7th National Conference on Electronic Structure (NCES 2024)

Organisers:

Department of Physics,

SRM University-*AP*

Date: November 21 – 23, 2024

Sponsors:

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SRM UNIVERSITY AP
Andhra Pradesh

Dr. P. Sathyanarayanan
Pro Chancellor

Message

It is with immense pleasure and pride that I extend a warm welcome to each and every one of you to the 7th National Conference on electronic structure (NCES-2024), hosted by SRM University - AP, from 21st - 23rd November 2024 in association with S N Bose centre for Basic Science, Kolkata and Tata Institute of Fundamental Research, Mumbai.

It is astonishing to witness the assembly of eminent speakers, brilliant and outstanding minds and novel and innovative ideas from across the globe under one roof. This conference serves as a top-notch platform for the exchange of valuable knowledge, unparalleled experiences, and breakthrough discoveries in the fascinating field of atomistic-level especially in electronic structure theory.

Our university takes great pride in being at the forefront of research and innovation, and delights by hosting this esteemed conference to underscore our commitment to fostering academic excellence and pushing the boundaries of scientific discovery in the versatile areas of expertise. I would like to express my heartfelt gratitude to the organizing committee, speakers, and all participants for their invaluable contributions in converting this idea of the conference into reality than mere dream.

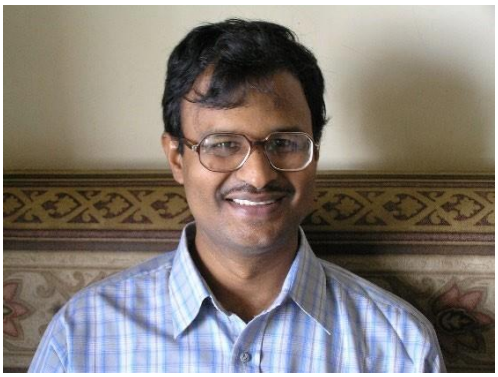
A special word of thanks is due to our esteemed collaborators, and the national conveners, for their unwavering support and involvement in organizing this event. Once again, a warm welcome to SRM University-AP. Let us join hands in embracing the spirit of inquiry, discovery, wisdom, and excellence as we embark on this enlightening journey together.

I wish this fruitful, triumphant and enriching conference will bring a one-of-kind experience to you all.

Warm regards,

Pro Chancellor

Preface by Prof. Kalobaran Maiti



Prof. Kalobaran Maiti
National Convenor

Message

Material research is the key to the technological advances. Recently, there have been additional emphasis on quantum materials, advanced materials, etc. to address the challenges of huge data processing, meet power requirements, green energy, protect environment etc. Electronic structure constitutes the microscopic origin of all material properties. Whether a solid is a metal, semiconductor, insulator, superconductor, magnet or topological material is determined by the properties of electrons and their interactions with varied degrees of freedom. Even the elastic and thermal properties depend on the electronic structure. Electron spectroscopy is one of the major and most important experimental tool to study material properties that will help designing new materials of technological importance as well as resolve long standing fundamental issues.

"National Conference on Electronic Structure – NCES" was conceived in 2016 to discuss experimental and theoretical advances in the fields involving electronic structure and related topics, and brainstorm future developments. This meeting also provides a platform for capacity building via discussion/encouragement of the younger generation from research Institutes, Universities and Colleges. Discuss the opportunities available in terms of accessing various state-of-the-art facilities available worldwide and plan for future mega-projects. It is wonderful to see that we had several highly successful meetings due to active participation of our colleagues and the community has grown significantly - first meeting (NCES 2016) at IOP Bhubaneswar (Toshali Sands), second meeting (NCES 2017) at IISER Bhopal, third meeting (NCES 2018) at SRM University Tamil Nadu, fourth meeting (NCES 2019) at SNBCBS Kolkata, fifth meeting (NCES 2022) at the University of Goa, and sixth meeting (NCES 2023) at IOP Bhubaneswar (Pramod Hotel, Odisha).

On behalf of the national conveners, I thank the local organizers (Prof. Ranjit Thapa and his team), the Director and the administration of SRM University, Amaravati for their splendid job to organize the 7th meeting and keep the spirit of the meeting up. My best wishes for a great success of this meeting and I sincerely hope that the tradition will be continued in the future.

Warm Regards

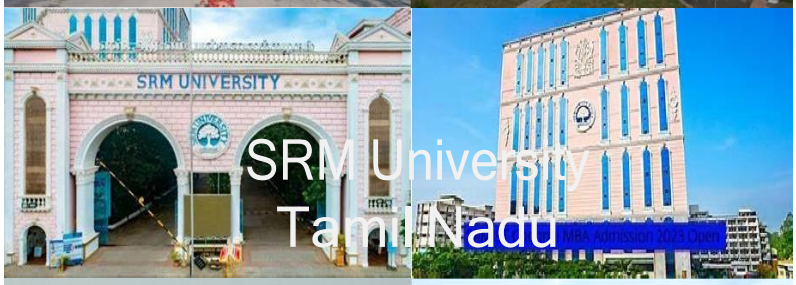
Prof. Kalobaran Maiti

Previous Events

1st NCES in 2016

2nd NCES in 2017

3rd NCES in 2018



4th NCES in 2019

5th NCES in 2022

6th NCES in 2023

Program Schedule

7th National Conference on Electronic Structure (NCES)

Organized by

Department of Physics & Centre for Computational and Integrative Sciences

SRM University – AP, Andhra Pradesh

In association with

Tata Institute of Fundamental Research, Mumbai

S. N. Bose National Centre for Basic Sciences, Kolkata

21- 23 November 2024

21st November, Thursday 2024

Venue: THEATRE, SR Block, SRM University -AP

8.30 a.m. to - 9.30 a.m.: Registration, **Theatre, SR Block**, SRM University-AP

9.30 a.m. - 9.45 a.m.: Inaugural Session, **Theatre, SR Block**, SRM University-AP

Morning Session: 9.45 a.m. – 1:00 p.m.

Session I & II

9.45 a.m. – 10.30 a.m.	**Theatre**	Invited Lecture 1	Prof. E. V. Sampathkumaran	Title: 4f hybridization induced exotic magnetism of Nd based compounds - An unexplored avenue.
10.35 a.m. – 11.05 a.m.	**Theatre**	Invited Lecture 2	Prof. Sugata Ray	Title: Unusual electro-resistance response accompanied by metal-insulator transition in a mixed-valent vanadate
Tea/Coffee Break 20 mints				
11.25 a.m. – 11.55 p.m.	**Theatre**	Invited Lecture 3	Dr. Bahadur Singh	Title: Obstructed atomic insulators: From concept to materials realizations
12:00 a.m. – 12:30 p.m.	**Theatre**	Invited Lecture 4	Dr. Debraj Choudhuri	Title: Volatile resistive-state switching in some titanate-spinel compounds
12:35 p.m. – 1.05 p.m.	**Theatre**	Invited Lecture 5	Dr. Preeti Bhobe	Title: Kondo-like transport and ferromagnetism in Mn substituted Fe2TiSn

20 min. lecture + 10 min. discussion

01. 05 p.m. – 2.00 p.m.: Lunch Break for all participants, In front of SR Block

Afternoon Session: 2.00 p.m. – 5.45 p.m.

Session III

2.00 p.m. – 2.30 p.m.	**Theatre**	Invited Lecture 6	Dr. Indranil Sarkar	Title: Interplay of electronic structure and spin dynamics of Ferromagnet/Nonmagnet interfaces
2.35 p.m. – 3:05 p.m.	**Theatre**	Invited Lecture 7	Dr. Surajit Saha	Title: Can spin-phonon coupling suppress an otherwise expected phase transition?
3.10 p.m. – 3.40 p.m.	**Theatre**	Invited Lecture 8	Dr. Dibyendu Bhattacharya	Title: Operando X-ray Absorption Spectroscopy measurements on energy materials using Indus-2 synchrotron radiation source

20 min. lecture + 10 min. discussion

Tea/Coffee Break 20 mints

Session IV

4.00 p.m. – 4.30 p.m.	**Theatre**	Invited Lecture 9	Prof. Krishna Kumar S R menon	Title: Magnetic domain imaging with magnetostriction: An electron microscopic approach
4:35 p.m. – 5:05 p.m.	**Theatre**	Invited Lecture 10	Dr. Sudipto Kanungo	Title: Berry curvature induced anomalous Hall state in the designed topological heterostructure
5:10 p.m. – 5.40 p.m.	**Theatre**	Invited Lecture 11	Dr. Soma Banik	Title: Electronic band engineering in Co1-xFexSn Kagome semimetal with doping

20 min. lecture + 10 min. discussion

Bus will leave to Red Fox Hotel at 6:00 p.m

Dinner for External Experts and Speakers at Red Fox Hotel

22nd November, Friday 2024

Venue: Theatre, SR Block, SRM University -AP

Session V

Morning Session: 9.30 a.m. – 12.45 p.m.

9.30 a.m. – 10:00 a.m.	**Theatre**	Invited Lecture 12	Prof. Biplab Sanyal	Title: Two-dimensional metallic ferromagnets: fundamental insights fromab initio theory
10.05 a.m. – 10:35 a.m.	**Theatre**	Invited Lecture 13	Dr. Anita Halder	Title: Half-metallic Transport and Spin-Polarized Tunneling in 2D Ferromagnets: Towards 2D
10:40 a.m. – 11.00 a.m.	Tea/Coffee Break 20 mints			

Session VI

11.00 a.m. – 11.30 p.m.	**Theatre**	Invited Lecture 14	Dr. Abir De Sarkar	Title: Sculpting Materials for Self-Powered Electronics
11.35 a.m. – 12.05 p.m.	**Theatre**	Invited Lecture 15	Dr. Krishna Prasad Maity	Electro-optical control of graphene magnetoresistance using ferroelectric substrate
12:10 a.m. – 12:40 p.m.	**Theatre**	Invited Lecture 16	Dr. Tanmoy Das	Title: Fractional and Quasi-Orbitals

20 min. lecture + 10 min. discussion

12:45 p.m to 1:00 p.m Group Photo

1.00 p.m. – 2.00 p.m.: Lunch Break, In front of SR Block

Afternoon Session: 2.00 p.m. – 5.40 p.m.:

Session VII

2.00 p.m. – 2.30 p.m.	**Theatre**	Invited Lecture 17	Dr. Ajay Kumar Shukla	Title: Design, development, and performance of a versatile graphene epitaxy system for the growth of epitaxial graphene on SiC
2.35 p.m. – 3:05 p.m.	**Theatre**	Invited Lecture 18	Prof. Vaitheeswaran	Title: Ferroelectric Properties in Layered Antiferromagnet $Cu(OH)_2$

3.10 p.m. – 3.40 p.m.	**Theatre**	Invited Lecture 19	Dr. J P Rajapandiyan	Title: Surface-enhanced Raman spectroscopy and its applications.

20 min. lecture + 10 min. discussion

Evening Session: 3.40 p.m. – 5.40 p.m.:

Poster session with Tea/Soft drinks in front of SR Block

Four best Poster will be selected by expert panel members

7.30 p.m. – 9.30 p.m.: Banquet Dinner at Lemon Tree Premier, Vijayawada

https://www.lemontreehotels.com/lemon-tree-premier/vijayawada/hotel-vijayawada

Bus will start at 6:00 P.M to venue for Banquet Dinner,

Please wear the conference ID card

23rd November, Saturday 2024

Venue: Tiered Classroom

Session VIII

Morning Session: 9.40 a.m. – 12.35 p.m.

9.40 a.m. – 10:10 a.m.	**Tiered Classroom**	Invited Lecture 20	Dr. Ravi Sankar Singh	Title: Origin of dimensional crossover in quasi-one-dimensional hollandite $K_2Ru_8O_{16}$
10.15 a.m. – 10:45 a.m.	**Tiered Classroom**	Invited Lecture 21	Dr. Jayita Nayak	Title: Electronic Structure and Magneto-transport Properties of Magnetic Topological Materials.
10:45 a.m. – 11.00 a.m.	Tea/Coffee Break 15 mints			

20 min. lecture + 10 min. discussion

Session IX

11:00 a.m. – 11:30 a.m.	**Tiered Classroom**	Invited Lecture 22	Prof. Sudhakar Chandran	Title: Li-Ion Conduction in Grain Boundary-Tailored Solid-State Electrolytes: Local Electronic and Structural Influences—A Case Study
11.35 a.m. – 12.05 p.m.	**Tiered Classroom**	Invited Lecture 23	Prof. Anjan K Gupta	Title: Gate tunable vortex transport regimes in hybrid devices of lead (Pb) and 2D materials
12.05 a.m. – 12.35 p.m.	**Tiered Classroom**	Invited Lecture 24	Dr. Siddhartha Ghosh	Title: Optical and Magnetic Properties of Cr doped CdSe Quantum Dots

20 min. lecture + 10 min. discussion

Overall Discussion and Closing of NCES 2024 and Certificate distribution:

12:35 p.m. to 1:15 p.m.

Lunch Break, In front of SR Block
1:15 p.m. – 2.00 p.m.

Tour – 2:00 to 6:00 p.m. – Durga Temple.

Dinner for external experts and speakers at Red Fox Hotel

Invited Speakers

IL-1

4f hybridization induced exotic magnetism of Nd based compounds – An unexplored avenue

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Abstract: 4f orbital in rare-earths (R) was historically believed to be localized well-within the ionic core. However, certain degree of 4f radial extension beyond the ionic core for the case of Ce systems and consequent 4f-hybridization results in several novel phenomena in condensed matter physics areas, in particular in magnetism, as discovered during the last five decades or so. Though there is now a consensus that the localization of the 4f orbital is gradual as one traverses from La to Gd, anomalous magnetism due to 4f hybridization has not been sufficiently demonstrated for Pr and Nd cases. In this talk, I will overview the status for Nd systems - such a Nd 4f hybridization leading to exceptional magnetism, with a focus on AlB_2- derived ternary hexagonal series, R_2TSi_3 (T= Transition-metals), to bring out the direction of Nd 4f hybridization effects is wide open for exotic properties.

IL-2

Unusual electroresistance response accompanied by metal-insulator transition in a mixed-valent vanadate

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Abstract: Colossal electro resistance (CER) in manganites, i.e., a large change in electrical resistance as a function of varying applied electric field or applied electric current, has often been described as complimentary to the colossal magnetoresistance (CMR) effect. Mixed valence vanadates with active *t*2g and empty *e*g orbitals, unlike manganites, have not naturally been discussed in this context, as double exchange based CMR is not realizable in them. However, presence of coupled spin and orbital degrees of freedom, metal-insulator transition (MIT) accompanied by orbital order-disorder transition, still make the vanadates important. Here we probe a Fe-doped hollandite lead vanadate series PbFe6-*x*V*x*O11 (PFVO), which exhibits a clear MIT as a function of temperature for certain *x* values. Most importantly, a giant fall in the resistivity, indicative of a CER, as well as a systematic shift in the MIT towards higher temperatures are observed with increasing applied current. Detailed structural, magnetic, thermodynamic, and transport studies point towards a complex interplay between the structural distortion, orbital order/disorder effect, and the resultant MIT and magnetic ordering in this system.

1. R. A. Saha et al., Phys. Rev. B **104,** 045149 (2021).
2. S. Halder et al., Int J Ceramic Eng Sci. **4**, 309 (2022).

IL-3

Obstructed atomic insulators: From concept to materials Realizations

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Abstract: A new paradigm for classifying materials according to their band topologies has led to the exciting discovery of topological states of quantum matter [1-2]. Extensive recent high-throughput searchers for topological band structures employing topological quantum chemistry and symmetry-indicators theories have identified many topological nontrivial materials. These topologically nontrivial materials support symmetry-protected metallic boundary modes that reflect the nontrivial winding of their associated bulk states. In this talk, we will introduce obstructed atomic insulators that are topologically trivial but support partially occupied boundary modes with filling anomaly along their specific edges [2]. Taking phosphorene and group-Va monolayers with puckered lattices, we will demonstrate how to identify obstructed atomic insulators within a first-principles framework and how these atomically thin obstructed atomic insulators transition to a state with substantial spin-Berry curvature. We will also discuss a topological phase transition from obstructed atomic insulators to a double quantum spin Hall state with the largest spin-Hall conductivity reported to date [2].

1. B. Singh, H. Lin, A. Bansil, Advanced Materials **35**, 2201058 (2023)
2. R. Verma, S. H. Huang, B. Singh, Phys. Rev. B **110**, 165122 (2024)

IL-4

Volatile resistive-state switching in some titanate-spinel compounds

D. Choudhury[1], A. Rahaman, P. Maji, A. Roy Chaudhuri
[1]*Indian Institute of Technology Kharagpur*
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Abstract: I will discuss some of our experimental results on the volatile resistive state switching in doped $MgTi_2O_4$ spinel system [1]. $MgTi_2O_4$ spinel oxide exhibits a rare concomitant magnetic (spin-singlet), structural and orbital-ordering (tetramer orbital ordering) transition driven by Jahn-Teller active $Ti^{3+}(3d^1)$ ions. In presence of a complimentary Jahn-Teller active ion ($V^{3+}(3d^2)$) doping, V-doped $MgTi_2O_4$ spinel exhibits a rare mixed-valent (containing Ti^{3+}, V^{3+}, Ti^{4+} and V^{2+} ions) ground state [2]. We will discuss the transport results revealing that both V-doped and vacancy-doped $MgTi_2O_4$ exhibits current/voltage -induced breakdown of their Mott insulating state to give way to a low-resistive state in presence of extremely-small threshold electric fields. Further lowering of the threshold fields for resistive-state transition can be realized by suitable tuning of the magnetic ground-state of the $MgTi_2O_4$ spinel by replacing the non-magnetic Mg-site with magnetic Mn^{2+} ions.

1. P. Maji *et al*. [*Manuscript under preparation*]
2. A. Rahaman *et al*. *Phys. Rev. B* **103,** 245145 (2021).

IL-5

Kondo-like transport and ferromagnetism in Mn substituted Fe_2TiSn

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Abstract: The coexistence of Kondo effect and ferromagnetism has typically been noticed with rare earth compounds, such as $UCu_{5-x}Pd_x$, $YbCu_2Si_2$, where strong correlations between localized *f*-electrons and conduction electrons play a crucial role. Interestingly, we have observed this rare phenomenon in a *3d* transition metal-based Heusler alloy, Fe_2TiSn. This $L2_1$ structured composition is an example of nonmagnetic Heusler that shows the heavy fermionic nature with an effective mass ~ 40 m_e. However, its physical properties are significantly affected by the intrinsic antisite disorder between Fe and Ti sites. Here we report our study of the antisite disorder-controlled Mn substituted $Fe_2Ti_{1-x}Mn_xSn$ compositions. The observation of Kondo-like scattering and electron-electron interaction in electrical transport at low temperatures will be discussed. Further, our magneto-transport measurements reveal a dominance of Kondo scattering compared to the electron-electron interaction. Additionally, the magnetic ground state of $Fe_2Ti_{1-x}Mn_xSn$ that can be described as a ferromagnet with wandering axis, consistent with random anisotropy model, will be presented.

1. Kulbhushan Mishra et al., *arXiv:2407.11576* [cond-mat.mtrl-sci]

IL-6

Interplay of electronic structure and spin dynamics of Ferromagnet/Non-magnet interfaces

Indranil Sarkar[1, *]
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Abstract: Heterostructures comprising of ferromagnet (FM) and nonmagnetic metal (NM) interfaces capable are crucial for next-generation ultrafast magnetic switching devices. Therefore, it is imperative to understand the interfacial electronic structure and spin physics of FM/NM heterostructure in juxtaposition to each other. In this talk I shall present examples from our spin polarized electronic structure and magnetization dynamics study on two important class of metallic FM/NM interfaces namely CoFeB/NM and CoFe/Ta. A pedagogical approach will be taken to demonstrate how the interplay of electronic structure of ferromagnetic layer vis-à-vis adjacent non-magnetic layer can be used to control various interfacial spin dynamics and transport parameters such as spin mixing conductance, magnetic damping, spin pumping and interfacial spin chemical potential.

IL-7

Can spin-phonon coupling suppress an otherwise expected phase transition?

Surajit Saha
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Abstract: Spin-phonon coupling in condensed matter systems is one of the most important topics of research having an immediate impact, not only on its fundamental understanding but also on various technological applications targeting the spin-relaxation time in a lattice. Here, for the first time, we experimentally demonstrate that spin-phonon coupling can be detrimental to an otherwise expected (structural) phase transition. We have also supported our observation with extensive theoretical simulations. If we look back at the literature, so far, we have seen various example systems that enhance our knowledge of the fundamentals of spin-phonon coupling. Historically, the coupling between the lattice (phonon) and spin degrees of freedom has been known to promote/trigger structural changes or distortions (i.e., symmetry breaking) in the host system, especially when there is magnetic frustration in the lattice. This is intuitive in nature and there are several examples of such cases, some of which are also reported in recent years [1-6]. Of course, there are also examples where even a large spin phonon coupling does not significantly affect the crystal structure [7-8]. Contrary to these, our study reveals an entirely new phenomenon putting forward a concept, *hitherto* unknown. We show, for the first time, that spin-phonon coupling could also have an effect that can *prevent* an otherwise expected structural transition that too in a system possessing strong magnetic frustration. It is very important to note that in a system where there are multiple ingredients (*viz.*, soft-phonon and strong magnetic frustration) present that can drive a structural phase transition, it rather avoids the expected transition down to low temperatures (~ 2K) due to an onset of spin-phonon coupling and its effect on the soft phonon as well as magnetic frustration. In order to establish this fundamental concept, we have chosen the model system of hexagonal double perovskite structure ($A_2BB'O_6$) - the non-magnetic Ba_2ZnTeO_6 that undergoes a structural (and ferroelastic) transition at ~ 150 K driven by a soft phonon arising from strong phonon anharmonicity [9] while its isostructural counterpart Ba_2NiTeO_6 avoids the phase transition down to low temperatures reported (2K) despite the presence of strong anharmonicity and strong magnetic frustration. We have shown experimentally that spin-phonon couplings develop right around the temperature where short-ranged spin-spin correlations appear with magnetic frustrations. The host lattice (Ba_2NiTeO_6) possesses a very strong phonon anharmonicity (which gives rise to a soft mode in the non-magnetic counterpart Ba_2ZnTeO_6), in addition to the magnetic frustration. As the spin-phonon coupling develops, it affects the phonon anharmonicity of the host lattice which in turn suppresses the instability i.e. the soft mode thus preventing the structural phase transition. We have performed extensive theoretical simulations to support the experimental observations. We believe that this is a unique and profound observation [10] and there are no such examples known to date, to the best of our knowledge. Therefore, we strongly believe that our observation is going to create a renewed thrust on spin-phonon coupling in condensed matter physics.

1. Zhao et al. Nature Communications 13, 2364 (2022),
2. Cazorla et al. Science Advances 3, e1700288 (2017),
3. Garcia-Flores et al. Physical Review Letters 108, 177202 (2012),
4. Lee and Rabe Physical Review Letters 104, 207204 (2010),
5. Shushkov et al. Physical Review Letters 94, 137202 (2005),
6. Bartolome et al. Journal of Magnetism and Magnetic Materials 31,1052-1054 (1983)
7. Calder et al. Nature Communications 6, 8916 (2015),
8. Chen et al. Physical Review B 52, R13130(R) (1995)
9. Badola et al. Physical Chemistry and Chemical Physics 24, 20152 (2022).
10. Badola et al. Physical Review B (Letter) 109, L060104 (2024).

IL-8

Operando X-ray Absorption Spectroscopy measurements on energy materials using Indus-2 synchrotron radiation source

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Abstract: Over the last few years several facilities have been created at the EXAFS beamlines (BL-08 & BL-09) of the 2.5 GeV, Synchrotron Radiation Source (Indus-2) at RRCAT, Indore, India for carrying out *operando* X-ray Absorption Spectroscopy (XAS) measurements. This includes facilities for (i) studying the initial stages of growth of nanoparticles from solution phase (ii) probing the structural changes in catalysts during a catalysis/photo-catalysis or electro-catalysis reaction and also (iii) for probing changes in electronic and geometric structures of electrode materials during the electrochemical reactions of rechargeable Li/Na ion batteries. The results of few such *operando* measurements carried out at Indus-2 synchrotron source on energy materials like Li ion batteries and electrocatalysts for hydrogen generation will be presented here alongwith glimpses of the facilities created [1-6]. *Operando* XAS measurements on (Mn,Ni) co-doped $LiFePO_4$/Carbon (LMNFP/C) cathodes during charging-discharging cycles of Li ion batteries revealed involvement of three principal components during delithiation or charging, LMNFP/C first converts to intermediate L_xMNFP/C phase where x is ~ 0.72, and then converts to MNFP/C. Further, *operando* XAS measurements on Li ion batteries with $MoSe_2$@rGO anode during the 1st discharge/charge cycle provides a detail insight into the intercalation/conversion processes that take place during lithiation/de-lithiation. It has been revealed that during the initial discharge process Li atoms are inserted into the $MoSe_2$ lattice leading to the formation of Li_xMoSe_2 which corresponds to the intercalation reaction mechanism and further Li induction is associated with the conversion reaction mechanism where Mo and Li_2Se are formed. The Li de-intercalation (charging process) shows oxidation of Mo to $MoSe_2$, though the process is found to be not fully irreversible and residual unreacted Mo and Se may lead to capacity fading of the batteries during long cycling. *Operando* XAS measurements at Co and Ni K edges have also been carried out during hydrogen evolution reaction (HER) of water splitting experiments on different phases of Co-Ni bimetallic alloy thin film electrocatalysts deposited on Ni foam substrates. It has been observed from the above studies that for the FCC phase alloy sample (CoNi), both Co and Ni cations participate in the HER, though for the HCP phase sample ($CoNi_4$), Co cations are the major electroactive sites participating in the HER.

1. Abharana N, C. Nayak, K. K. Halankar, S. N. Jha and **D. Bhattacharyya**, Nucl. Instrum. Meth. In Phys. Res. A 969 (2020) 164032.
2. C. Nayak, Abharana N., B. Modak, K. Halankar, S. N. Jha and **D.Bhattacharyya**, Phys. Chem. Chem. Phys., 23 (2021) 6051-6061.
3. Abharana N, K. K. Halankar, Velaga Srihari, Brindaban Modak, S. N. Jha and **D.Bhattacharyya** Sol. St. Ionics 398 (2023) 116270.
4. Abharana N., K.K. Halankar, Ankita Pathak and **D.Bhattacharyya**, J. Alloy & Comp. 976 (2024) 173096.
5. C. Nayak,V. Bhasin, K. K. Halankar, S. Banerjee, A. Bute, S.N. Jha and **D. Bhattacharyya** J. Electroanaltytical Chem. 969 (2024) 118536.
6. C. Nayak, A. Biswas, R.Kumar, S. K. Sarkar and **D. Bhattacharyya** Electrochimica Atca 492 (2024) 14433.

IL-9

Magnetic domain imaging with magnetostriction: An electron microscopic approach

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Abstract: Studying magnetic domains on surfaces and thin films is vital for their fundamental understanding and various applications. Magnetic domain imaging with nanometer resolution is a challenging area with limited options, especially for compensated materials, such as ferrimagnets and antiferromagnets. Here, we develop a new way to image the magnetic domains based on the magnetostrictive lattice facets generated at surfaces using a Low Energy Electron Microscope (LEEM). We demonstrate the antiferromagnetic domain imaging on a prototypical system, Nickel Oxide (NiO), using this method on the surfaces and from the buried interfaces. We show the ability of this method to detect tiny magnetostrictive surface displacements in the picometer length scales and to resolve the detailed twin domain structure. We believe this electron microscopy approach might find applications in different phase transitions in the material systems.

IL-10

Berry curvature induced anomalous Hall state in the designed topological heterostructure

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Abstract: The coupling between topology and magnetism can explore rich physics with fundamental interest. Passing through the phase of Bi-based topological insulators magnetized by the 3*d*/4*f* transition metal doping, currently the fabrication of quantum heterostructures by suitable new-generation 2D materials, has emerged as a prospective alternative. Following the current trends, the present investigation deals with the atomistic designing and investigation of the quantum heterostructures of the newly predicted massive Dirac semimetal and layered ferromagnetic insulator using the first-principles density functional theory calculations supplemented by the low energy tight-binding model Hamiltonian. Proximity effect induces magnetic interactions, breaks the time-reversal symmetry at the interface, and leads to Berry curvature-driven tunable intrinsic anomalous Hall conductance (AHC) at the Fermi energy. Our analysis reveals the electrons with high Fermi velocity (~10^6 m s^{-1}) in the heterostructures and the band topology at the Fermi level can be tuned effectively using very small external gate voltage or homogeneous electric field.

1. Surasree Sadhukhan and Sudipta Kanungo, J. Phys. Cond. Matter **35,** 455601 (2023).

IL-11

Electronic band engineering in $Co_{1-x}Fe_xSn$ Kagome semimetal with doping

Soma Banik
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Abstract: Kagome materials have attracted significant attention due to the topologically protected linear dispersive band with Dirac fermions and dispersionless flat bands in the electronic structure, which leads to novel transport properties and energy-efficient spintronic applications. There has been immense interest in these materials for band engineering, which involves tuning the Dirac fermions and flat bands with doping to achieve enhanced transport properties. In this talk, I will present the results of the electronic structure investigation on $Co_{1-x}Fe_xSn$ kagome semimetal to explain the changes observed in the magnetization and magnetotransport properties. CoSn has Pauli paramagnetism while FeSn has antiferromagnetic ordering. The intermediate compositions in the range $0<x\leq0.4$ showed spin glass behaviour while in the range $0.4\leq x<1$ showed canted antiferromagnetism. Doping Fe in CoSn is like hole doping which is reported to move the flat band close to the Fermi level (E_F), however, the microscopic effect of doping in the electronic states has not been explored. Detailed electronic structure studies have been performed using synchrotron-based photoelectron spectroscopy at ARPES beamline BL-10, Indus-2. Systematic variation in magnetoresistance has been observed for $0<x\leq0.4$ compositions which depends on both the structural changes associated with an increase in the lattice parameters and the electronic modifications associated with the origin of quasilocalized states near the E_F[1]. Antiferromagnetic transition temperature for the compositions $0.4\leq x<1$ was found to increase with the increase in x and has been associated with the decrease in the correlation effects with doping [2]. The density of states showed different natures of localized states with dominating screening effects on the surface and dominating correlation effects in the bulk for the Fe-doped compositions which gives rise to the origin of valence fluctuation, complex magnetism, and topological properties in this system [3]. The change in energy position of the Dirac fermions and the flat bands is attributed to the presence of localized-quasilocalized phenomena which arise due to the interplay between the Coulomb correlation and hybridization. The detailed quantum phenomena of the electronic interactions in the kagome lattice of $Co_{1-x}Fe_xSn$ will be discussed here.

[1] Kritika Vijay, L. S. Sharath Chandra, Kawsar Ali, Archna Sagdeo, Pragya Tiwari, M. K. Chattopadhyay, A. Arya, and Soma Banik, Applied Physics Letters 122, 233103 (2023).
[2] Kritika Vijay, Kawsar Ali, Kranti Kumar, Archna Sagdeo, Ashok Arya, and Soma Banik, Physical Review B, 110, 085163 (2024).
[3] Kritika Vijay, Kawsar Ali, Najnin Bano, Anju Ahlawat, Mukul Gupta, R. J. Choudhary, D. K. Shukla, Ashok Arya, Soma Banik, Unpublished results (2024).

IL-12

Two-dimensional metallic ferromagnets: fundamental insights from ab initio theory

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Abstract: In recent years, the realization of magnetic long-range order in atomically thin 2D materials has shown a big potential in spintronic applications in ultrathin magnets due to the possibility of manipulation of magnetism by external fields, strain or proximity effects in van der Waals heterostructures. Specifically, the family of metallic magnets Fe_nGeTe_2 (n=3, 4, 5) has attracted huge attention due to their high Curie temperatures and intriguing properties. In this talk, I will review the status of this research field, highlighting our own research by ab initio density functional theory, calculations of interatomic exchange interaction parameters and Monte Carlo simulations. A particular emphasis will be given on the systematic study of the electronic structure and magnetism of Fe_nGeTe_2 magnets along with some critical discussions on the importance of electron correlation with the aid of dynamical mean field theory, spin-orbit coupling and effects of transition metal doping. Finally, some results on the spin-polarized quantum transport will be shown for PtTe2/Fe4GeTe2/PtTe2 van der Waals heterostructures.

[1] S. Ghosh, S. Ershadrad, V. Borisov, B. Sanyal, *npj comp. mat.* **2023**, *9*, 86-101.
[2] S. Ershadrad, S. Ghosh, D. Wang, Y. Kvashnin, B. Sanyal, *J. Phys. Chem. Lett.* **2022**, *13*, 4877-4883.
[3] S. Ghosh, S. Ershadrad, B. Sanyal, *2D materials* **11** 035002 (2024)
[4] M. Davoudiniya, B. Sanyal, Nanoscale Advances (2024)
[5] R. Ngaloy et al., ACS Nano 18, 5240 (2024)

IL-13

Half-metallic Transport and Spin-Polarized Tunneling in 2D Ferromagnets: Towards 2D Spintronics

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Abstract: In recent years, the discovery of ferromagnetic two-dimensional (2D) van der Waals (vdW) materials, particularly FenGeTe2 (FGT) [1] (n = 3–5), has attracted significant attention for potential spintronic applications due to their high Curie temperatures. Using density functional theory (DFT) and Nonequilibrium Green's Function (NEGF) methods, we investigate the spin-dependent transport properties of Fe4GeTe2 (FGT4). Our findings [2] reveal that the conductance exhibits remarkably high spin polarization (SP), attributed to the unique half-metallic nature of the band structure along the direction perpendicular to the 2D vdW layer. Notably, this high SP remains robust when transitioning from the bulk material to a single layer interfaced with model Au electrodes. Furthermore, we observe a substantial spin-polarized current whenthe system is driven out of equilibrium under significant bias. Importantly, this spin-dependent transportis largely unaffected by the presence of spin-orbit coupling and electron-electron correlation effects. The spin-filtering capability of monolayer FGT4 provides a promising opportunity for designing magnetic tunnel junctions (MTJs) using 2D vdW materials, offering high tunnel magnetoresistance (TMR). Our study demonstrates that an MTJ device employing model Au electrodes, with the vdW gap serving as an insulating barrier between two FGT4 layers, can achieve a TMR of nearly 500%. Additionally, we extend our analysis [3] to other materials in this family, such as Fe3GaTe2. Our findings show that all these compounds exhibit strong spin-filtering properties, stemming from their unique electronic structures along the transport direction. This creates the possibility of designing MTJs using two different vdW ferromagnets, which could facilitate easier switching of the magnetization direction due to their differing magnetic anisotropy. We anticipate that these findings will inspire further theoretical and experimental efforts to design more practical spintronic devices, replacing conventional ferromagnets with 2D vdW materials.

[1] Z. Fei et al. Nat. Mater. **17**, 778 (2018).
[2] A. Halder, D. Nell, A. Sihi, A. Bajaj, S. Sanvito, A. Droghetti. Nano Letters **24**, 30 (2024).
[3] A. Halder, D. Nell, A. Bajaj, S. Sanvito, A. Droghetti. (Under Preparation)

IL-14

DFT perspectives on piezoelectricity and spin-orbitronics in selected functional 2D materials

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Abstract: Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of materials. HfN_2 monolayers [1] exhibit valleytronic properties complementary to that in single-layer MoS_2, while the merger of spin (valley) Hall effect with the Rashba effect is observed in h-NbN, h-TaN and monolayers screened via high throughput studies [2, 3]. Out-of-plane piezoelectricity is induced at the interfaces of 2D semiconducting planar monolayers, which show in-plane piezoelectricity individually and zero out-of-plane polarization/piezoelectricity, such as GaN and boron monophosphide (BP) monolayers. The understanding reached in GaN/BP van der Waals heterobilayers (vdWHs) has been reinforced on MoS_2/BP and MoSSe/BP vdWHs. Experimental verification of these theoretical predictions is encouraging. The origin of negative piezoelectricity at the interfaces of 2D dialkali oxide and chalcogenide monolayers has been elucidated [4] together with strain tunability in ultrahigh shear piezoelectricity in superflexible non–van der Waals graphitic ScX monolayers (X = P, As, Sb) [5]. Conflux of ferroelectricity, ferroelasticity and large in- plane piezoelectricity is noted in AlXY (X=S, Se; Y=Cl, Br, I) monolayers [6]. Last but not least, intrinsic carrier mobility estimation via several models in selected 2D materials can be discussed, as mobility plays a crucial role in determining the performance of electronic devices [7].

1. M. K. Mohanta, A. De Sarkar, Phys. Rev. B, 102, 125414 (2020).
2. A. Arora, S. Sharma, A. De Sarkar, J. Appl. Phys., 136, 124301 (2024).
3. R. Ahammed, A. De Sarkar, Phys. Rev. B, 105, 045426 (2022).
4. A. Arora, A. Rawat, A. De Sarkar, Phys. Rev. B, 107, 085402 (2023).
5. H. Seksaria, A. Kaur, A. De Sarkar, Phys. Rev. B, 108, 075426 (2023).
6. N. Tripathy, A. De Sarkar, Phys. Rev. B, 109, 125414 (2024).
7. A. Arora, A. De Sarkar, Appl. Phys. Lett. 124, 082101 (2024).

IL-15

Electro-optical control of graphene magnetoresistance using ferroelectric substrate

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Abstract: The charge transport in graphene is strongly influenced by the environmental sensitivity of its π-electrons. Using ferroelectric materials as gate substrates enhances charge doping in the semiconducting channel due to their inherent electrical polarization. In this presentation, I will discuss how both electrical and purely optical methods can be employed to modify the magnetoresistive response of CVD-deposited graphene through electrostatic interactions with a photoferroelectric substrate. Electrically, switching the ferroelectric polarization can alter graphene's magnetoresistance by up to 67%, driven by a shift in the Fermi level and associated changes in charge mobility. Similarly, this control can be achieved optically through light irradiation with energy exceeding the substrate's bandgap, leveraging the photovoltaic effect. Additionally, an all-optical approach enables the reversible modulation of graphene's magnetoresistance and magnetic control over its transconductance. These insights expand the use of photoferroelectric control in 2D materials to magnetic applications, advancing wireless functionalities for sensors and field-effect transistors.

IL-16

Fractional and Quasi-Orbitals

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Abstract: Fractional particles do not exist individually but are entangled among themselves or coupled to emergent gauge fields. Similarly, quasi-particles are excitations of the many-body wavefunctions that are restricted to follow single-particle statistics. Obtaining their local orbital description is challenging. In this talk, I introduce a systematic method for constructing low-energy lattice models that capture the dynamics of these exotic orbitals. Unlike traditional ad-hoc geometric approaches, our method systematically eliminates high-energy states through virtual hopping, deriving the super exchange-like one-body (gauge) potential. We apply the theory to study Majorana orbitals in the Kitaev spin model and Bogolyubov orbitals in superconductors. We introduce a gauge-invariant mean-field theory for interacting Majorana/Bogolyubov particles, resulting in correlation-induced (fractional) Chern insulators

IL-17

Design, development, and performance of a versatile graphene epitaxy system for the growth of epitaxial graphene on SiC

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Abstract: The realization of graphene, a single-atom-thick sheet of carbon atoms arranged in a hexagonal lattice, ignited immense interest due to its extraordinary electrical, mechanical, and thermal properties, promising a diverse range of applications. Graphene has emerged most studied quantum material over the years. However, conventional methods like micromechanical exfoliation, while yielding high-quality graphene, faced limitations in scalability and reproducibility. Chemical vapor deposition, though cost-effective, presented challenges in achieving large-area, high-crystallinity graphene and required transfer to target substrates. Epitaxial graphene (EG), grown directly on silicon carbide (SiC) by high-temperature Si sublimation, emerged as a solution, offering large-area, single-crystalline graphene seamlessly integrated with the substrate, thereby overcoming the limitations of previous methods. A versatile graphene epitaxy (GrapE) system has been engineered to facilitate the growth of EG on SiC under diverse environmental conditions, ranging from high vacuum to atmospheric argon pressure. Leveraging radio-frequency induction heating, the GrapE system achieves temperatures up to 2000 °C with precisely controlled ramp rates as high as 200 °C/s. The details of critical design aspects and temperature characteristics of the GrapE system will be discussed. This automated platform has enabled the growth of high-quality EG monolayers and turbostratic EG via various methodologies, including confinement-controlled sublimation (CCS), open configuration, polymer-assisted CCS, and rapid thermal annealing. The quality and structural characteristics of the synthesized EG were rigorously assessed using atomic force microscopy, Raman spectroscopy, and low-energy electron diffraction, confirming the versatility and efficacy of the GrapE system in producing high-quality EG.

1. Rev. Sci. Instrum. **95**, 063901 (2024)

IL-18

Ferroelectric Properties in Layered Antiferromagnet $Cu(OH)_2$

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Abstract: Ferroic orders and their structural phase transitions play a key role in elucidating numerous unconventional phenomena in condensed matter systems. Our study examines the polymorphic ferroelectric phase transitions of Copper(II) hydroxide, $Cu(OH)_2$, considering its antiferromagnetic ground state. Through the first-principles studies and group theory analysis, we have provided a systematic theoretical investigation of vibrational properties in the hypothetical *Cmcm* high-symmetry phase to identify the symmetry-allowed ferroic phases. We identified a non-polar to polar ($Cmc2_1$) phase transition, in which the displacive transformation is primarily responsible for the phase change induced by two B_{1u} (i.e. Γ^-_2) phonon modes within the centrosymmetric phase. The two polar structures have the same space group with different atomic arrangements. These structures correspond to different degrees of polarization (i.e. P_s = 3.06 μC·cm^{-2} and P_s = 42.41 μC·cm^{-2}), emerging from the parent high symmetry structure. The structure corresponding to phonon branch-3, at Γ, matches with experimentally determined polar structure which is not the ground state and possess polarization of 42.41 μC·cm^{-2}. Here ferroelectricity is geometric by nature and is driven by the Γ^-_2 mode in which the O- and H-sites displacements lead the polar distortion with a minor contribution from the Cu-sites. Interestingly, the $3d^9$:Cu^{2+} Jahn–Teller distortion coupled with the orientational shifts of O–H atoms enhance the polarization.

IL-19

Surface-enhanced Raman spectroscopy and its applications

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Abstract: Surface-enhanced Raman scattering (SERS) is a powerful vibrational spectroscopic technique that can offer chemical and structural information about the adsorbed molecules on plasmonic nanostructures (Ag, Au, or Cu).[1] In this talk, I will introduce the fundamentals of SERS and different types of SERS substrates. In particular, how SERS technique can be used for surface analysis of materials.[2,3] Moreover, selected applications of SERS and SHINERS in energy materials will be discussed.[2] Finally, the future directions of SERS technique will be explained in detail.[4]

1. Panneerselvam, R. et al. Chem. Commun. 54, 10–25 (2018).
2. Ding, S.-Y. et al. Nat. Rev. Mater. 1, 16021 (2016).
3. Zhang Y. J. et al., J. Phys. Chem. C, 120, 37, 20684–20691, (2016).
4. Wang H. L. et al., Light: Science & Applications, 10, 161, (2021).

IL-20

Origin of dimensional crossover in quasi-one-dimensional hollandite $K_2Ru_8O_{16}$

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Abstract: Electronic dimensionality has dramatic consequences on the ground state of the interacting electron systems. Owing to the strong correlation in one-dimensional (1D) systems, a metallic system is described by the Tomonaga-Luttinger liquid (TLL) theory instead of the Fermi-liquid theory. The TLL state has been experimentally observed in quantum wires, carbon nanotubes, *etc*. In quasi-1D materials, the transverse / interchain electron hopping plays a decisive role in their properties. These interactions can induce a transition from a 1D electronic behaviour to a 3D electronic behaviour, *i.e.* a dimensional crossover as observed in several quasi-1D materials. The understanding of such crossover has been subject of research interest. In this talk, I will present our results on the electronic structure of quasi-1D hollandite $K_2Ru_8O_{16}$. We highlight the importance of electron correlation on the electronic structure and unravel the dimensional crossover using high resolution photoemission spectroscopy and theoretical framework within density functional theory combined with dynamical mean-field theory.

IL-21

Electronic structure and magneto transport properties of magnetic topological materials

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Abstract: The quest for magnetic topological systems attracts large interest and is the most interesting research topic in the field of topological materials. It is important for both fundamental research (merging the topological matter with magnetism) and possible applications in spintronics. We have investigated MnSb8Te13 and MnSb12Te19, members of the MnSb2nTe3n+1 family by magneto-transport techniques, theory and angle resolved photoelectron spectroscopy, good candidates for the ferromagnetic topological material. The magnetic susceptibility experiments identify pronounced ferromagnetic transitions at temperatures T1 = 22 K, T2 = 12.9 K, and T3 = 4 K in MnSb8Te13. The Hall resistivity measurements indicate the hole-dominated behavior, which was also confirmed by ARPES measurements. Density functional theory calculations demonstrate that MnSb8Te13 is a ferromagnetic topological insulator with termination- dependent surface states. However, magnetic measurements indicate weak ferromagnetism due to the deficiency of Mn atoms and the disorder within the sample [1]. Interestingly, magnetic susceptibility experiments in MnSb12Te19, identify ferromagnetic transitions at temperature Tc =18.7 K, consistent with heat capacity measurements (T=18.8 K). The anomalous Hall effect (AHE) is observed for the field along the c-axis below Tc. Shubinikov-de-Haas (SdH) oscillations provide evidence for Dirac fermions with π Berry phase. MnSb12Te19 exhibits an FM ground state along with AHE, and hole-dominated transport properties consistent with ARPES measurements [2].

[1]. Magnetotransport and electronic structure of the axion insulator MnSb8Te13, Mohit Mudgal, Debasis Dutta, Priyanka Meena, Venkateswara Yenugonda, Vishnu Kumar Tiwari, Vivek Kumar Malik, Jens Buck, Sanjoy Kr Mahatha, Amit Agarwal, and **Jayita Nayak**, ***Phys. Rev. B* 110**, 045124 (2024).
[2]. Magnetotransport and angle-resolved photoemission spectroscopy of MnSb12Te19: a new member of MnSb2nTe3n+1 family, Mohit Mudgal, Priyanka Meena, Vishnu Kumar Tiwari, Venkateswara Yenugonda, Vivek Kumar Malik, Jens Buck, Kai Rossnagel, Sanjoy Kr Mahatha and **Jayita Nayak**, **JPCM 36** 50LT01 (2024).

IL-22

Li-Ion Conduction in Grain Boundary-Tailored Solid-State Electrolytes: Local Electronic and Structural Influences—A Case Study

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Abstract: Understanding lithium-ion dynamics in solid electrolytes is crucial for enabling its application in solid state batteries. By using samples processed via conventional isothermal sintering (CIS) and spark plasma sintering (SPS) the role of defect-rich grain boundaries (GB) in $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ [LATP] solid electrolytes are examined. Using X-ray absorption spectroscopy (XAS) and electron energy loss spectroscopy (EELS), we identify local electronic and structural changes in the GB region. Results reveal distinct spectral features linked to octahedral symmetry and oxidation states, with LATP-SPS exhibiting higher Li content and enhanced ionic conductivity ($\sigma_{gb,300K}$ ~$1.36 10^{-3}$ S/cm) compared to LATP-CIS ($\sigma_{gb,300K}$ ~$3.84 10^{-5}$ S/cm). Molecular dynamics study performed on different crystallites indicates higher ionic migration in the case of an amorphous grain boundary due to increased lithium resulting from bond breakage. The study underscores the critical role of GB structural distortion in influencing Li-ion transport properties.

IL-23

Gate tunable vortex transport regimes in hybrid devices of lead (Pb) and 2D materials

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Abstract: Josephson junction (JJ) arrays with tunable junction parameters are valuable model systems for investigating vortex dynamics and quantum phase transitions in granular superconductors (SCs) and high-Tc SCs. I plan to begin with our recent works on gate tunable transport in a hybrid device of lead (Pb) and graphene that leads to Josephson coupled Pb islands on graphene due to poor wettability of Pb on graphene. At zero magnetic field, a crossover between a vortex-ineraction and vortex-pinning dominated regimes with cooling below the superconductivity onset in Pb at 7 K is found. The former regime is described using Berezinskii-Kosterlitz-Thouless (BKT) physics while the latter fits well with Ambegaokar-Halperin model of thermally activated phase slips or vortex depinning. The gate tunability arises from the gate-voltage control on the temperature-dependent Josephson coupling EJ between the Pb-islands. While above the crossover temperature TX the inter-vortex interaction dictates the dissipation while below TX, the dynamics of the free vortices, existing due to a distribution in EJ, in this disordered JJ array is dicated by the depinning physics [1]. The magetotransport is shows a field dependent critical temperature described by Werthamer-Helfand-Hohenberg (WHH) theory at low fields which goes through different vortex regimes. Near the upper critical field a gate-dependent quantum critical point is found where the finite-size scaling analysis indicates that this transition falls within the (2 + 1)D-XY universality class and without disorder [2]. If time permits I shall also try to discuss some of the results on MoS2-Pb hybrid system where a superinsulator regime is found.

1. Suraina Gupta , Santu Prasad Jana , Rukshana Pervin, and Anjan K. Gupta, Phys. Rev. B110, 024506 (2024).
2. Suraina Gupta , Santu Prasad Jana , Rukshana Pervin, and Anjan K. Gupta, Supercond. Sci. Technol. 110, 115027 (2024).

IL-24

Optical and Magnetic Properties of Cr doped CdSe Quantum Dots

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Abstract: Substitution of semiconductor quantum dots (QDs) by a small number of transition-metal ions having magnetic properties gives rise to magnetic doped semiconductor. With the balance of optical and magnetic properties, these magnetic semiconductors are widely used in spintronics, bio-imaging and magnetic resonance imaging (MRI) applications. To facilitate their usage in bio applications, it is critical to synthesize water soluble magnetic QDs with stabilized structure while maintaining their optical and magnetic properties. Here in our work, we developed a facile substituted synthetic route to achieve Cr doped CdSe (Cr-CdSe) via a facile hydrothermal method. The effects of doping on the structural, optical, and magnetic properties of the Cr-CdSe were studied using X-ray diffraction, UV-Visible spectroscopy, photoluminescence lifetime. We then explored their chemical nature and morphology change with increase in doping concentration via X-ray photoelectron spectroscopy and transmission electron microscopy. Water soluble QDs have been used as a bio-imaging probe for the past few decades due to their strong fluorescence, photostability and improved tissue or cellular penetration. However, incorporating magnetic material into fluorescent entity harnesses the ability to control strengths of both modalities that enhance the diagnostic accuracy and facilitate its application in bio-systems especially in early accurate diagnosis. Finally, we demonstrate the competency of Cr-CdSe as a dual imaging probe with fluorescent cellular.

Poster Participants

Electronic structure of layered nickelates using density functional theory calculations

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Abstract: Ruddlesden-Popper series of lanthanum nickelates, $La_{n+1}Ni_nO_{3n+1}$ are made up of n conducting perovskite layers ($LaNiO_3$) separated by insulating rock-salt layers (LaO) along the crystallographic *c*-axis. We study the electronic structure of this series for n = 1, 2, 3 and ∞ using density functional theory (DFT) and (DFT+*U*). We focus our study on understanding the evolution from an antiferromagnetic insulating state for n = 1 to a paramagnetic metallic state for n = ∞. We present the detailed computational results on the electronic structure to understand the role and interplay of dimensionality, crystal structure, and electron correlation in these systems.

Manifestation of incoherent-coherent crossover and non-Stoner magnetism in the electronic structure of Fe_3GeTe2

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Abstract: Two-dimensional (2D) van der Waals ferromagnets have gained enormous interest due to their potential applications as next-generation spintronic devices and provide a platform to explore the fundamental physics behind 2D magnetism. With Curie temperature of about 220 K, ferromagnetic Fe_3GeTe_2 having layered structure exhibits highly-anisotropic electronic and magnetic properties, persisting down to the monolayer limit. Here, we present the temperature evolution of electronic structure of Fe_3GeTe_2 using high-resolution photoemission spectroscopy in conjunction with density functional theory and dynamical mean field theory and further provide substantial evidence for non-Stoner magnetism. We unveil the appearance of quasiparticle peak and its evolution in the vicinity of Fermi energy, and empirical evidence of incoherent-coherent crossover at around 125 K. Interestingly, an increase in vacancy at Fe sites leads to suppressed transition temperature. Moreover, substitution of other 3*d* transition metals at the place of Fe leads to considerable change in its magnetic as well as electronic properties, for example, Ni_3GeTe_2 is paramagnetic down to lowest temperature measured. Hence, we also present the effects of cobalt doping on the electronic structure of ferromagnet Fe_3GeTe_2.

Correlated surface states in Dirac semimetal NiTe2

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Abstract: Here we investigate the electronic structure of 1*T* $NiTe_2$ using angle resolved photoemission spectroscopy in conjunction with *ab initio* results. Bulk electronic structure probed using *x*-ray photoemission spectroscopy could be efficiently captured within density functional theory. Angle resolved photoemission spectroscopic measurement exhibits anisotropic Fermi surface and suggests that the type-II bulk Dirac point appears in close vicinity of Fermi energy. Band dispersion along with three-fold bulk Fermi surface could also be well captured within density functional theory. Surface state at the Fermi level were observed along Γ-*M* direction forming six-fold symmetric Fermi surface. Interestingly Dirac cone formed by the surface states at Γ point much below the Fermi level was found to be at higher binding energy than estimated from the calculated surface band structure within density functional theory. We show that the correlation effects at the surface are enhanced and are important to understand the surface state in this topological system. We also study the role of disorder and spin orbit coupling on the electronic structure of other 1*T* type *M*TeSe (M = Ni, Rh, Pd, Pt).

Probing the Magnetic Ground State of Ba2YIrO6: Impact of Nonmagnetic Dopants and Spin-Orbit Coupling

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Abstract: Strong spin-orbit coupling (SOC) in iridates has long been predicted to lead to exotic electronic and magnetic ground states. Ba2YIrO6 (BYIO) has attracted particular attention due to the expectation of a Jeff = 0 state for Ir5+ ions under the jj-coupling scheme. However, controversies surround the actual realisation of this state, as finite magnetic moments are consistently observed experimentally. We explore the effects of nonmagnetic Sb^{7+} doping in place of Ir^{7+} in Ba2YIrO6, which was supposed to form resonating valance bond singlets. Despite similar charge and ionic radii, Sb^{7+} doping appears highly inhomogeneous, coexisting with a fraction of nearly pure BYIO regions, as confirmed by X-ray diffraction (XRD). Remarkably, even minor Sb^{7+} doping (10–20%) results in increased magnetisation, indicating the breakdown of dynamic singlets formed by magnetic Ir ions in BYIO. The steady rise in magnetisation with higher Sb^{7+} content challenges the expected Jeff = 0 states

and suggests the persistence of individual $Ir7^{+}$ moments. These findings indicate that SOC in BYIO may not be strong enough to be fully described by the jj-coupling scheme, prompting further exploration of its electronic and magnetic properties.

Synergistic effects of strain and vacancy on electronic and magnetic properties of single-layer Chromium Tri-iodide

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Abstract: Strain and defects are two important tools to tune the physical properties of materials. In general, the effects are dominant in low-dimensional systems, such as one-dimensional nanotube, two-dimensional (2D) graphene-like monolayers. The combination of strain and vacancy can also lead to interesting properties in a material. Chrromium tri-iodide (CrI3) monolayer is the first experimentally discovered 2D ferromagnetic material and attracted much attention due to its potential use in spintronics applications. In this work, we use first-principles calculations to study the synergistic effects of vacancy and biaxial strain on the electronic and magnetic properties of the ferromagnetic CrI3 monolayer. We considered the different possible vacancies, namely I, Cr, CrI3, and CrI6 along with applied biaxial stain (both compressive and tensile) ranging from -4% to +4% in steps of 2%, on the CrI3 monolayer. We observed that the magnetic moment is retained in the defective structures and are robust under applied external strain in all four vacancies, while at the same, the band gap of the system can be tuned via external applied strain.

Stain induced evolution of band edge alignment and excitonic lifetime in vdW heterostructure: A case study of CrMo3S8/CrW3S8

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Abstract: In this study, we present the first-principles calculations to investigate the excitonic properties and band edge alignment of the CrMo3S8/CrW3S8 van der Waals heterostructure, with a particular focus on the impact of strain. Firstly, Density functional theory (DFT) based first-principles electronic

structure calculations is conducted on the heterostructure, enabling us to examine the band edge alignment. Due to the crucial role of excitonic effects in optoelectronic devices we calculate the exciton energies and its strengths by GW-Bethe Salpeter Equation (BSE) method. This information allows us to further determine the exciton radiative lifetime. The influence of lateral strain on the heterostructure is then systematically explored.We analyse how strain modifies the band edge alignment, potentially altering the charge transfer dynamics. Additionally, we examine the strain-induced changes in exciton radiative lifetime. The ability to predict and control radiative lifetimes in these 2D materials through strain offers promising avenues for their application in solar energy conversion and other optoelectronic technologies. By understanding the interplay between strain, band alignment, and excitonic behaviour, we aim to contribute to the development of advanced, tunable devices based on van der Waals heterostructures.

1. Marco Bernardi, Maurizia Palummo, and Jeffrey C. Grossman*, Extraordinary Sunlight Absorption and One Nanometer Thick Photovoltaics Using Two-Dimensional Monolayer Materials, Nano Letters (2013)
2. Maurizia Palummo, Marco Bernardi,and Jeffrey C. Grossman,Exciton Radiative Lifetimes in Two-Dimensional Transition Metal Dichalcogenides, Nano Letters (2015)
3. Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Dimple, Raihan Ahammed, and Abir De Sarkar,Interfacing Boron Monophosphide with Molybdenum Disulfide for an Ultrahigh Performance in Thermoelectrics, Two-Dimensional Excitonic Solar Cells, and Nanopiezotronics, ACS 2019

Ion Migration in Halide Perovskites: Pathways to Neuromorphic Memristive Devices

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Abstract: Neuromorphic computing requires low-energy, highly parallel systems that surpass traditional CMOS (Complementary Metal–Oxide Semiconductor) circuits in complexity and efficiency. Halide perovskites, with their ability to handle both ions and electronic charges, are found to emerge as promising candidates for such computing systems, offering unique switching behaviours ideal for neuromorphic hardware [1, 2]. Ion migration, a key mechanism in these materials, can be controlled by adjusting the cation size and configuration in the perovskites, allowing for tuneable energy barriers and reliable memristive switching. This makes halide perovskites suitable for creating artificial synapses and neurons, which opens new possibilities for adaptive computing networks. By modifying the type or arrangement of cations in the perovskite, the migration of halide ions can be controlled, thereby tuning the energy barriers for this migration. This study investigates the correlation between the cationic interplay and ion migration pathways in halide perovskites, utilizing optimization techniques like the doubly-nudged elastic band (d-NEB) method as implemented in OPTIM code. This method systematically builds a complete minimum-saddle-minimum sequence by accurately locating transition states and mapping out migration pathways [3]. By better handling the forces along the transition paths,

this method yields more accurate migration barriers and faster convergence compared to traditional approaches. Our results highlight the complex energy landscape of ion migration in perovskites and demonstrate how tuning of these pathways can lead to the development of materials with neuromorphic functionalities. This investigation opens avenues for using halide perovskites in energy-efficient and adaptive computing architectures, where controlled ion migration plays a pivotal role in mimicking synaptic behaviour.

1. Vasilopoulou, M., Mohd Yusoff, A.R.b., Chai, Y. et al. Neuromorphic computing based on halide perovskites. Nat Electron **6**, 949–962 (2023).

2. John, R.A., Demirağ, Y., Shynkarenko, Y. et al. Reconfigurable halide perovskite nanocrystal memristors for neuromorphic computing. Nat Commun **13**, 2074 (2022).

3. Wales, David J. "Energy landscapes: calculating pathways and rates." International Reviews in Physical Chemistry 25.1-2 (2006): 237-282.

Cationic Interplay for the Halide Ion Migration: Implication to Neuromorphic Computing

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Abstract: Neuromorphic computing, which aims to replicate the neural architecture and functionalities of the human brain, relies heavily on materials that can emulate synaptic behaviour through reliable memristive switching. In recent times, halide perovskites have emerged as promising candidates to be used in such memristive devices[1,2] due to their unique ionic-electronic properties. This study focuses on the role of cationic interplay in halide ion migration, a critical factor influencing the stability and performance of perovskite-based memristors. Using first-principles based electronic structure calculations in conjunction with climbing image Nudged Elastic Band (CI-NEB) approach, we investigate the energy barriers and all possible migration pathways of halide ions under various cationic configurations. The simulations reveal that modifying the cationic environment one can effectively control the ion migration which in turn helps to reduce the energy barriers and thus enhances the consistency of resistive switching. These findings are crucial for developing high-performance memristive devices capable of fast and reliable switching, which are essential for neuromorphic computing applications. By fine-tuning cationic interactions, this research provides a comprehensive strategy for engineering next-generation perovskite-based neuromorphic systems, advancing the field of artificial intelligence and enabling more efficient and sophisticated computing architectures.

1. K. Sakhatskyi, R. A. John, A. Guerrero, S. Tsarev, S. Sabisch, T. Das, G. J. Matt, S. Yakunin, I. Cherniukh, M. Kotyrba, Y. Berezovska, M. I. Bodnarchuk, S. Chakraborty, J. Bisquert, M. V Kovalenko, “Assessing the Drawbacks and Benefits of Ion Migration in Lead Halide Perovskites”, ***ACS Energy Letters***, 7 (2022) 3401.

2. S. K. Vishwanath, B. Febriansyah, S. Ng, T. Das, J. Acharya, R. A. John, D. Sharma, P. A. Dananjaya, M. Jagadeeswararao, N. Tiwari, M. R. C. Kulkarni, W. S. Lew, S. Chakraborty, A. Basuf and N. Mathews, High-Performance One-Dimensional Halide Perovskite Crossbar Memristors and Synapses for Neuromorphic Computing, ***Material Horizons***, 11, 2643–2656, 2024.

Scanning Tunnelling Microscopy & Spectroscopy study in Antiferromagnetic Topological Insulator $MnBi_4Te_7$

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Abstract: Recently discovered antiferromagnetic topological insulator $MnBi_4Te_7$ (MBT) offers a novel material platform to achieve topologically protected quantum states in stoichiometric magnetic materials [1]. Several recent report confirms that the controlling native defects and Fermi levels is critical for establishing MBT as topological quantum Anomalous Hall insulator [2-3]. We used scanning tunnelling microscopy and spectroscopy to visualize surface structures, atomic terminations and native defects in the single crystalline antiferromagnetic topological insulator $MnBi_4Te_7$. High resolution surface topography on the *insitu* cleaved crystal surfaces reveals a multiple atomic scale insight about the local atomic and electronic structures and their correlation with native defects. The spatially inhomogeneous cation (Mn-Bi) intermixing impacts the distribution of Mn atoms, explaining this phenomenon.

1. Otrokov, M. M., I. I. Klimovskikh, H. Bentmann, D. Estyunin, A. Zeugner, Z. S. Aliev, S. Gaß, A. U. B. Wolter, A. V. Koroleva, and A. M. Shikin et al., Nature (London) 576, 416 (2019).

2. Yan, J. Q., Liu, Y. H., Parker, D. S., Wu, Y., Aczel, A. A., Matsuda, M., ... & Sales, B. C. (2020), Physical Review Materials, 4(5), 054202

3. Liu, Y., Wang, L. L., Zheng, Q., Huang, Z., Wang, X., Chi, M., ... & Yan, J. (2021), Physical Review X, 11(2), 021033.

Ab-intio insight on the fermiology of d1 transition metals on the honeycomb lattice: Hierarchy of hopping pathways and spin-orbit coupling.

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Abstract: Recently, the physics of J=3/2 electrons on a honeycomb lattice has received attention with the suggestion of hosting an SU (8) Dirac semi metallic state. Motivated by this, in this work we provide a systematic study of the interplay of various hopping pathways and atomic spin-orbit coupling for the low-energy electrons in candidate d1 transition-metal halides MX3 (M=Ti, Zr,Hf; X=F,Cl,Br). By combining first-principles calculations and a minimal hopping Hamiltonian, we uncover the role of dominant direct metal-metal hopping on top of indirect metal-halide-metal hopping. This sets up a hierarchy of hopping pathways that centrally modify the SU (8) picture for the above materials. These hopping interactions, along with the spin-orbit coupling, lead to a plethora of exactly compensated metals instead of the SU (8) Dirac semimetal. Remarkably, the same can be understood as descendants of a topological insulator obtained by gapping out the SU (8) Dirac semi metallic phase. The resultant compensated metals have varied Fermi surface topology and are separated by Lifshitz phase transitions. We discuss the implications of the proximate Lifshitz transition, which may be accessed via strain, in the context of the relevant materials.

Theoretical and experimental investigations on Fe doped Bi_2Se_3 topological insulator

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Abstract: Induction of magnetism in topological insulators (TI's) through doping of transition metal (TM) impurities break the time reversal symmetry causing opening of the energy gap in surface states at Dirac point. This leads to realization of novel physical phenomena such as magnetic monopoles, quantum anomalous hall effect, giant magneto-optical Kerr effect and Majorana fermion

and may also lead to the development of new devices based on spintronics and several efforts have been given in recent years to grow and study transition metal doped Bi_2Se_3 crystals[1,2]. In this work, ab-initio electronic structure calculations using Density Functional Theory (DFT) were conducted using the Vienna Ab-initio Simulation Package (VASP) on Fe doped Bi_2Se_3 system. Calculations have been carried out assuming both substitutional and various configurations of interstitial doping and formation energy calculations with optimized structural parameters indicates that the van der Waals (vdW) gap between successive quintuple layers of Bi_2Se_3 lattice is the most favorable doping site for Fe atoms. Simulated electronic band structure of Bi_2Se_3 with Fe doping in the above interstitial sites shows a bandgap value similar to that of pristine Bi_2Se_3, while the substitutional doping at Bi sites exhibits lower bandgap. Subsequently high-quality single crystals of undoped, 2%, 4%, and 6% Fe-doped Bi_2Se_3 were grown, XRD patterns of cleaved surfaces of the crystals show only (00l) (l =3n, where n is an integer) type of reflections over 2θ of 10°-80° indicating that all layers have grown with the c-axis perpendicular to the surface and have a single-phase rhombohedral structure with space group (R3m). X-ray near-edge structure (XANES) and Extended X-ray absorption fine structure (EXAFS) measurements of the samples were done in transmission mode at Bi L_3-edge and Se K-edge and in fluorescence mode at Fe K-edge at the Energy-Scanning EXAFS beamline (BL-09) of Indus-2 synchrotron source. Absorption edge of Bi in Fe-doped Bi_2Se_3 aligns closely with that of pure $BiFeO_3$ standard, indicating a +3 oxidation state for Bi in the sample while Se absorption edge of the crystals is found to lie at lower energy compared to that of the Se foil in conformity with the fact that Se ions are present in -2 oxidation state. Notably, the Fe absorption edges of Fe-doped Bi_2Se_3 samples are found to fall between those of Fe metal and Fe_2O_3. This data effectively dismisses the possibility of Fe metallic clusters or oxides formation in the doped samples. The EXAFS data have been analyzed following the standard procedure using ATHENA subroutine available within the IFEFFIT software package. The dissimilarity of the fourier transformed EXAFS spectra or $\chi(R)$ versus R plots shows different local structures around Bi and Fe atoms in the sample and thus clearly establishes that Fe ions have not occupied the Bi sites. Finally, the effect of doping on the electronic band structure of the samples have been investigated using angle-resolved photoelectron spectroscopy (ARPES) measurements at the ARPES beamline (BL-10) of Indus-2 synchrotron source using He I_α lamp ($h\nu$ = 21.2 eV) and synchrotron radiation of $h\nu$ = 32.4, 49 and 69 eV at a temperature of 20 K. ARPES data of the samples reveal that the bandgap reduction is minimal in the doped samples compared to the pristine sample. Thus, the above investigations, incorporating DFT simulations, XANES, EXAFS and ARPES measurements, suggest that Fe atoms preferentially occupy the vdW gap sites during doping in Bi_2Se_3.

1.R. Kumar, Soma Banik, Shashwati Sen, S.N. Jha and D. Bhattacharyya, Phys Rev. Mater. **6** (11), 114201 (2022).
2.R. Kumar and D. Bhattacharyya, Superlattices and Microstructures 159 (2021) 107033.

Layer-dependent electronic structures and magnetic ground states of polar-polar $LaVO_3/KTaO_3$ (001) heterostructures

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Abstract: Employing a first-principles and model Hamiltonian approach, we work out the electronic properties of polar-polar $LaVO_3/KTaO_3$ (LVO/KTO, 001) heterostrctures[1], with up to six layers of KTO and five layers of LVO. Our analyses indicate the existence of multiple Lifshitz transitions (LTs) within the t_{2g} bands, which can be fine-tuned by adjusting the number of LVO layers or applying gate voltage. Contrary to the experimental report, spin-orbit coupling is found to be negligible, originating solely from the Ta $5d_{xy}$-derived band of KTO, while the $5d_{xz}$ and $5d_{yz}$ bands are considerably away from the Fermi level while LVO overlayers having no role in it[2]. Magnetic properties of the heterostructures, due to Vanadium ions, exhibit a pronounced sensitivity to the number of LVO and KTO layers. Our calculations indicate that the interlayer AFM, (so called A-AFM), is energetically most favorable. This is further supported by ground state energy calculations on extended $\sqrt{2}$ x $\sqrt{2}$ supercells. Moreover, we find that an insulator to metal transition at the interface requires four LVO layers, corroborating the experimental observation. The interfaces featuring ferromagnetic (FM) ground states turn out to be *half-metallic* after the critical thickness is reached. Considerations of the magnetic interactions appear crucial for the experimentally observed critical thickness for metallicity.

1. N. Wadehra et al. Nat. Commun. 11, 874 (2020).

Material-specific investigations of strongly correlated electron systems through DFT+DMFT

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Abstract: Strongly correlated electron systems (SCES) have traditionally been investigated through effective, low-energy many-body Hamiltonians such as the Hubbard and the periodic Anderson model. While such toy models offer great insight into phenomena such as the Mott metal-insulator

transition and heavy fermion physics, these types of investigations are not material-specific. The advent of dynamical mean field theory (DMFT) three decades ago followed by quantum cluster theories, opened possibilities of predictive modeling of SCES through a combination with density functional theory. In my poster, I will begin by reviewing some of the progress made through the DFT+DMFT approach. Subsequently, I will discuss our work on the development and application of a fast and inexpensive, albeit perturbative, impurity solver that yields results directly on the real frequency axis and scales polynomially with the number of orbitals. I will summarize with a discussion of the utility of such a solver in large unit cell systems such as multiorbital materials, disordered systems, and Moire lattices.

Identification of Griffiths Singularity in Swedenborgite compounds Dy(1−x)ErxBaCo4O(7+δ) (x = 0.00, 0.25, 0.50, 0.75, 1.0)

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Abstract: In the given work, we study the Griffiths phase phenomenon in the Swedenborgite compound Dy(1−x)ErxBaCo4O(7+δ) (x = 0.00, 0.25, 0.50, 0.75, 1.0). DyBaCo4O7, one of which becomes immersed in the Griffiths phase, is best known to be a Griffiths phase, whereas its Er-substituted analogous ErBaCo4O7 behaves differently according to the difference in x. The systematic mixing of the added Er, or this is, the values of x are the objects that serve as a variable in our investigations, and through this we intend to find the answer to the question as to what the reason for wiping out the Griffiths phase is and how the local structural distortions and ionic radius are going to influence the magnetic ordering. A bunch of our research tools are employed such as X-ray diffraction, magnetic susceptibility, μSR, and heat capacity measurements on the series to attract the behavior of the structural, magnetic, and electronic properties discussed clearly in the series. Our results showed that the Griffiths phase is repressed very slowly coming from or towards cobalt content, thus we have shown the disorder is lower and the antiferromagnetic mechanism is stronger, so they become more effective as they approach each other, etc. Moreover, our studies reveal some other important aspects regarding the Griffiths phase; e.g. abnormal interactions and disorder involve the competition of interactions improving the magnetic behavior of the geometrically frustrated systems

Kondo Effect and Magnetic Property Studies in CVD Grown Uniform 2D VSe2 Thin Films

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Abstract: Vanadium diselenide (VSe2), a van der Waals (vdW) layered material, has potential application across diverse fields, including electronics, spintronics, memory devices and energy application due to its unique physical and chemical properties, such as high electrical conductivity [1], charge density wave (CDW) [1] and intrinsic ferromagnetism in mono to few-layers [2], distinct from its bulk counterpart. However, synthesizing high-quality uniform 2D VSe2 thin film for potential applications remains a significant challenge. Here, we present a method to grow large area (~ 1cm × 1cm) uniform 1T-VSe2 thin films on Si/SiO2, using chemical vapor deposition (CVD) method. A highly crystalline thin film without any impurity phases and the thickness of ~100 nm is realized. Low temperature electrical and magneto-transport studies demonstrate the presence of localized magnetic moments, originating from the interlayer V ions in metallic multilayer VSe2 thin film. These localized magnetic moments, play a crucial role in scattering of conduction electrons, leading to Kondo effect [3]. This weak Kondo effect is confirmed by the negative Magnetoresistance (MR) at low temperature (< 5 K), regardless the direction of magnetic field applied to the sample plane. Moreover, VSe2 thin film exhibits soft ferromagnetic behaviour at room temperature with saturation magnetization, MS ~ 2 $\times 10^{-5}$emu, likely originating from the interlayer V ions. Also, temperature-dependent zero-field-cooled (ZFC) and field-cooled (FC) magnetization measurements show a ferromagnetic nature sustaining well above 300 K. The large area continuous VSe2 thin film holds promise for next-generation electronics and spintronics application.

1.Y. Xue *et al.*, "Thickness-dependent magnetotransport properties in 1T VSe2 single crystals prepared by chemical vapor deposition," *Nanotechnology*, vol. 31, no. 14, Jan. 2020, doi: 10.1088/1361-6528/ab6478.
2. M. Bonilla *et al.*, "Strong roomerature ferromagnetism in VSe2 monolayers on van der Waals substrates," *Nat. Nanotechnol.*, vol. 13, no. 4, pp. 289–293, Apr. 2018, doi: 10.1038/s41565-018-0063-9.
3. S. Barua, M. C. Hatnean, M. R. Lees, and G. Balakrishnan, "Signatures of the Kondo effect in VSe2," *Sci. Rep.*, vol. 7, no. 1, Dec. 2017, doi: 10.1038/s41598-017-11247-4.

Blocking transition of $SrTiO_3$ surface dipoles in $MoS_2/SrTiO_3$ field effect transistors with counterclockwise hysteresis

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Abstract: A counterclockwise hysteresis is observed at room temperature in the transfer characteristics of SrTiO3 (STO) gated MoS2 field effect transistor (FET) and attributed to bistable dipoles on the STO surface. The hysteresis is expectedly found to increase with increasing range, as well as decreasing rate, of the gate-voltage sweep. The hysteresis peaks near 350 K while the transconductance rises with rising temperature above the room temperature. This is attributed to a blocking transition arising from an interplay of thermal energy and an energy-barrier that separates the two dipole states. The dipoles are discussed in terms of the displacement of the puckered oxygen ions at the STO surface. Finally, the blocking enables a control on the threshold gate-voltage of the FET over a wide range at low temperature which demonstrates it as a heat assisted memory device.

Anomalous magnetoresistance, metamagnetic transition and magnetoelastic coupling in metallic canted antiferromagnet

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Abstract: Present a comprehensive study of the cubic Heusler alloy $Mn_{1.7}Fe_{1.3}Si$, highlighting its complex magnetic and electronic transport behavior. Magnetic measurements reveal a paramagnetic

to ferromagnetic transition at 85 K, followed by a spin reorientation transition between 65 K and 55 K, and a canted antiferromagnetic state below 55 K. Isothermal M(H) measurements at T < 30 K show field-induced metamagnetic transitions, accompanied by a butterfly-like magnetoresistance curve with an open hysteresis loop. Neutron diffraction suggests that spin reorientation is driven by magnetoelastic coupling, while the anomalous MR behavior stems from phase coexistence of AFM and FM states after field cycling. These results shed light on the intricate electronic structure and phase transitions in $Mn_{1.7}Fe_{1.3}Si$, with potential relevance for spintronic applications.

Structural, Optical and Electronic Structure Investigations of Cu Substituted NiO Solid Solutions

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Abstract: NiO is a p-type semiconductor with a wide optical gap (~4.0 eV). Its inherent p-type conductivity, which arises from metal vacancies, is neither very stable nor easily tunable. To enhance its p-type conductivity and to improve its stability, NiO has been intentionally doped with acceptor impurities such as Li, Cu, and Ag. The observed increase in conductivity with Cu substitution is attributed to small polaron hopping conduction. Additionally, it is also reported that the conductivity of Cu doped NiO improves due to the delocalization of holes in the valence band (VB) because of the replacement of Ni^{2+} ions with Cu^{+}ions. Electronic structure investigations are thus necessary to investigate how the VB and conduction band (CB) states of NiO are modified with the Cu substitution, which may find implications in the observed enhancement of p-type conductivity in NiO. Ternary solid solutions of $Ni_{1-x}Cu_xO$ (x = 0, 0.06, 0.10, 0.15, 0.22, 0.25) were synthesized using solid state reaction method. The phase purity and crystal structure of the solid solutions were determined by X-ray diffraction (XRD), where all the solid solutions are found in single phase with cubic rock-salt (RS) crystal structure. In addition, a linear variation of lattice parameter is noted as a function of Cu substitution. The optical gap of the solid solution was investigated by diffuse reflectance spectroscopy (DRS), which is found to decrease almost linearly with the Cu content in NiO. However, even with 25% of Cu substitution, the optical gap decreases only by 0.2 eV. To understand this minor change in the optical gap, electronic structure of unoccupied (CB) and occupied (VB) states of Cu substituted NiO were investigated by X-ray absorption near edge structures (XANES) at oxygen K-edge and Photoelectron spectroscopy (PES) at beamlines, BL-01 and BL-10, Indus-2, RRCAT, respectively. The onset of the CB edge is found to decrease by ~ 0.2 eV with the 25% of

Cu substitution. This small change in the onset of CB band edge may be attributed to the dominance of the localized nature of Ni 3d states. The Cu and Ni K-edges XANES spectra indicate that the valency of Cu and Ni cations in the solid solution do not change upon Cu substitution. A comparative study of the VB structure of NiO, CuO and $Ni_{0.75}Cu_{0.25}O$ was carried out using PES technique.Top of the VB is found to be dominated by the localized Ni 3d states indicating no significant changes on the onset of VB of NiO upon Cu substitution. Since, no significant change is observed at the onset of the VB, and there is only ~0.2 eV shift at the CB edge upon 25% of Cu substitution, the small decrease (~ 0.2 eV) in the optical gap can be attributed to solely by change in the CB edge dominated by localized Ni 3d state. Resonant PES is also performed to determine the nature of Cu derived states in the VB of $Ni_{1-x}Cu_xO$, which is may be responsible for the enhancement of the conductivity. This will be discussed during poster presentation.

Growth and local electronic structure of Sn on WS2 surface: A case of substitutional doping

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Abstract: In this work, we study the growth and local electronic properties of Sn on the WS2 surfaces by performing in-situ low energy electron diffraction (LEED), scanning tunneling microscopy (STM) and spectroscopy (STS) measurements, and first principles ab-initio calculations. The LEED and high resolution STM studies on the bare WS2 display hexagonal symmetry with 1×1 diffraction spots and an atomically resolved hexagonal surface with a lattice periodicity of 0.34 nm in real space [1]. The STS studies reveal the local electronic structure of the pristine WS2 crystal surface, with the valence band (VB) and conduction band edges lying at around -0.2 and 1.1 eV respectively, demonstrating an indirect band gap of ~1.3 eV. The growth of Sn on the WS2 surface was carried out under ultra high vacuum (UHV) conditions at room temperature (RT) for different coverages. The Sn grown WS2 surface exhibits similar 1×1 LEED patterns, however, a gradual change in the angles corresponding to the hexagonal symmetry is observed with Sn coverages. This change in the angles indicates a stretched hexagonal surface lattice with strain developing in the system with Sn growth. The intact hexagonal symmetry without any evidence of extra diffraction spots in the LEED measurements even after prolonged Sn deposition conveys that Sn is growing nearly commensurately on the WS2 surface. STM measurements, along with density functional

theory (DFT) calculations, reveal that the initial growth of Sn is a case of substitutional doping at the top `S' sites via the formation of monomers (U) and dimers (P) with the distance between two adjacent Sn atoms being 0.34 nm and 0.293 nm respectively. Atomically precise RT STS measurements exhibit the local electronic states of the `S' defects, as well as the Sn grown surface for `U' and `P'- like adsorptions. We observe modulated in-gap electronic states after Sn deposition for coverages less than a monolayer [2]. These in-gap electronic states slowly disappear with Sn growth, and evidence of new local electronic states emerges in the STS spectra. The experimental results, along with DFT calculations will be presented here.

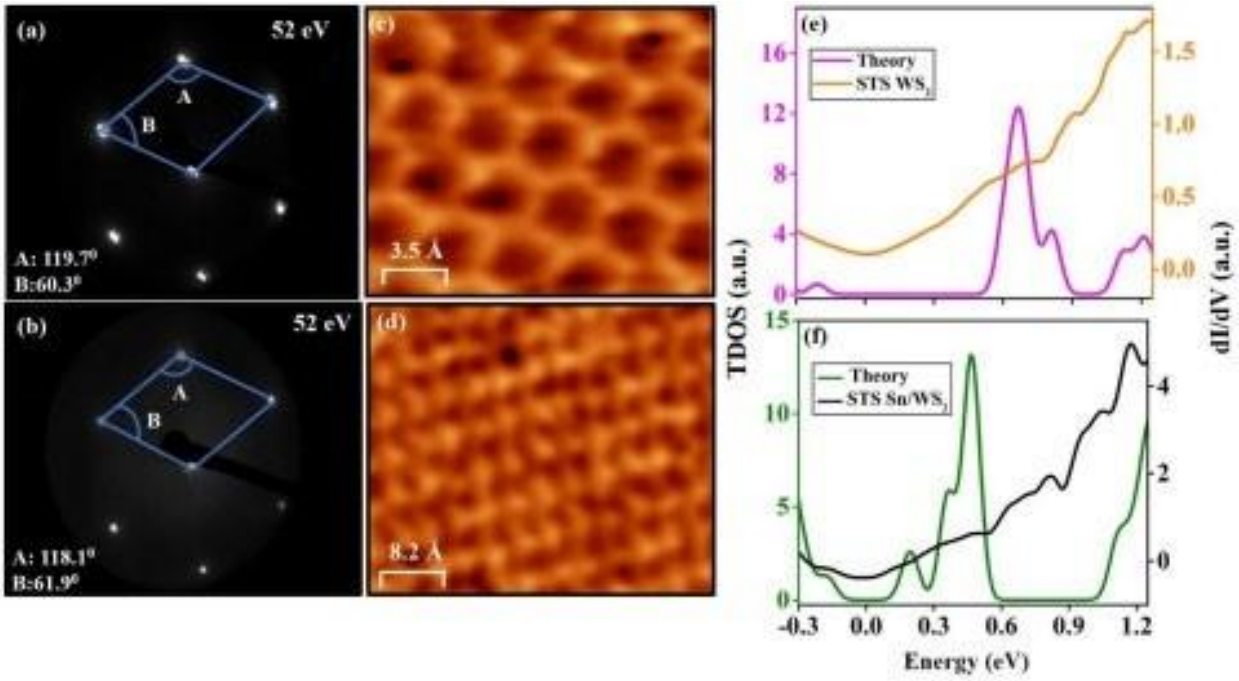

Fig.1. *LEED patterns for (a) bare WS2 surface, (b) ~3 ML of Sn deposition on the WS2 surface. The measured angles are shown in the figure. The corresponding STM images are shown in (c), and (d). Experimental STS spectra along with the calculated electronic states for bare WS2 and ~3 ML of Sn deposition are shown in (e) and (f).*

1. Manu Mohan, Vipin Kumar Singh, Reshmi S, Sudipta Roy Barman, Kuntala Bhattacharjee, Atomic adsorption of Sn on mechanically cleaved WS2 surface at room temperature, Surface Science **701**, 121685, (2020) https://doi.org/10.1016/j.susc.2020.121685

2. Manu Mohan, Vipin Kumar Singh, Reshmi S, Mihir Ranjan Sahoo, Sudipta Roy Barman, Kuntala Bhattacharjee, Local hybridized states of adsorbed atomic Sn on WS2 substrate, Applied Surface Science **635**, 157765 (2023)
https://doi.org/10.1016/j.apsusc.2023.157765

Exploring the 1T phase of TaSeTe: From Synthesis to CDW-Induced Electronic Structure

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Abstract: Among the transition metal dichalcogenides (TMDCs), the polytypes of tantalum diselenides (TaSe2) provide an excellent platform for studying the coexistence of a charge density wave (CDW) and superconductivity, both stemming from electron-phonon coupling and instabilities at the Fermi surface. Unlike the typical system, TaSe2, we observed that the doping induces Se/Te disorder, which leads to the emergence of short-range charge and magnetic correlations in TaSeTe [1]. Here, we successfully synthesized the 1T phase in TaSeTe using the chemical vapour transport (CVT) method with iodine as a transport agent. The X-ray diffraction (XRD) patterns of TaSeTe single crystals exhibit only (00l) reflections, suggesting the presence of a well-ordered stacking of this layered material along the c-axis. The resistivity curve mimics the behavior already reported in the 1T-TaSe2-xTex solid solution, thereby confirming the 1T structure [2]. The electronic structure of 1T-TaSeTe single crystal is investigated using synchrotron-based photoemission spectroscopy. The core-level spectra indicate that each peak of the spin-orbit-split Ta 4f doublet is further splitted due to the presence of CDW. Additionally, the band structure analysis reveals that the CDW induces band folding in the 1T phase, which is distinctly visible in the valence bands along the Γ-M direction. Further magnetic and magneto-transport measurements of this system may prove to be of considerable interest.

1.Liu, Yu, et al. "Nature of charge density waves and superconductivity in 1T− TaSe2−xTex: A review." Physical Review B **94**.4 045131 (2016).
2. Huixia Luo, et al. "Polytypism, polymorphism, and superconductivity in TaSe2−xTex: A review." Proceedings of the National Academy of Sciences **112.**11 E1174-E1180 (2015).

Terahertz crystal electric field transitions in a Kondo-lattice antiferromagnet

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Abstract: The interplay between the Kondo effect and Ruderman-Kittel-Kasuya-Yosida leads to the emergence of many intriguing phenomena in strongly correlated systems. Metallic materials doped with magnetic impurities are ideal for such studies. These impurities interact with the crystal electric field (CEF) produced by neighbouring ions, lifting the degeneracy of their energy levels and creating CEF states. The hybridization between these CEF states and the conduction band often determines the magnetic phase of the system. Therefore, identifying these states and understanding their impact on the material's ground state is crucial [1]. Given that CEF excitations occur in the millielectronvolt (meV) range, the terahertz (THz) frequency range is particularly suited for these investigations. Using time-domain THz reflection spectroscopy, we show the first direct evidence of two low-energy CEF transitions at 0.6 THz (2.5 meV) and 2.1 THz (8.7 meV) in $CeAg_2Ge_2$, a prototype Kondo-lattice antiferromagnet. The presence of low-frequency infrared-active phonon modes further manifests as a Fano-modified line shape of the CEF conductivity peak. In addition, we also observe that the lower CEF transition peak undergoes a blue-shift once the sample enters into the antiferromagnetic phase. The temporal spectral weights obtained directly from the THz time traces corroborate the corresponding CEF energy scales of the compound [2].

1. S. Pal, C. Wetli, F. Zamani, O. Stockert, H. v. Löhneysen, M. Fiebig, and J. Kroha, *Phys. Rev. Lett.* **122**, 096401 (2019).
2. P. Shee, C.-J. Yang, S. K. Pandey, A. K. Nandy, R. Kulkarni, A. Thamizhavel, M. Fiebig, and S. Pal, *Phys. Rev. B* **109,** 075133 (2024).

Transport evidence of Novel Two-Dimensional Surface State in CoSn_2 single crystal

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Abstract: We propose the transport evidence for the emergence of novel 2D topological surface state in CoSn_2 single crystal. The magnetotransport uncovers a metallic behaviour and a clear slope change around 35 K in zero field. Magnetoresistance (MR) at high fields shows a crossover from quadratic dependence to linear dependence below 35 K. In addition to linear magnetoresistance (LMR) at high magnetic fields, we have also observed weak antilocalization (WAL) cusp in magnetoresistance at low magnetic fields. Angle dependence of WAL analysis shows that the

conducting channels are confined to two dimensions, consistent with a surface state origin. Using Density Functional Theory (DFT), we demonstrate the emergence of surface states originating from nodal point near the Fermi level, whose effect has been seen in transport. Furthermore, angular-dependent magnetoresistance measurements confirm the presence of a 2D surface state, as the symmetry of the angular magnetoresistance transitions from fourfold to twofold. These observations reinforce the presence of a two-dimensional topological surface state and shed light on the unique low-temperature transport behavior in CoSn_2.

Novel Cylindrical Substrate-Assisted SERS Detection of Rhodamine B in Food samples

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Abstract: Surface-enhanced Raman spectroscopy (SERS) can provide fingerprint information of chemical and biological molecules with ultrahigh sensitivity, down to the single-molecule level. However, the reproducibility and sensitivity of SERS substrates remain a great challenge. Herein, we demonstrate the fabrication of Ag nanoparticle (AgNP) assemblies on a novel cylindrical copper rod (CuR) substrate using a drop casting method. The droplet volume, analyte nanoparticle ratio, and reaction conditions were systematically examined to determine the optimum parameters. The cylindrical substrate can confine the analyte at the tip of the SERS surface by showing sufficient hydrophobicity, which eliminates the issue of aqueous samples spreading on most SERS substrates. The required volume of the sample could be as low as 5 μL without the need for a drying step in the procedure. By aligning the cylindrical SERS substrates into a 3D printed holder, an array of cylindrical substrates was produced for mass analysis of the aqueous samples. This new substrate improved both the reproducibility and sensitivity of detection in aqueous samples with a relative standard deviation of 8.6%. Using the optimized conditions, a carcinogenic dye, Rhodamine B, was detected with a low threshold of 10^{-9} M (1 nanomolar) in aqueous and real-world samples.

1. Lin, Xiu-Mei, Yan Cui, Yan-Hui Xu, Bin Ren, and Zhong-Qun Tian. "Surface-enhanced Raman spectroscopy: substrate-related issues," Anal Bioanal Chem, **394**, 1729-1745, (2009).

2. Rajapandiyan, Panneerselvam, and Jyisy Yang. "Sensitive cylindrical SERS substrate array for rapid microanalysis of nucleobases," Anal. Chem, **84**, 10277-10282, (2012)

Development of a low-cost digital lock-in amplifier and application to kelvin probe microscopy.

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Abstract: At its core, the contact potential difference (CPD) determines device characteristics, especially in devices that involve junctions between different materials. By vibrating a reference and sample of interest, the CPD can be straightforwardly measured using the Kelvin probe technique. In this setup, the distance between the reference and sample is varied by vibrating one of the two, which is attached to a disc piezoelectric actuator. The compensation, or nullification voltage, that minimizes the current through the parallel plate capacitor is determined, which is approximately equal to the work function difference between the sample and reference. Due to the very small inherent signal generated by the capacitor action, a lock-in amplifier is essential for the measurement. Lock-in amplifiers are generally indispensable in scientific laboratories for measuring the amplitude and phase of weak signals embedded in significant noise. In this poster, we present the design and development of a budget-friendly lock-in amplifier using digital signal processing, with a target application in Kelvin probe. The electronic circuit consists of a trans-impedance amplifier (TIA) with a gain of 10^8 V/A, a Teensy 4.1 microcontroller for digitizing the TIA output at 80 ksps, and a Raspberry Pi for interfacing the complete system, where signal processing for the lock-in detection is carried out using Python programming. The performance of the lock-in amplifier is verified by estimating the capacitance of commonly available capacitors (in the pF to nF range) by measuring the current through them at low input voltages. The lock-in amplifier is then utilized to measure the CPD of a brass-aluminum junction, and further applications, such as its use in scanning tunnelling spectroscopy, are discussed.

Identification of C3N/Silicene heterostructure as anode materials for Li-ion battery and its origin

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Abstract: The design and development of new and light weight two-dimensional (2D) heterostructures as anode materials is necessary to enhance the electrochemical performance for Li-ion batteries (LIB's) but finding a correct combination is a challenge. In this work, using first-principles study, we have demonstrated that the ratio of two-dimensional polyaniline (C3N) and silicene in the multilayer heterostructures plays a major role to define the Li storage properties and to provide metallicity for easy conduction of electrons and increase the stability and specific capacity with moderate open circuit voltage. The volume expansion for fully lithiated heterostructures is within 22 %. The proposed 2D heterostructures could be a future material for anode in LIB's and the description of the interface effect on Li storage properties will help for further development of 2D heterostructure materials. The low interlayer diffusion energy of Li-ion makes all the heterostructure as a potential anode material. The proposed study will help to understand the Li storage properties of the C3N/silicene based composite to develop the anode materials with a certain approach.

Aqueous Based Ultra-Small Magnetic Doped Semiconductor as a Potential Dual Imaging Probe in Biomedicine

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Abstract: Substitution of semiconductor quantum dots (QDs) by a small number of transition-metal ions having magnetic properties gives rise to magnetic doped semiconductor. With the balance of optical and magnetic properties, these magnetic semiconductors are widely used in spintronics, bio-imaging and magnetic resonance imaging (MRI) applications. To facilitate their usage in bio applications, it is critical to synthesize water soluble magnetic QDs with stabilized structure while maintaining their optical and magnetic properties. Here in our work, we developed a facile substituted synthetic route to achieve Cr doped CdSe (Cr-CdSe) via a facile hydrothermal method. The effects of doping on the structural, optical, and magnetic properties of the Cr-CdSe were studied using X-ray diffraction, UV-Visible spectroscopy, photoluminescence lifetime. We then explored their chemical nature and morphology change with increase in doping concentration via X-ray photoelectron spectroscopy and transmission electron microscopy. Magnetic properties of Cr-CdSe sample were analysed through magnetic property measurement system (MPMS). Water soluble QDs have been used as a bio-imaging probe for the past few decades due to their strong fluorescence, photostability and improved tissue or cellular penetration. However, incorporating magnetic material into fluorescent entity harnesses the ability to control strengths of both modalities that enhance the diagnostic accuracy and facilitate its application in bio-systems especially in early accurate diagnosis. Finally, we demonstrate the competency of Cr-CdSe as a dual imaging probe with fluorescent cellular imaging and MRI applications.

Hydrophobic To Hydrophilic Transition of Laser Annealed rGO Thin Film Synthesized By Pulsed Laser Deposition

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Abstract: Reduced graphene oxide (rGO) has captivated the scientific community due to its exceptional electrical conductivity, high specific surface area, and excellent mechanical strength. The physical properties of reduced graphene oxide (rGO) are strongly dependent on the presence of different functional groups in its structural framework along with surface roughness. In this study, laser annealing was employed by a nanosecond Nd:YAG laser to investigate the impact of varying laser energies on the wettability and conductivity of reduced graphene oxide (rGO) samples grown by pulsed laser deposition. The rGO films were annealed with different laser fluences like 10, 20, 30, 38, 48, 55, and 250 mJ/cm^2. Our results reveal a notable transition in wettability, transforming the initially hydrophobic rGO samples into a hydrophilic state. Also, changes in conductivity were observed, suggesting a correlation between the surface roughness and the electrical properties of rGO. The presented findings not only contribute to the understanding of laser-induced modifications in rGO but also highlight the potential applications of controlled laser annealing in tailoring the surface properties of graphene-based materials for diverse technological advancements.

Core Diameter influence in Fe_3O_4@NiO for Oxygen Evolution Reaction

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Abstract: The oxygen evolution reaction (OER) is an electrochemical process where singletOH^-/H_2O co nverts to triplet O_2, influenced by spin dynamics. However, the slow pace of this reaction hinders its effi ciency in electrochemical water splitting. Although the theoretical equilibrium potential of water splitting is only 1.23V in standard conditions, a high overpotential is required due to the sluggish reaction kinetics of OER. Therefore, the development of efficient electrocatalysts for water splitting is of vital importance. To date, noble metal-based materials, such as Pt, IrO_2, and RuO_2, are regarded as efficient electrocatalysts for OER, however, their scarcity and high cost hinder their applications. Herein, we developed a core-shell structure of Fe_3O_4@NiO via hydrothermal synthesis as an efficient oxygen evolution reaction catalyst. Experimental results exhibit an outstanding OER performance, with overpotential of only 94mV at a current density of 10 mA cm^{-2}. Furthermore, the 18 hour Chronoamperometry test confirmed its stability. This hetero-structural catalyst boosts the Oxygen evolution reaction due to its substantial surface area, which plays a crucial role in enabling the exposure of greater number of active sites leading to augmented contact area between catalyst and electrolyte.

A DFT Study of Structural, Electronic, and Quantum Geometric Properties of Transition Metal Dichalcogenides TMDs (MX2 and MXY)

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Abstract: This study presents a comprehensive analysis of the structural, electronic, and geometric properties of Group VI transition metal dichalcogenides (TMDs) in two distinct combinations: MX2 and MXY (where M = Mo or W, and X, Y = S, Se, or Te). TMDs, known for their unique electronic properties. While the structural and electronic properties of these materials have been extensively studied, the Berry curvature and other geometric quantities, which provide insights into their topological properties, remain relatively unexplored. Using first-principles calculations, we investigate the electronic band structures and geometrical characteristics of these materials. In addition, we delve into the Berry curvature of these TMDs to get insights into their topological characteristics. The inclusion of Berry curvature analysis provides deeper insights into the potential applications of these materials in spintronics and quantum computing. The comparative approach offers a thorough understanding of how the structural and electronic properties of MX2 and MXY compounds evolve, contributing to the broader knowledge of topological materials.

F, B, N-Doped Defective Carbon As Metal-Free Electrocatalyst: Synergistic Effect Augmented Electrochemical Ammonia Synthesis

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Abstract: Ammonia (NH_3) is crucial in the agricultural industry, serving as a key component in the production of various synthetic materials. Traditionally, the Haber-Bosch process, which converts atmospheric nitrogen (N_2) and hydrogen (H_2) from natural gas into ammonia using iron-based catalysts, requires high pressures and temperatures.[1] Despite its efficiency, this method is energy-intensive and accounts for about 1.5% of global energy consumption, significantly contributing to CO_2 emissions [1] As an alternative, the electrochemical nitrogen reduction reaction (NRR) offers a promising solution by enabling ammonia production under ambient conditions using renewable electricity, with water as the hydrogen source. The metal-free carbonaceous material incorporating heteroatoms and defects presents a promising avenue for electrocatalysts for green ammonia production, offering a sustainable and efficient alternative to traditional metal-based catalysts. Their abundance, cost-effectiveness, and tunable properties make them ideal candidates for electrochemical nitrogen reduction reactions (NRR). In this study, we synthesize a defective N-doped carbon material with boron and fluorine as secondary dopants (FBDG). Boron, being electron deficient, serves as the primary active center, while the carbon atoms adjacent to fluorine acquire a partially positive charge, creating additional active sites for nitrogen adsorption. The synergistic effect of three heteroatoms and defects in the catalyst enhances electron-donor behavior, improving π bonding within the carbon framework and facilitating the electron transfer processes during NRR, resulting in a Faradaic efficiency of 38.1 %. Theoretical calculation of charge density distribution reveals that FBDG possesses sufficient charge density to reduce nitrogen at a low overpotential. The electrocatalyst follows an alternating free energy pathway with a minimal limiting potential. This study elucidates the impact of different heteroatoms in the structure of carbon material and their influence on NRR activity and kinetics.

Linear and Non-Linear Intrinsic AC Orbital Hall Conductivity in Broken-Inversion Symmetric System

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Abstract: We investigate the intrinsic linear and nonlinear AC orbital Hall (OH) conductivity in a two-dimensional system, arising from the transverse motion of electrons with finite orbital angular momentum in an applied electric field. Using the quantum kinetic approach, we show that the total OH conductivity comprises both interband and intraband contributions. However, the interband contribution

dominates over the intraband in the high-frequency regime. Our analysis predicts that the interband part of the linear OH conductivity is governed by the Fermi Sea contribution. Meanwhile the nonlinear responses, including second harmonic and rectification effects, stem from the interplay between the Fermi Sea and Fermi surface contributions. We find that the broken-inversion symmetry in the system yields non-zero orbital angular momentum and consequently the orbital Hall response. In addition, the linear OH conductivity exhibits a resonant peak and a sign transition depending on the gap and Fermi energy values relative to the incident energy. Unlike the linear, the second harmonic OH conductivity shows two sign conversions as the incident energy approaches to the gap value and twice its value. These findings shed light on the modulation of field-driven orbital Hall conductivity with frequency, Fermi energy, and band gap.

Designing Site-Specific Electrocatalysts: Unveiling Active Sites for Oxygen Reduction and Evolution Reactions

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Abstract: Oxygen electrocatalysis involving oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) is a key process occurring in many renewable energy conversion and storage technologies. The development of metal-free, inexpensive, stable, and bifunctional electrocatalysts is the major requirement of the hour. The heteroatom-doped defective electrocatalysts are pondered as the efficient catalyst for bifunctional activity in fuel cells and metal-air batteries. However, the identification of active sites individually for both ORR and OER is still vague. We reported in this study that metal-free N-doped carbonaceous material with topological defects derived from triazene derivative exhibited excellent bifunctional activity with a remarkable ΔE value (0.72 V). Showing 0.37V overpotential for OER and 0.52V for ORR theoretically. Here, the pyridinic-N is responsible for ORR and graphitic-N contributes towards OER. Further, the reaction intermediates of ORR and OER are well-characterized by in-situ attenuated total reflection-Fourier Transform Infrared (ATR-FTIR) spectroscopy. Our work sheds light on the path of designing metal-free site-specific electrocatalysts with particular activity for practical significance.

Anomalous hall conductivity on tilted Dirac Nodal Line Semimetals

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Abstract: The anomalous Hall conductivity, particularly in relation to transport properties, has been extensively studied in three-dimensional topological semimetals, including Dirac, Weyl, and nodal line semimetals (NLSMs). In the case of NLSMs, the presence of a symmetry-protected nodal ring adds an additional layer of complexity, making the investigation of their transport properties both challenging and insightful. This study focuses on exploring the effects of inversion-symmetry-breaking tilt and $\mathcal{PT}$-symmetry-breaking mass terms on the transport properties of Dirac nodal line semimetals. By employing quantum kinetic theory, we analyze these effects in detail, addressing both the intrinsic (Fermi sea) and extrinsic (Fermi surface) contributions to interband conductivity with equal consideration. Our findings reveal that the intrinsic contribution to interband conductivity exhibits a prominent peak at low chemical potential, while at higher chemical potentials, the extrinsic contribution becomes dominant. Furthermore, the effect of tilt is evident in the intrinsic contribution, where the presence of multiple kinks indicates different frequency domains arising from the competition between the tilt and Fermi energy. Our study proposes the presence of disorder can significantly influence the total conductivity, making it a crucial factor for the study of the overall response of a three-dimensional system.

Electronic and energy descriptors to identify the dual metal center catalyst for CO_2ER towards C_2 product

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Abstract: Electrocatalytic CO_2 reduction (CORR) is pivotal for producing valuable multi-carbon (C_{2+}) products, yet achieving high performance in this area remains challenging. In this study, we explore the catalytic efficiency of transition metals (TM_1: Cu, Zn, W, Tc; TM_2: Ag, Pd, Au, Pt, Fe, Ni, Co, Os, Sc, Ti, Ir, La, Hf, Y, Nb, Mo, Cd, Ta, Rh, Re) anchored to N-doped graphene (TM_1TM_2@NG) through first-principles calculations. Our research reveals that the d-band center significantly influences CO molecule binding and serves as a key descriptor for coupling free energy and CO-CO adsorption energy. Notably, among 54 combinations, WW@NG, WFe@NG, and WIr@NG stand out as the most promising candidates for ethanol production, with low overpotentials of 0.51, 0.53, and 0.49 eV, respectively. This work offers valuable insights for designing effective dual-atom catalysts for CORR.

An Asymmetric Optical Cryptosystem Using C-Point Polarization Singularity Speckles and Equal Modulus Decomposition

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Abstract: In this paper, we propose a new asymmetric cryptosystem using bright C-point polarization singularity speckle (BCPSs) patterns. These unique speckles are difficult to replicate and serve as

security keys. In encryption, the input image is converted to a phase image and modulated with the phase mask synthesized using BCPSs to obtain a complex image. This image is illuminated using a plane wave, and the complex wavefront is recorded. The resultant image is decomposed using Equal Modulus Decomposition (EMD), providing a private key and the other part undergoing pixel scrambling. Numerical simulations are shown to validate the proposed technique.

Site Specific Descriptor for Metals for Oxygen Evolution Reaction Activity on Single Atom Catalysts Using QMML

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Abstract: Descriptors are properties or parameters of a material that is used to explain the any catalytic activity both computationally and experimentally. Such descriptors aid in designing the materials property to obtain efficient catalyst. d-band center, given by Hammer and Norskov in 1995, explained the binding strength of oxygen atom on pure transition metals [1]. For transition metals, d-band center is a well known descriptor that shows Sabatier type relation for several catalytic reactions. It is well known that, when the dimensions of a system is lowered the states become narrow and localized. In such systems, the d-band center does not explain the catalytic activity well and it is an open research problem [2]. Studies reveals the d-band center works well for metals across the group under same electronic environment (facets, substrate, phase, etc.,) but fails for a same metal under varying conditions and in nano dimensions. Following the criteria of localized states, single atom catalysts (SAC) are the materials, where the metal atom states are localized. Low dimensional carbon has been used as the host for SAC and extensively studied towards several catalytic reactions. Some of these synthesis involves the use of organic polymers instead of graphene as precursor material have made synthesis and structural engineering possible. In the carbon class, the graphene nanoribbons (GNRs) with width variation and doping make them good support for SACs. SAC on GNRs could be used to test the impact of GNRs on electronic properties of SAC and obtain multiple electronic parameters that can be utilized in machine learning to do a deeper search for a better descriptor that could explain as well as predict the catalytic activity. To address this, density functional theory was used for single atom catalysts (SACs) [2] embedded on armchair and zigzag graphene nanoribbons (AGNR and ZGNR). By varying the anchoring nitrogen atoms' orientation and considering pristine and doped cases 432 active sites were used to test the oxygen evolution reaction [3] activity. It was observed that S and SO_2 dopant helps in reducing the overpotential on Co-SAC (η = 0.28 V). Along with the d-band center, a total of 105 possible descriptors were tested individually. Machine learning process were employed to narrow down

unique descriptors and several algorithms were trained on the two obtained descriptors. Among the models, support vector regression model showed highest performance with R^2 = 0.89 on test data. This work shows the necessity of a multi-descriptor approach to explain OER catalytic activity on SAC and the approach would help in identifying similar descriptors for other catalytic reactions as well.

1. Hammer, Bjørk, and Jens K. Norskov. "Why gold is the noblest of all the metals." *Nature* 376.6537 (**1995**): 238-240.
2. Kapse, Samadhan, Shobhana Narasimhan, and Ranjit Thapa. "Descriptors and graphical construction for in silico design of efficient and selective single atom catalysts for the eNRR." *Chemical Science* 13.34 (**2022**): 10003-10010.
3. Borah, Munu, et al. "Stable and boosted oxygen evolution efficiency of mixed metal oxide and borate planner heterostructure over heteroatom (N) doped electrochemically exfoliated graphite foam." *Catalysis Today* 370 (**2021**): 83-92.

Studying critical phenomena using inequality index

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Abstract: Critical phenomena are ubiquitous in nature. Critical points or phase transition points, where a system completely changes its macroscopic behavior due to a minute change in the driving parameter for example, ferromagnetic materials like iron, cobalt and nickel etc. completely lose their magnetic properties above the Curie temperature. Thus, finding it is crucial for systems from condensed matter to biophysics, geophysics. Here we present a method where this can be done by measuring inequality namely, the Gini index from the fluctuation of order parameter. The order parameter for a continuous transition shows diverging fluctuation near the critical point. It can be shown, through numerical simulations and scaling arguments, that the inequality between the values of an order parameter, measured near a critical point, is independent of the system size. Quantification of such inequality through Gini index (g), therefore, leads to a scaling form g=GF-FCN1dν , where F denotes the driving parameter for the transition (e.g., temperature T for ferro-para transition at Tc, or lattice occupation probability p near percolation threshold pc), N is the system size, d is the spatial dimension and is the correlation length exponent. Using this method, identification of critical point and the correlation length exponent can be done for any equilibrium or nonequilibrium systems showing continuous phase transition.

1.S. Das, S. Biswas, A. Chakraborti, and B. K. Chakrabarti, Finding critical points and correlation length exponents using finite size scaling of Gini Index, Phys. Rev. E., 109, 024121, 2024.
2. S. Das and S. Biswas, Critical scaling through Gini Index, Phys. Rev. Lett., 131, 157101, 2023.
3. C. Gini, Measurement of Inequality of incomes, The Economic Journal, vol 31, no. 121, 1921.

In situ Synthesis of Robust Copper-Zinc Sulphide (Cu/ZnS) Metal Alloy for Enhanced the Hydrogen Evolution via Water Splitting

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Abstract: Due to the high demand for green energy, water splitting is the most advantageous and cleanest method of producing green hydrogen without emitting carbon dioxide into the environment. Erecting a highly active, recyclable, and low-cost photocatalysts for the hydrogen evolution reaction (HER) under visible light is critical for direct conversion of solar energy to chemical fuels for a wide range of green energy applications. It is highly challenging yet crucial for a photocatalyst to simultaneously boost visible-light absorption and inhibit photogenerated electron-hole recombination while also maintaining high stability and recyclability in such applications. Herein, we successfully synthesized Cu/ZnS nano-composite as a photocatalyst via simple hydrothermal technique. The enhanced optical and electronic properties of the photocatalyst was confirmed by various characterization such as., UV-Visible, X-ray diffraction (XRD), high resolution scanning electron microscopy (FE-SEM), high resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS). The photocatalytic activity was investigated by splitting of water containing an aqueous Na_2SO_4 solution under visible light irradiation. Among the prepared photocatalysts, the hydrogen evolution rate reaches the maximum of about 2915 ppm for Cu/ZnS whereas the bare ZnS is only 700 ppm for 12 h continues irradiation of sunlight and also Cu/ZnS is photo-catalytically stable for 15 h.

Boosting Selective Nitrogen Oxidation to Nitric Acid by Synergizing Cobalt Phthalocyanine on Carbon Nitride Surface

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Abstract: The Ostwald process, which is producing HNO_3 for commercial use, involves the catalytic oxidation of NH_3 and a series of chemical reactions conducted under severe operating conditions. Due to their energy-intensive nature, these activities play a major role in greenhouse gas emissions and global energy consumption. In response to the urgent requirements of the global energy and environmental sectors, there is an increasingly critical need to develop novel, highly efficient, and environmentally sustainable methods. Herein, we show CoPc/C_3N_4 system, integrating CoPc nanotubes with C_3N_4 nanosheets. The CoPc/C_3N_4 electrocatalyst demonstrates yield rate of 871.8 µmol h^{-1} g_{cat}^{-1} at 2.2V, with corresponding Faradaic efficiency (FE) of 46.4% at 2.1V, which notably surpasses that of CoPc. Through a combination of experimental investigations and density functional theory (DFT) calculations, our study shows that CoPc anchored on C_3N_4 effectively simplifies the adsorption and activation of chemically inactive nitrogen molecules. The improved catalytic activity for hybrid system might be the reason of re-distribution of charges over the CoPc, tuning the valence orbital of Co-centre due to the presence of 2D layer of C_3N_4. This mechanism significantly lowers the energy barrier required for critical breaking of inert N_2, ultimately leading to a significant improvement in N_2 oxidation efficiency.

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Qualitative electronic descriptor to identify Cu based FCC-FCT alloy nanoparticles towards C_2 product over C_1 product on (111) plane

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Abstract: Obtaining C_2 product (possessing higher energy density and more industrial values than C_1 products) in CO_2ER is greatly worthwhile but remains a challenge. In addition, the product distribution in electrochemical reduction of CO_2 (CO_2ER) towards C_1 or C_2 products on the catalyst depends on the nature of the active site, type of surface facet, nature of the plane, morphology, binding strength of different intermediates etc. Cu is the only metal which can reduce CO_2 beyond CO into single carbon products (C_1) or double carbon products (C_2) products but the selectivity towards final product remains as a challenge due to several and overlapping pathways. In general, bulk Cu in (100) plane favor C_2

production while its (111) plane promotes C_1 product formation. Conversely, (111) plane of Cu nanoparticle (Cu NP) favor C_1 or C_2 products depending on the size and shape of the active plane. Introducing new metal atom by forming alloys can influence the CO_2ER towards different final product by tuning the properties of the intermediates. Finding any descriptor to predict ethanol formation as C_2 product in (111) plane is highly demanding.

Here we report the Cu NP based FCC-FCT alloys with Ag and Zn as the alloy element to selectively promote the ethanol product formation on (111) plane via *CO-*CO dimerization. Finally, two different descriptors are studied to explain the fundamental criteria as well as predict the possibility of ethanol formation in CO_2ER. These two simple descriptors also significantly reduced computational costs as it required only one SCF calculation of the optimized model. Moreover, the role of different host layers is also studied to elucidate possible underlying mechanism of different hosts to find a general host for CO_2ER towards ethanol production.

1. Anjana Tripathi, Ranjit Thapa. Carbon 208 (2023), 330-337.
2. Asif Iqbal, Anjana Tripathi, Ranjit Thapa. Inorganic Chemistry 2024, 63, 2, 1462-1470.

Exploring Bi_2O_2Se/Rubrene Heterostructures for Enhanced Optoelectronic Performance

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Abstract: The integration of two-dimensional (2D) materials with organic semiconductors offers a promising avenue for advancing electronic and optoelectronic devices. However, the performance of these devices is often hindered by challenges such as large noise current, slow photo-response, and low photocurrent on/off ratios. We aim to overcome these limitations by investigating the interface between Bi_2O_2Se, a 2D material with great potential, and rubrene, an organic semiconductor. We synthesized Bi_2O_2Se by both chemical vapor deposition (CVD) and hydrothermal techniques and subsequently integrate it with rubrene to form heterostructures.

To understand the charge transfer dynamics at the Bi_2O_2Se/rubrene interface, we plan to employ advanced characterization techniques, including atomic force microscopy (AFM), scanning electron microscopy (SEM), scanning tunneling microscopy (STM), Kelvin probe force microscopy (KPFM), X-ray photoelectron spectroscopy (XPS), and ultrafast transient absorption spectroscopy (TAS). Examining Bi_2O_2Se/rubrene interface with the above-mentioned techniques we will be able to understand surface morphology, interfacial quality, and electronic properties of the heterostructures. We have also investigated Bi_2O_2Se/rubrene interface with Density Functional Theory to explore band alignment and energy level matching between Bi_2O_2Se and rubrene at their interfaces. Our studies will facilitate to develop a multifunctional device by optimizing electronic properties at Bi_2O_2Se/rubrene

interface and significantly contribute to the advancement of next-generation electronic and optoelectronic technologies.

1. Hossain M T, Das M, Ghosh J, Ghosh S, Giri PK. Understanding the interfacial charge transfer in the CVD grown $Bi_2O_2Se/CsPbBr_3$ nanocrystal heterostructure and its exploitation in superior photodetection: experiment vs. theory. *Nanoscale*. ***2021***;13(35):14945-59
2. Dang L Y, Liu M, Wang G G, Zhao D Q, Han J C, Zhu J Q, Liu Z. Organic Ion Template-Guided Solution Growth of Ultrathin Bismuth Oxyselenide with Tunable Electronic Properties for Optoelectronic Applications. *Adv. Func. Mater. 2022*; 32(31): 2201020

Carbon Nanotube Assisted Device Performance Improvement in a Flexible

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Abstract: A hybrid nanogenerator (HNG) offers both high output performance and flexibility by utilizing the synergy between piezoelectric and triboelectric mechanisms. Achieving high output performance, reproducibility, and mechanical stability in an HNG device is still a major challenge. Here, we demonstrate the design and fabrication of a flexible HNG device based on the composite of lead-free piezoelectric ceramic and triboelectric polymer polydimethylsiloxane (PDMS). The piezoelectric ceramic oxide $(Bi_{0.785}\ K_{0.035}Ba_{0.180})(Fe_{0.750}Ti_{0250})O_3$ (BKBFT/MPB-piezo) exhibits improved piezoelectric properties at the morphotropic phase boundary (MPB) in the $BiFeO_3$ – $Bi_{0.5}K_{0.5}TiO_3$ – $BaTiO_3$ ternary phase diagram. We find that composite 90 wt% PDMS – 10 wt% MPB-piezo offers optimum device performance and flexibility. Interestingly, the incorporation of multi-walled carbon nanotubes (MWCNT), a conducting filler, significantly enhances the device's performance without the aid of electric field poling. MWCNT forms nano-electrical bridges that aid charge transfer and improve the composite's structural homogeneity. The 89 wt% PDMS – 10 wt% MPB-piezo – 1 wt% MWCNT composite displays a peak-to-peak open circuit voltage (*Vpp*), short-circuit current (*Isc*) and power density (*U*) of 22 V, 1.8 μA, and 72 nW respectively.

Synthesis of Molybdenum and Copper Selenide for sensing application.

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Abstract: Thin films of Copper and Molybdenum were deposited onto glass substrates by using thermal evaporation and sputtering methods. These thin films were subjected to selenization by heating selenium powder in Chemical Vapor Deposition setup. For comparison powder samples of copper and molybdenum selenide were synthesized via chemical route namely Solvothermal method. Powder samples and selenized thin films were characterized by X-ray Diffraction and Raman Spectrometer. The broad XRD peaks of molybdenum selenide(powder) indicates the formation of a few layered hexagonal $MoSe_2$. Whereas Highly crystalline XRD peaks of copper selenide(powder) indicates the formation of hexagonal crystal structure. Raman peaks of molybdenum selenide correspond to the out of plane vibration A_{1g} mode. Preliminary I-V characterization of these thin films was carried out by using two probe methods. Also, Powder samples were drop-casted onto glass substrates for I-V characterization.

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