposites

Sushil Kumar Behera<sup>1</sup>, Maheswar Panda<sup>1,\*</sup>and Dinesh Kumar Shukla<sup>2</sup>

<sup>1</sup>Multifunctional Polymer Nanocomposites Laboratory, Department of Physics, Dr. Harisingh Gour Vishwavidyalaya (A Central University), Sagar, M.P-470003, India.

<sup>2</sup>UGC-DAE Consortium for Scientific Research, Indore, M.P-452001, India.

\*Corresponding Author: mpanda@dhsgsu.edu.in

Keywords: Core-Shell, Dielectric Loss, Impedance and Modulus

Abstract: As purchased PVDF and Synthesized BaTiO<sub>3</sub>@Al<sub>2</sub>O<sub>3</sub> Core-Shell by heteronucleation method were used to synthesize the Cold -pressed PVDF/ BaTiO<sub>3</sub>@Al<sub>2</sub>O<sub>3</sub> Polymer nanocomposite (PNC). The structure/ core-shell microstructures were confirmed through XRD/FESEM/TEM. Due to the cold pressing PVDF spherulites were preserved which led to an increase in the effective dielectric constant and due to the thickened insulating shell layer suppression of dielectric loss~0.04 obtained for the addition of 20 wt% of BaTiO<sub>3</sub>@Al<sub>2</sub>O<sub>3</sub> in PVDF matrix. AC conductivity is well-fitted with Jonscher's power law and modulus spectra show a non-Debye type of broad relaxations with stretching coefficients  $\beta(0.3 \text{ to } 0.41) < 1$ . These PVDF/BaTiO<sub>3</sub>@Al<sub>2</sub>O<sub>3</sub> PNC may be used as a high-performance dielectric materials for next-generation capacitors and other energy storage devices.

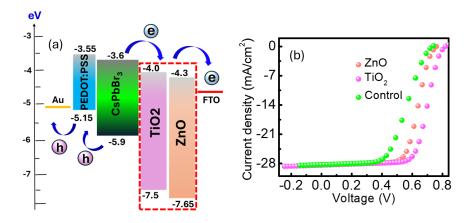
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#### Exploring the Synergistic Photophysical Properties of CsPbBr<sub>3</sub> Nanocrystals with ZnO and TiO<sub>2</sub> Nanoparticles for Advanced Optoelectronic Devices

Priyanka Dubey and Manas Kumar Sarangi<sup>\*</sup> Affiliation Indian Institute of Technology Patna, Bihar, India, 801106 \*Contact: mksarangi@iitp.ac.in

Keywords: Perovskite nanocrystal, Electron transport layer, Hole transport layer, Power conversion efficiency.

The efficiency of optoelectronic devices based on lead halide perovskite nanocrystals (PNCs) is greatly influenced by the rapid and efficient interfacial charge transfer (CT), which significantly boosts energy conversion. This study delves into the CT process in CsPbBr<sub>3</sub> PNCs when paired with ZnO and TiO<sub>2</sub> nanoparticles (NPs), both of which serve as excellent electron acceptors due to their optimal energy level alignment with the PNCs. Through a combination of steady-state and time-resolved spectroscopic techniques, along with current sensing atomic force microscopy, we observe smooth electron transfer (ET) from the P-NCs to both ZnO and TiO<sub>2</sub>. To further highlight the impact of ET on the performance of PNC-based photovoltaic devices, we simulate three device configurations: FTO/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (control), FTO/ZnO/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (with ZnO), and FTO/TiO<sub>2</sub>/CsPbBr<sub>3</sub>/PEDOT:PSS/Au (with TiO<sub>2</sub>). The results reveal a remarkable enhancement in device performance—efficiency, current density, open circuit voltage, and fill factor—when ZnO and TiO<sub>2</sub> are incorporated, surpassing the control device. However, TiO<sub>2</sub> stands out with its superior ET rate, improved electrical conductivity, and overall better device performance, owing to its more favorable energy level alignment with the PNCs. This study underscores the critical role of optimizing interlayer charge transfer to maximize the performance of perovskite-based photovoltaic devices.



**Figure 1:** (a) Energy band alignment of the photovoltaic device and (b) the corresponding current-voltage curve for control device, device with ZnO and TiO<sub>2</sub>.

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#### Magnetism & Superconductivity

## Ni<sub>12</sub>(HPO<sub>4</sub>)<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub>: A compound with coupled frustrated hexagons of alternating ferromagnetic and antiferromagnetic interactions

<u>V. K. Sahu</u>,<sup>1</sup> S. Gayen,<sup>2</sup> K. Boya,<sup>1</sup> V. K. Singh,<sup>1</sup> M. Barik,<sup>3</sup> P Khuntia,<sup>3</sup> S. K. Panda,<sup>2</sup> B. Koteswararao<sup>1,\*</sup>

<sup>1</sup>Department of Physics, Indian Institute of Technology Tirupati, Tirupati-517619 <sup>2</sup>Department of Physics, Bennett University, Greater Noida, 201310, India <sup>3</sup>Department of Physics,Indian Institute of Technology Madras, Chennai, 600036, India \*koteswararao@iittp.ac.in

Category: Poster

Keywords: frustration, hexagonal ring, magnetization, specific heat, DFT

The compounds built by the hexagons, such as honeycomb lattice, are of special interest due to the exciting physics associated with robust quantum fluctuations [1,2]. In this work, we introduced a hexagonal lattice compound with a new kind of magnetic frustration. We present an example of an S = 1 hexagonal spin system where the magnetic frustration comes from the alternating ferromagnetic (FM) and antiferromagnetic (AFM) interactions in the hexagonal ring. We report the synthesis, structural features, and magnetic properties of S = 1 frustrated system Ni<sub>12</sub>(HPO<sub>4</sub>)<sub>6</sub>(PO<sub>4</sub>)<sub>2</sub>(OH)<sub>6</sub> (NPOH) through magnetization and specific heat measurements, along with the theoretical density functional theory calculations. The electronic structure calculations reveal that the hexagonal rings have alternative ferromagnetic ( $J_1$ ) and antiferromagnetic ( $J_2$ ) interactions, along with non-negligible three-dimensional inter-hexagonal ring interactions. The system orders at 61 K despite the presence of strong AFM ( $\theta_{CW} \approx -250$  K) interactions. The frustration parameter, f value, is about 4 (indicating a moderate level of magnetic frustration). The origin of magnetic frustration is due to the incompatible inter-hexagon interactions lead to the magnetic order with moderate magnetic frustration.

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#### Structural and Physical Insights into Rare Earth Iron Garnets

Meghana Mishra<sup>1</sup>, Manjushree Maity, Rakesh Kumar Nayak, Rajeev Singh and Biswanath Bhoi\*

Department of Physics, I.I.T. (BHU) Varanasi, Varanasi - 221005, India

Email of presenting author: meghana.jra.phy24@itbhu.ac.in

\*Email of corresponding author: biswanath.phy@iitbhu.ac.in

Category: Poster

Keywords: Rare Earth Iron Garnets, Microwave & Magneto-optical Devices, Low Damping

Garnet has been a prominent material in scientific research for many years, and its ongoing advancements and broadening applications keep it a central topic of interest for scientists even today. Their unique properties such as low dielectric loss, high resistivity, and low magnetic damping make garnets the material of choice for advanced microwave and magneto-optical devices [1]. This development has triggered renewed scientific interest in exploring the structural and physical properties of Rare Earth Iron Garnets [2] (RIG or  $R_3Fe_5O_{12}$ , R= Y, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu). In this study, we have synthesized a range of RIG using conventional solid state reaction method. The crystallographic structures of the samples were analyzed using an X'pert Pro (PW 3040) X-ray diffractometer, and the Rietveld profile refinement method was employed to confirm the formation of the cubic structure. Room temperature magnetic characterization was carried out using a physical properties measurement system. A comprehensive study of the electrical properties such as capacitance, dielectric constant, dielectric loss, AC conductivity, complex impedance, and modulus was performed on all the samples over a range of frequencies and temperatures using a high-precision LCR meter.

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#### Josephson diode effect in a quantum dot junction

#### Debika Debnath<sup>1</sup>, Paramita Dutta<sup>1</sup>

<sup>1</sup> Physical Research Laboratory, Navrangpura, Ahmedabad–380009, India

We theoretically study the Josephson diode effect (JDE) in a quantum dot (QD)–based Josephson junction (JJ) in the presence of an external magnetic field and Rashba spin-orbit interaction (RSOI). In order to achieve the diode effect in the JJ we break the time-reversal symmetry through the Zeeman field and the inversion symmetry is broken by RSOI. We calculate the Josephson current using the Keldysh nonequilibrium Green's function technique. Our QD with RSOI induces JDE in the heterojunction with a large rectification coefficient (RC) that can be tuned to be as high as 70% by an external gate potential, indicating a giant JDE in our QD junction. Our result also shows that the rectification property could be enhanced with the inclusion of chirality in the QD. Interestingly we find that the sign and magnitude of the RC are highly controllable by the magnetic field and RSOI. We also investigate the role of electronelectron correlation to the Josephson diode by incorporating an interacting QD as the intermediate tunneling medium. Our proposed QD–based Josephson diode (JD) has the potential to be an efficient superconducting device component.

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#### Growth of Low Coercivity Lithium Ferrite Thin Films for Device Applications

Abhishek Kumar<sup>1\*</sup>, Vivek K Malik<sup>2</sup>, Debangsu Roy<sup>1</sup>

<sup>1</sup> Indian Institute of Technology, Rupnagar-1400001, Punjab, <sup>2</sup> Indian Institute of Technology, Roorkee- Roorkee 247667, India

Keywords: Lithium Ferrite, Pulsed Laser Deposition, Ultra-Low Damping, X-ray Reflectivity

#### Abstract:

Lithium ferrite (LiFe<sub>2</sub>O<sub>4</sub>) thin films are increasingly recognized for their potential in advanced electronic and magnetic devices due to their tunable magnetic properties and high chemical stability. This study investigates the growth of lithium ferrite thin films with low coercivity and explores their impact on device performance, particularly focusing on the relationship between coercivity, ultra-low magnetic damping, and ferromagnetic resonance (FMR) properties.

We utilized pulsed laser deposition (PLD) to fabricate lithium ferrite thin films with reduced coercivity. By optimizing key growth parameters, such as deposition temperature, oxygen partial pressure, and post-deposition annealing conditions, we successfully produced films with significantly lower coercivity. Structural characterization, conducted using X-ray diffraction (XRD) and atomic force microscopy (AFM), confirmed that the films possess a well-defined spinel structure, characterized by smooth surfaces and high uniformity.

Magnetic properties were assessed using superconducting quantum interference device (SQUID) magnetometry, revealing a marked reduction in coercivity to approximately 10 Oe. This low coercivity is directly related to the ultra-low magnetic damping observed in the films, a crucial factor that enhances their performance in dynamic applications <sup>1, 2</sup>. Additionally, ferromagnetic resonance (FMR) measurements were performed to further investigate the magnetic dynamics of the films. The FMR data revealed narrow resonance linewidths, indicative of low magnetic damping and high-quality magnetic behaviour. These results highlight the impact of ultra-low damping on reducing energy losses and improving efficiency in devices. The reduced magnetic storage and microwave components. Preliminary findings also indicate significant improvements in device efficiency and response due to the enhanced magnetic properties and reduced energy losses from ultra-low damping and optimal FMR characteristics.

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Physics 2024	
Day-1: 8 <sup>th</sup> December 2024 (Sunday)	
Event	

Time	Day-1: 8 <sup>11</sup> December 2024 (Sunday) Event				
9:00-10:00	Event Conference Registration (Central Lecture Hall)				
10:00-10:40	Inauguration of the Conference (Felicitation by dignitaries, Lighting of lamp, welcome addresses), Venue: LT003				
10:40-11:05	High Tea				
11:05-11:50	Plenary Talk: Prof. S. M. Yusuf				
11:50-12:40	Keynote Talk: Prof A Sriniyasan Director CIT Kokraihar				
12:40-13:30	Session Chair: Prof. S.M. Yusuf Keynote Talk: Prof. Hiroyuki Nojiri, ICC-IMR				
13:30-14:15					
	Parallel Session-A (LT-001) Session Chair: Prof. Surendra Singh	Parallel Session-B (LT-002) Session Chair: Prof. Jayakumar Balakrishnan	Parallel Session-C (LT-003) Session Chair: Prof. Saket Asthana		
Theme	Plasma and Solid-State Physics	Physics of Functional Material	Emerging Area in Solid state Physics		
14:15-14:45	Invited Talk: Prof. Bibhuti Bhusan Sahu IIT Delhi Title: "Advanced magnetron sputtering plasma processes for the control of growth and properties of ITO films"	Invited Talk: Prof. Somnath Chanda Roy IIT Madras	Invited Talk: Prof. Rudra Sekhar Manna IIT Tirupati Title: "Tunning phases with pressure for strongly correlated systems"		
14:45-15:15	Invited Talk: Prof. Subhra Sen Gupta Shiv Nadar Institution of Eminence Title: "The Nature of Eigenstates in Disordered Quantum Many-body Systems and some Special Random Matrix Models"	Invited Talk: Prof. Jitendra Sharma Shri Mata Vaishno Devi University, Katra Title: "Luminescent Nanoparticles and Composites!"	Invited Talk: Prof. Rumi De IISER Kolkata Title: "Stick-slip motion and mechanosensitivity of migrating cells"		
15:15-15:30	Participant: Dr. Rohit Soni IISER Berhampur Title: "Size Effects on Statics and Dynamics of Ferroelectric Domain Walls"	Invited Talk: Prof. Rakesh Joshi UNSW, Sydney	Invited Talk: Prof. R. B. Choudhary IIT(ISM) Dhanbad Title: "Nature-Inspired Viable Electrode Materials for Electrochemical		
15:30-15:45	Participant: Mr. Priyanuj Rajbongshi IIT Tirupati Title: "Topological Properties in a Curved Space-Time Su-Schrieffer-Heeger Model"		Energy Storage Devices"		
15:45-16:00	Participant: Dr. Atikur Rahman NIT Srinagar Title: "Enhancing the hot corrosion resistance of nickel-based superalloy in real service environment via hafnium oxide nano-coating"	Participant: Dr. Jagannath Sutradhar Bar Iian University, Israel Title: "Singlet, triplet, and mixed all-to-all pairing states emerging from incoherent fermions"	Participant: Bibek Ranjan Satapathy INST Mohali		
16:00-16:15		Tea Break			
16:15-17:00	Keynote Talk: Prof. Rajeev Ahuja, IIT Ropar,	Title: "Computational materials science and its application of the second statement of the second se	ations in the area of materials for energy"		
17:00-18.30	Session Chair: A. Srinivasan, Venue: LT003         Young Scientist Award Talks         Session Chair: Prof. Rajeev Ahuja, Venue: LT003         1.       Invited Talk: Prof. Tiantian Zhang         Chinese Academy of Science       Chinese Academy of Science         Title: "Catalogue of topological electronic materials and exploration of topological phonons"       2.         Invited Talk: Prof. Chang Yang Kuo       National Yang Ming Chiao Tug University, Taiwan         Title: "Study of NéMl Vector in Room Temperature Multiferroic BiFeO3"       "				
		3. Invited Talk: Prof. Junzhang Ma City University of Hong Kong			
	Title: "Discovery and	nd Deep Investigation of Novel Quasiparticles in Variou Systems"	us Quantum		
T:	Day-	2:9 <sup>th</sup> December 2024 (Monday)			
Time	Donallel Session A (LT 001)	Event	Parallel Session-C (LT-003)		
	Parallel Session-A (LT-001) Session Chair: Prof. Venkata Kamalakar	Parallel Session -B (LT-002) Session Chair: Prof. Saurabh Basu	Session Chair: Prof. Ashish Arora		
Theme	Semiconductor and Related Area	Quantum Materials and Related Area	Magnetism and Strongly Correlated Electron System		
9:30-10:00	Invited Talk: Prof. Pratap Sahoo NISER Bhubaneswar Title: "Defects-activated CDW and excitonic luminescence in 2D quantum materials"	<b>Invited Talk: Prof. Ravindra Pandey</b> Michigan Technological University, US	Invited Talk: Prof. Kaushik Ghosh INST Mohali Title: "Multifunctional 2D Material- Based Sensors and Energy Harvesting Systems"		
10:00-10:30	Invited Talk: Prof. Jayakumar Balakrishnan IIT Palakkad Title: "Thermal Transport in 2D materials"	Invited Talk: Prof. Kartikeshwar Senapati NISER Bhubaneswar Title: "Signatures of non-reciprocal supercurrent transport across Nb-Pt-Ni-Pt-Nb Josephson junctions"	Invited Talk: Prof. Jyoti Prasad Borah NIT Nagaland Title: "Dipolar Interactions and Magnetic Anisotropy: Key Factors in Optimizing		





		1193103 2027	
			Self-Heating Efficiency for Magnetic Hyperthermia with Rare Earth- Substituted Ferrites"
10:30-11:00	Invited Talk: Prof. Aveek Bid IISC Bangalore Title: "Universality of quantum phase transitions in the integer and fractional quantum Hall regime"	Participant: Priya Kaith NISER Bhubaneswar Title: "Signatures of non-reciprocal supercurrent transport across Nb-Pt-Ni-Pt-Nb Josephson junctions" (15min)	Invited Talk: Prof. Saket Asthana IIT Hyderabad Title: "Cation Substitution-Driven Polar Phase Engineering for High-Energy Storage and Actuator Application in Green Ferroelectrics"
11:00-11:15		Tea Break	i chockettes
	Parallel Session-A (LT-001) Session Chair: <b>Prof. Pratap Sahoo</b>	Parallel Session-B (LT-002) Session Chair: Prof. Kartikeshwar Senapati	Parallel Session-C (LT-003) Session Chair: Prof. Koushik Ghosh
Theme	Semiconductor and Related Area	Quantum Materials and Related Area	Magnetism and Strongly Correlated Electron System
11:15-11:45	Invited Talk: Prof. M Venkata Kamalakar UPPSALA University, Sweden Title: "Exploration of Spin Currents and Orbital Current"	Invited Talk: Prof. Nirmal Ganguly IISER Bhopal Title: "Nonsymmorphic-symmetry-driven quantum materials for technology"	Invited Talk: Prof. Ashish Arora IISER Pune Title: "Novel high-performance differentia magneto-spectroscopy techniques: results and challenges"
11:45-12:15	Invited Talk: Prof. Atindra Nath Pal SNBNCBS, Kolkata Title: "Light-matter interaction driven enhanced photo-response in 2D-0D hybrid"	Invited Talk: Prof. Udo Schwingenschlögl KAUST, Saudi Arabia Title: "Exciton Dissociation by Topological Edge States"	Invited Talk: Prof. Anil Kumar Yadav CCSU, Meerut Title: "Investigation of anisotropic superconducting properties of diagonally grown FeTxSe (T: Fe, Cr) single crystals via electrical transport measurements"
12:15-12:45	Invited Talk: Prof. Subhadeep Datta IACS, Kolkata Title: "Robustness of the Half-metallic Behavior under Disorder in Co2MnAl System"	Invited Talk: Prof. Pawan Kumar Mahatma Gandhi Central University Title: "Impact of Oxygen Vacancy on Dieletric Properties of Ca and Mn co-doped Nanocrystal line Bismuth Ferrite"	Invited Talk: Prof. Sandeep Shrivastava CIT Kokrajhar, Assam Title: "Magnetic Properties of Fe-Pt-Co Ternary Alloys Thin Films"
12:45-13:00	Participant: Dr. Mrityunjay Pandey RWTH Aachen University, Germany Title: "Magneto-phonon Raman spectroscopy of Graphene (C13) encapsulated by Graphene (C12)	Participant: Dr. Pradip Das Guru Ghasidas Vishwavidyalaya, Bilaspur Title: "Topological Nodal Line Features in NiSe Semimetal"	Invited Talk: Prof. S. K. Pandey DRDO Title: "Research opportunities in AR&DB
13:00-13:15	Participant: Dr. Rohit Kumar IIT Bombay Title: "Hyperbolic Phonon Polariton for Molecular Sensing"	Participant: Dr. Geetika Sahu BITS Pilani Hyderabad, Telangana Title: "Growth mechanism of Colloidal MoS2 Quantum Dots: Influence of reaction time and precursor concentration"	
13:15-15:00	Lunch Poster Session (Theme: Topological condense matter, Quantum materials, 2D material Soft condense matter, Analytical tools, Artificial intelligence, and Other emerging areas) Session Chair: Dr. A.D. Thakur and Dr. S. J. Ray Venue: Central Lecture Hall		
	Parallel Session-A (LT-001)	Parallel Session-B (LT-002) Session Chair: Prof. Aveek Bid	Parallel Session-C (LT-003)
Theme	Session Chair: Prof. Ravindra Pandey Strongly Correlated System and Emerging Area of CMP	Energy Materials and Related Topics	Session Chair: Prof. Sandeep Shrivastava Theoretical CMP and Other Emerging Area
15:00-15:30	Invited Talk: Prof. Anupam Kundu ICTS-TIFR, Bangaluru Title: "Restarting can expedite target search"	Invited Talk: Prof. Kaushik Parida IIT Roorkee Title: "Textile-based Wearable Nanogenerators	Invited Talk: Prof. Saurabh Basu IIT Guwahati Title: "Quasiperiodic potential induced
15:30-16:00	Invited Talk: Prof. Saroj Nandi, TIFR Hyderabad	for Next-generation Electronics" Invited Talk: Prof. Sashi Bhushan Singh IISER Berhampur Title: "Utilizing Flexible MXene Composites for Photo- and Piezoelectric- Induced Sur-face Enhanced Raman Scattering"	corner states in a quadrupolar insulator Invited Talk: Prof. Siddhartha Lal, IISER Kolkata Title: "Exploring the patterns of Entanglement within Quantum Matter"
16:00-16:30	Invited Talk: Prof. Sayantan Majumder Raman Research Institute, Bengaluru Title: "Local Rigid Clusters Encode Mechanical Memories in Shear-Jammed Dense Suspensions"	Invited Talk: Prof. Debangsu Roy IIT Ropar Title: "Reconfigurable Spin Logics and High- density Multistate Memory in a Single Spin-orbit Torque Device"	Invited Talk: Prof. Akshay Singh IISC Bangaluru Title: "2D Materials for Quantum and Neuromorphic Technologies"
16:30-17:00	Invited Talk: Prof. Jatis Kumar Dash SRM University Title: "Efficient Photocatalytic Green Hydrogen	Invited Talk: Prof. Manoj Kumar Singh University of Allahabad Title: "Crystal field induced band gap tuning with	Participant: Dr. Chithra H. Sharma Kiel University, Germany (15min)





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	Production using Borophene based Nanostructures under Visible Light"	enhanced energy storage in cobalt modified BiFeO3"	Participant: Habeebur Rahman IIT Roorkee (15min)
17:00-17:30	Invited Talk: Prof. V. Ravi Chandra NISER Bhubaneswar Title: "Resistively detected electron spin	<b>Participant: M. K. Jha</b> (15min) TU, Kirtipur, Nepal	<b>Participant: Dr. Atanu Nandy</b> APC college, Kolkata (15min)
	resonance and g factor in few-layered exfoliated MoS2 devices"	Participant: Dr. Arun Kumar IISER Pune (15min)	Participant: Dr. Sambhunath Bera BML Munjal University (15min)
17:45-19:30	Cultural	program	Venue: Guest House
19:30 onwards		Dinner	
	Day-3	3: 10 <sup>th</sup> December 2024 (Tuesday)	
Time	Parallel Session -A (LT001)	Event Parallel Session -B (LT002)	$\mathbf{D}_{\mathrm{rest}} = \{1, 2, 2, 3, 5, 7$
	Session Chair: Prof. Oleg Tretiakov	Session Chair: Prof. Srimanta Middey	Parallel Session -C (LT003) Session Chair: Prof. Debakanta Samal
Theme	Magnetism and Related Area	Semiconductor, Sensors and Thin Films	Light-Matter Interaction and Photonics
9:30-9:55	Invited Talk: Prof. Neeraj Shukla	Invited Talk: Prof. Aloke Kanjilal	Invited Talk: Prof. Abhishek Kumar
	NIT Patna	Shiv Nadar Institute of Eminence, Delhi	JNCASR, Bangaluru
	Title: "An Overview of Ion Beam Induced	Title: "Opportunities of ZnO@b-SiC based	Title: "Enhancing the performance of
	Ferromagnetic Ordering in 2D Materials:	Memristor for Neuromorphic Computing"	topological photonic devices through
	Experimental and First		artificial intelligence"
0.55.10.20	Principles Investigations"		
9:55-10:20	Invited Talk: Prof. Masashi Tokunaga	Invited Talk: Prof. Archana Tiwari	Participant: Dr. Nilakantha Tripathy
	The University of Tokyo	BHU Title: "Synthesis of Cu/CuO nanoparticles using	INST Mohali
	Title: "Field-induced strongly correlated state in BiSb"	laser ablation: effect of fluence and solvents"	Participant: Mrs. Neha Pandey
10:20-10:45	Invited Talk: Prof. Rohit Ranjan Shahi	Invited Talk: Prof. N. Kamaraju	DAU Indore Invited Talk: Prof. Sumilan Banerjee,
10.20-10.45	CUSB, Gaya	IISER Kolkata	IISC, Bangalore
	Title: "Magnetic Properties of TiFeNi-Based	Title: "Probing Magnetic Ordering in intrinsic	Title: "Quantum oscillations in the
	High Entropy Alloys"	magnetic topological insulator, MnBi2Te4 using	magnetization and density of states of
	8 · · · · · · · · · · · · · · · · · · ·	ultrafast and THz Spectroscopy"	an interacting insulator"
10:45-11:00		Tea Break	
11:00-11:40	K	eynote Talk: Prof. Kwang-Yong, Venue: LT003	
	Parallel Session -A (LT001)	Parallel Session -B (LT002)	Parallel Session -C (LT003)
	Session Chair: Prof. Udo Schwingenschlögl	Session Chair: Prof. Anupam Kundu	Session Chair: Prof. Masashi Tokunaga
Theme	Strongly Correlated System and Emerging Area of CMP	Emerging Area in CMP	Magnetism and Related Area
11:40-12:05	Invited Talk: Prof. Debakanta Samal	Invited Talk: Prof. Srimanta Middey	Invited Talk: Prof. Niharika Mohapatra
	IOP, BBSR	IISC Bangaluru	IIT BBSR
		Title: "Embracing disorder in quantum materials	
12:05-12:30		design"	
12:05-12:30	Invited Talk: Prof. Joydeep Bhattacharjee	Invited Talk: Prof. Tushar Kanti Dey	Invited Talk: Prof. Oleg Tretiakov
	NISER Bhubaneswar	IIT(ISM) Dhanbad	University of New South Wales,
	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter	Title: "Frustrated magnetism in 3d and 5d-based	University of New South Wales, Australia
	NISER Bhubaneswar		University of New South Wales, Australia Title: "Bimerons in Magnetic
12:30-12:55	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter from Geometric Phases of Electrons"	Title: "Frustrated magnetism in 3d and 5d-based triple perovskite materials"	University of New South Wales, Australia Title: "Bimerons in Magnetic Topological Materials"
	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter	Title: "Frustrated magnetism in 3d and 5d-based	University of New South Wales, Australia Title: "Bimerons in Magnetic
	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter from Geometric Phases of Electrons" Invited Talk: Prof. Surendra Singh	Title: "Frustrated magnetism in 3d and 5d-based triple perovskite materials" Invited Talk: Prof. Preeti Bhobe	University of New South Wales, Australia Title: "Bimerons in Magnetic Topological Materials" Invited Talk: Prof. Ajay Tripathy
	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter from Geometric Phases of Electrons" Invited Talk: Prof. Surendra Singh BARC, Mumbai	Title: "Frustrated magnetism in 3d and 5d-based triple perovskite materials" Invited Talk: Prof. Preeti Bhobe IIT Indore	University of New South Wales, Australia Title: "Bimerons in Magnetic Topological Materials" Invited Talk: Prof. Ajay Tripathy Sikkim University, Sikkim Title: "Synthesis of Cu/CuO nanoparticles using laser ablation: effect
12:30-12:55	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter from Geometric Phases of Electrons" Invited Talk: Prof. Surendra Singh BARC, Mumbai Title: "Interface-Driven Magnetization in Isovalent Manganite Heterostructures"	Title: "Frustrated magnetism in 3d and 5d-based triple perovskite materials" Invited Talk: Prof. Preeti Bhobe IIT Indore Title: "Electronic Transport in two-dimensional single crystalline SnSe2"	University of New South Wales, Australia <i>Title: "Bimerons in Magnetic</i> <i>Topological Materials"</i> <b>Invited Talk: Prof. Ajay Tripathy</b> Sikkim University, Sikkim <i>Title: "Synthesis of Cu/CuO</i> <i>nanoparticles using laser ablation: effect</i> <i>of fluence and solvents"</i>
	NISER Bhubaneswar Title: "Distribution of Charge Centers in Matter from Geometric Phases of Electrons" Invited Talk: Prof. Surendra Singh BARC, Mumbai Title: "Interface-Driven Magnetization in Isovalent Manganite Heterostructures" Invited Talk: Prof. Rakesh Kr. Singh,	Title: "Frustrated magnetism in 3d and 5d-based triple perovskite materials" Invited Talk: Prof. Preeti Bhobe IIT Indore Title: "Electronic Transport in two-dimensional single crystalline SnSe2" Invited Talk: Prof. Anurag Sahay	University of New South Wales, Australia <i>Title: "Bimerons in Magnetic</i> <i>Topological Materials"</i> Invited Talk: Prof. Ajay Tripathy Sikkim University, Sikkim <i>Title: "Synthesis of Cu/CuO</i> <i>nanoparticles using laser ablation: effect</i> <i>of fluence and solvents"</i> Invited Talk: Prof. Samrat
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Theme	Magnetism and Related Area	Ferroelectrics and Related Area	Emerging Area in Solid State Physics
16:15-16:30	Participant: Dr. Vinod Ashokan	Participant: Dr. Takumi Kihara	Participant: Dr. Nitin Pratap Singh
	NIT Jalandhar, Punjab	RIIS, Okayama University, Japan	Jaipur National University
	Title: "Many-body correlation effects in quasi		Title: "Role of scattering processes in
16:30-16:45	one-dimensional quantum wire"		lattice thermal conductivity of MgB2"
10:30-10:45	Invited Talk: Prof. Akhyaya Pattnaik VSSUT, Odisha	Participant Dr. M.D. Lokman Ali Pabna University of Science, Bangladesh	Participant Dr. Rakesh Kumar Sahoo
	v 550 i, ouisiu	Title: "Investigation of Grain Boundary	Government Women's College,
		Segregation and Short-Range Chemical Ordering	Sambalpur
		in Multi Principal Element Alloy"	Sunsupur
16:45-17:00	Participant Ms. Purba Dutta	Participant: Dr. Km Swati Rani	Participant Dr. Priyanka Mitra
	IISER Bhopal	Charan Singh University Meerut	BITS Pilani, Hyderabad
	Title: "Rashba-like spin splitting at the interface	<i>Title: "Photoluminescence properties of Eu3+ and</i>	Title: "Enhanced physical properties of
	of Antiferromagnet-WS2 van der Waal	Dy3+ doped SrCO3 nanophosphors synthesized by	BiFeO3-modified Bi4Ti3O12 thin film
	Heterostructure"	hydrothermal method"	prepared by pulsed laser deposition technique for memristor devices"
17:00-17:15	Participant: Dr. Aiswarya Priyambada	Participant: Dr. Rajendra Prasad Giri	Participant Dr. Bhanu Ranjan
11100 11110	KIIT BBSR	IIT(ISM) Dhanbad	IIT Roorkee
		<i>Title: "Unravelling the structure and dynamics of</i>	
		nano-bio interfaces and liquid surfaces	
		by X-ray scattering"	
17:15-17:30	Participant: Dr. M. D. Naiyar Perwez	Participant: Dr. Sweety Supriya	Participant Dr. Pintu Bhatacharya
	R.N. College, Hajipur	LS College, Muzaffarpur	L.N College, Bihar
	Title: "Electron energy in nanowires and	Title: "Cobalt Ferrite as a Promising Material for High-Performance Lithium-Ion Batteries"	Title: "Fermi Level of Intrinsic and
	rectangular nanorods in q-deformed calculus"	ingn-i erjormance Lanuan-1011 Datteries	Extrinsic Semiconductors in q-deformed calculus"
17:30-17:45	Participant: Dr. Debika Debnath,	Participant: Dr. Jyotirekha Mallick	Participant Dr. Pachineela Rambabu
	PRL Ahmedabad	IIT Bombay	GGV, Koni, Bilaspur
	Title: "Josephson diode effect in a quantum dot		Title: "Berry curvature driven
	junction"		Anomalous (Hall, Nernst) effects in half-
			metallic FeRu-CrSi: A first principles
17:45-18:00		Tea Break	study"
18.00-19:00	Evening Ta	alk: Prof. Arun Kumar Grover (Honorary Professor,	PEC)
	-	volution of research in physics in India since circa 185	
			······
		nue: LT003 (Session Chair: Dr. Raghavan K. E.)	·····
	Day	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday)	· · · · · · · · · · · · · · · · · · ·
Time	Day	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall	· · · · · · · · · · · · · · · · · · ·
Time	Day	uue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event	
Time	Day Parallel Session -A (LT001)	uue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002)	Parallel Session -C (LT001) Session Chair: Prof. Samrat
	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee
Time Theme	Day Parallel Session -A (LT001)	uue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002)	Parallel Session -C (LT001) Session Chair: Prof. Samrat
	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>III</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>III</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min)
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>III</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications"	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min)
<i>Theme</i> 9:30-10:00	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications"	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra
Theme	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury IIT Kharagpur	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee
<i>Theme</i> 9:30-10:00	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar       (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur       Title: "Resistive transition and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra
<i>Theme</i> 9:30-10:00	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury IIT Kharagpur	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra IIT Roorkee (15min)
<i>Theme</i> 9:30-10:00	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar       (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur       Title: "Resistive transition and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra IIT Roorkee (15min) Participant: Dr. Goverdhan Reddy Turpu
<i>Theme</i> 9:30-10:00	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar       (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur       Title: "Resistive transition and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra IIT Roorkee (15min) Participant: Dr. Goverdhan Reddy Turpu GGU, Bilaspur
<i>Theme</i> 9:30-10:00 10:00-10:30	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury IIT Kharagpur Title: "Resistive transition and superconductivity in V-doped MgTi2O4 spinel"	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices"	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra IIT Roorkee (15min) Participant: Dr. Goverdhan Reddy Turpu GGU, Bilaspur (15min)
<i>Theme</i> 9:30-10:00	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury IIT Kharagpur Title: "Resistive transition and superconductivity in V-doped MgTi2O4 spinel" Invited Talk: Prof. Devkumar Mahato	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)         Participant: Mr. Atul Kumar
<i>Theme</i> 9:30-10:00 10:00-10:30	Day Parallel Session -A (LT001) Session Chair: Prof. Tusharkanti Dey Strongly Correlated System Invited Talk: Prof. Ashis Nandy (NISER) Bhubaneswar (NISER) Bhubaneswar Invited Talk: Prof. Debraj Chowdhury IT Kharagpur Title: "Resistive transition and superconductivity in V-doped MgTi2O4 spinel"	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan IIT Delhi (15min)	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)         Participant: Mr. Atul Kumar         NIT Patna
<i>Theme</i> 9:30-10:00 10:00-10:30	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IT Kharagpur         Title: "Resistive transition and         superconductivity in V-doped MgTi2O4 spinel"         Invited Talk: Prof. Devkumar Mahato         NIT Patna	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>th</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)
<i>Theme</i> 9:30-10:00 10:00-10:30	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur         Title: "Resistive transition and         superconductivity in V-doped MgTi2O4 spinel"         Invited Talk: Prof. Devkumar Mahato         NIT Patna         Title: "Development of PZT powders and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan IIT Delhi (15min) Title: "Low Lattice Thermal Conductivity-Driven	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)         Participant: Mr. Atul Kumar         NIT Patna         (15min)         Title: "Layered Perovskites type         oxides for transport membrane
Theme         9:30-10:00         10:00-10:30         10:30-11:00	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur         Title: "Resistive transition and         superconductivity in V-doped MgTi2O4 spinel"         Invited Talk: Prof. Devkumar Mahato         NIT Patna         Title: "Development of PZT powders and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>III</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan IIT Delhi (15min) Title: "Low Lattice Thermal Conductivity-Driven Promising Thermoelectric Figure of Merit in NaSrSb and NaBaSb Zintl Phases"	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)         Participant: Mr. Atul Kumar         NIT Patna         (15min)         Participant: Mr. Atul Kumar
<i>Theme</i> 9:30-10:00 10:00-10:30	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur         Title: "Resistive transition and         superconductivity in V-doped MgTi2O4 spinel"         Invited Talk: Prof. Devkumar Mahato         NIT Patna         Title: "Development of PZT powders and         fabrication of multi-layered piezo actuators"	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>In</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan IIT Delhi (15min) Title: "Low Lattice Thermal Conductivity-Driven Promising Thermoelectric Figure of Merit in NaSrSb and NaBaSb Zintl Phases"	Parallel Session -C (LT001) Session Chair: Prof. Samrat Mukherjee Functional Materials Participant: Dr. Chandan Kumar Nagoya University, Japan (15min) Participant: Mr. Rohit Kumar IIT Bombay (15min) Participant: Dr. Kumar Kaushlendra IIT Roorkee (15min) Participant: Dr. Goverdhan Reddy Turpu GGU, Bilaspur (15min) Participant: Mr. Atul Kumar NIT Patna (15min) Title: "Layered Perovskites type oxides for transport membrane application"
Theme         9:30-10:00         10:00-10:30         10:30-11:00	Day         Parallel Session -A (LT001)         Session Chair: Prof. Tusharkanti Dey         Strongly Correlated System         Invited Talk: Prof. Ashis Nandy         (NISER) Bhubaneswar         Invited Talk: Prof. Debraj Chowdhury         IIT Kharagpur         Title: "Resistive transition and         superconductivity in V-doped MgTi2O4 spinel"         Invited Talk: Prof. Devkumar Mahato         NIT Patna         Title: "Development of PZT powders and	nue: LT003 (Session Chair: Dr. Raghavan K. E.) 4: 11 <sup>III</sup> December 2024 (Tuesday) Venue: Central Lecturer Hall Event Parallel Session -B (LT002) Session Chair: Prof. Alpana Nayak Applications of CMP Invited Talk: Prof. Rajan Jha IIT BBSR Title: "Plasmonics and Plexcitonics Systems for Optoelectronic Applications" Invited Talk: Prof. Paramjit Kour, BITS MESRA Title: "Ultralight absorption domination green electromagnetic shielding to protect human tissues and other electronic devices" Participant: Mr. Mohd Zeeshan IIT Delhi (15min) Title: "Low Lattice Thermal Conductivity-Driven Promising Thermoelectric Figure of Merit in NaSrSb and NaBaSb Zintl Phases"	Parallel Session -C (LT001)         Session Chair: Prof. Samrat         Mukherjee         Functional Materials         Participant: Dr. Chandan         Kumar         Nagoya University, Japan         (15min)         Participant: Mr. Rohit Kumar         IIT Bombay         (15min)         Participant: Dr. Kumar Kaushlendra         IIT Roorkee         (15min)         Participant: Dr. Goverdhan Reddy         Turpu         GGU, Bilaspur         (15min)         Participant: Mr. Atul Kumar         NIT Patna         (15min)         Participant: Mr. Atul Kumar         NIT Patna         (15min)         Title: "Layered Perovskites type         oxides for transport membrane





Theme	Ferroelectrics and Strongly Correlated System	Applications of CMP	Emerging Area of CMP
11:15-11:30	Participant: Mr. Tupan Das IIT Patna	Invited Talk: Prof. S. K. Pradhan BITS, Mesra Title: "Tailoring PVDF-Based Composites with PZT	Participant: Dr. Sunil Kumar BRABU, Bihar
11:30-11:45	Participant: Mr. Amod Kumar IIT Patna	and Derived PZT Fillers for Enhanced Dielectric, Ferroelectric, and Piezoelectric Performance in Advanced Sensor Applications"	Participant: Mr. Indranil Maity IIT Patna
11:45-12:00	Participant: Mr. Anant Shukla IIT Patna	Participant: Mr. Gulshan Kumar IIT Patna	Participant: Mr. Subham Sahoo IIT Patna
12:00-12:15	Participant: Mr. Khasti Dutta Pandey IIT Patna	Participant: Mr. Rohit Kumar IIT Patna	
12:15-13:00	Valedictory Session, Venue: LT003		
13:00-14:00		Lunch (Central Lecture Hall)	









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