Workshop and International conference on Electronic Structure Theory of Emergent Spin Orbit Driven Phenomenon

Organizers: Department of Metallurgical Engineering and Materials Science, IIT Bombay

Date: 11th November to 15th November, 2024

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Programme

ESTESODP – 2024 School Schedule (11th -12th Nov 2024)

Time	Session	Speaker
11-Nov-2024 (Monday) Chairperson: Prof. G. P. Das Venue: SJSOM		
08:00 AM - 09:00 AM	**Registration**	
09:00 AM - 10:15 AM	Fundamentals and application of density functional theory	Prof. Biplab Sanyal
10:15 AM - 11:30 AM	Density functional theory across different length scales: Quantum and classical	Prof. Swapan Ghosh
11:30 AM - 12:00 PM	**Tea Break**	
12:00 PM - 01:15 PM	An introduction to spin-orbit driven emergent phases	Prof. Indra Dasgupta
01:15 PM - 02:30 PM	**Lunch Break**	
Tutorials Venue: Bits and Bytes Lab		
02:30 PM - 04:00 PM	**Tutorial 1:** Basics of DFT calculations - self consistent loops and geometry optimization	
04:00 PM - 04:30 PM	**Tea Break**	
04:30 PM - 06:00 PM	**Tutorial 2:** Electronic structure using DFT - band structures and density of states	
Dinner		
12-Nov-2024 (Tuesday) Chairperson: Prof. Biplab Sanyal Venue: SJSOM		
09:00 AM - 10:15 AM	Introduction to classical and Ab initio molecular dynamics simulation	Prof. Dilip Kanhere
10:15 AM - 11:30 AM	Berry phase in quantum physics of solids with some case studies	Prof. Gour Prasad Das
11:30 AM - 12:00 PM	**Tea Break**	
12:00 PM - 01:15 PM	Exploring electronic structure through spectroscopy	Prof. Kalobaran Maiti
01:15 PM - 02:30 PM	**Lunch Break**	
Tutorials Venue: Bits and Bytes Lab		
02:30 PM - 04:00 PM	**Tutorial 3:** Magnetism using DFT - magnetic ground states and anisotropy	
04:00 PM - 04:30 PM	**Tea Break**	
04:30 PM - 06:00 PM	**Tutorial 4:** Calculation of isotropic magnetic exchange by energy mapping method	
Dinner		

ESTESODP – 2024 Conference Schedule (13th -15th November 2024)

Day 1, 13/11/2024 (Wednesday)	
09:00 AM – 09:30 AM	**Registration**
09:30 AM – 10:00 AM	**Welcome Address by Organizers, DD-ART, Dean R&D, HoD MEMS**
Session Chair: Alok Shukla (IIT, Bombay) **Venue: P C Saxena**	
10:00 AM – 10:45 AM	**Shobhana Narasimhan (JNCASR, Bangalore)** **Title:** At Cross Purposes: Spin-crossover systems on metal substrates
10:45 AM – 11:15 AM **Tea Break**	
11:15 AM – 11:30 AM **Director's Address**	
Session Chair: K. G. Suresh (IIT, Bombay) **Venue: P C Saxena**	
11:30 AM – 12:00 PM	**Swapan K. Pati (JNCASR, Bangalore)** **Title:** Computational modelling of transport phenomena in a few semiconductors
12:00 PM – 12:30 PM	**Abir De Sarkar (INST, Mohali)** **Title:** DFT perspectives on spin-orbitronics and piezotronics in selected functional 2D materials
12:30 AM – 01:00 PM	**Prasenjit Ghosh (IISER, Pune)** **Title:** Theoretical prediction of ZrHfCoNiSnSb high entropy half Heusler alloy with low lattice thermal conductivity
01:00 PM – 02:00 PM **Lunch Break**	
Session Chair: Ashok Arya (BARC, Mumbai) **Venue: SJSOM**	
02:00 PM – 02:30 PM	**Debjani Karmakar (BARC, Mumbai)** **Title:** Intriguing role of spin-orbit coupling on magnetic chirality of systems with broken inversion symmetries: Two examples
02:30 PM – 03:00 PM	**Mukul Kabir (IISER, Pune)** **Title:** Hole-doped two-dimensional magnets
03:00 PM – 03:30 PM	**Sayantika Bhowal (IIT, Bombay)** **Title:** Spin-orbit coupling in ferroaxial materials: Driving the fourth ferroic order and hidden spin polarization
03:30 PM – 04:00 PM **Tea Break**	
Session Chair: Swapan Pati (JNCASR, Bangalore) **Venue: SJSOM**	
04:00 PM – 04:30 PM	**Ashok Arya (BARC, Mumbai)** **Title:** Probing magnetic and defect structures in oxides/mixed oxides

04:30 PM – 05:00 PM	**Subhradip Ghosh (IIT, Guwahati)** **Title:** Non-volatile electrically switchable half-metallicity in multiferroic TMDC-MXene heterostructures
05:00 PM – 05:30 PM	**Dipanshu Bansal (IIT, Bombay)** **Title:** Strong orbital-selective spin-orbital-phonon coupling in $CrVO_4$
Contributed oral 05:30 PM to 06:30 PM	**Soheil Ershadrad (Uppsala University, Sweden)** **Title:** Ab initio study of magnetic properties in 2D metallic magnets: A case study of the Fe_nGeTe_2 family and $FeNbTe_2$
	Ted Trewick (Victoria University of Wellington, New Zealand) **Title:** Anisotropic magnetoresistance in Gadolinium Nitride
	Krishnaraj K (IIT, Bombay) **Title:** Unraveling the Rashba-Dresselhaus effect and spin switching in ferroelectric AIO_3 (A=K, Rb, Cs, Tl) perovskites
	Bishal Das (IIT, Bombay) **Title:** Coexistence of altermagnetism and Topological Weyl fermions in GdAlSi
07:30 PM – 09:30 PM **Dinner at Padma Vihar**	

Day 2, 14/11/2024 (Thursday)	
Session Chair: Shobhana Narasimhan (JNCASR, Bangalore) **Venue: SJSOM**	
09:00 AM – 09:45 AM	**Lars Nordström (Uppsala University, Sweden)** **Title:** Spin-orbit coupling and its dependence on magnetic symmetry applied to the enigmatic case Mn_3Sn
09:45 AM – 10:30 AM	**Priya Mahadevan (SNBNCBS, Kolkata)** **Title:** Examining the ground state of the Slater insulator $NaOsO_3$
10:30 AM – 11:00 AM **Tea Break**	
Session Chair: Hridis Kumar Pal (IIT, Bombay) **Venue: SJSOM**	
11:00 AM – 11:30 AM	**Bahadur Singh (TIFR, Mumbai)** **Title:** Spin U(1) quasi-symmetry in materials with a quantized spin Hall effect
11:30 AM – 12:00 PM	**Awadhesh Narayan (IISc, Bangalore)** **Title:** Non-linear hall effect in flatlands and chiral crystals
12:00 PM – 12:30 PM	**Swarup Panda (Bennett University, Delhi)** **Title:** Spin-spiral magnetism in Honeycomb lattice of $CaMn_2P_2$ - A first-principles and monte carlo perspective
Contributed oral 12:30 PM – 01:00 PM	**Rajnarayan De (BARC, Andhra Pradesh)** **Title:** Electronic and thermoelectric properties of 1-quintuple layer chalcogenides
	Kausar Ali (BARC, Mumbai) **Title:** First-principles study of Titanite-Type $CaTiSiO_5$ under pressure
01:00 PM – 02:00 PM **Lunch Break**	
Session Chair: Avradeep Pal (IIT, Bombay) **Venue: SJSOM**	

02:00 PM – 02:30 PM	**Shouvik Chatterjee (TIFR, Mumbai)** **Title:** Controlling Hall response in epitaxial Mn_3Sn thin films
02:30 PM – 03:00 PM	**Jackson Miller (Victoria University of Wellington, New Zealand)** **Title:**Experiment, computation, and a possible quantum critical point in SmN
03:00 PM – 03:30 PM	**Titas Dasgupta (IIT, Bombay)** **Title:** A refinement-based approach for extracting electronic band structure information and its application in thermoelectric materials and devices
03:30 PM – 05:45 PM	**Tea Break** **&** **Poster presentations by student participants**
06:00 PM – 10:30 PM **Banquet Dinner**	

Day 3, 15/11/2024 (Friday)	
Session Chair: Gopalan Rajaraman (IIT, Bombay) **Venue: SJSOM**	
09:30 AM – 10:00 AM	**Ankit Jain (IIT, Bombay)** **Title:** Phonon thermal transport in low- and high-thermal conductivity solids
10:00 AM – 10:30 AM	**Chiranjib Majumdar (BARC, Mumbai)** **Title:** Nano-ring to Nano-barrel: structural evolution of CuO clusters
10:30 AM – 11:00 AM	**Ranjit Thapa (SRM University, Amravati)** **Title:** Beyond d-band center to identify the catalyst for oxygen evolution reaction
11:00 AM – 11:30 AM **Tea Break**	
Session Chair: Priya Mahadevan (S. N. Bose, Kolkata) **Venue: SJSOM**	
11:30 AM – 12:00 PM	**Saurabh Ghosh (SRM University, Chennai)** **Title:** Polarization coupled magnetization switching in oxide perovskites
12:00 PM – 12:30 PM	**Partha Sarathi Ghosh (BARC, Mumbai)** **Title:** Coupling of the structure and magnetism to spin splitting in hybrid organic-inorganic perovskites
12:30 PM – 01:00 PM	**B. R. K. Nanda (IIT, Chennai)** **Title:** Realizing Friedel oscillation in the orbital channel: valley driven physics of $NbSe_2$ with a magnetic impurity
01:00 PM – 02:00 PM **Lunch Break**	
Session Chair: Saumya Bera (IIT, Bombay) **Venue: SJSOM**	
02:00 PM – 02:30 PM	**Rudra Banerjee (SRM University, Chennai)** **Title:** Data-driven discovery of quantum compatible deep centers in semiconductors
02:30 PM – 03:00 PM	**Sudipta Kanungo (IIT, Goa)** **Title:** Strategic role played by the SOC in emerging magnetic and topological phases in oxides and alloys

03:00 PM – 03:30 PM	**Arnab Bose (IIT, Kanpur)** **Title:** Generation of efficient spin currents in topological and altermagnetic materials
03:30 PM – 04:00 PM **Tea Break**	
Session Chair: Saurabh Ghosh (SRM University, Chennai) **Venue: SJSOM**	
Contributed oral 04:00 PM – 05:15 PM	**Shovan Gayen (Bennett University, Delhi)** **Title:** Pressure induced electronic and magnetic transition in antiferromagnetic NiS: A combined DFT+U and Monte-Carlo study
	Dipanwita Bhattacharjee (IIT, Bombay) **Title:** Effect of spin-orbit coupling on the thermoelectric power factor of CoBi based half-Heusler compounds
	Jagjit Kaur (HRI, Allahabad) **Title:** Unraveling Rashba effect through spin-texture evolution in unidimensional-confined halide-perovskite under compression
	P. Gayathri (SRM University, Chennai) **Title:** Machine learning and atomistic simulations for predicting ferroelectric switching in hybrid improper ferroelectric double perovskites oxides
	Joydeep Majhi (IIT, Bombay) **Title:** Investigating magneto-caloric effect and exchange interaction in $NdMnO_3$ perovskite: A computational study
05:15 PM - 05:45 PM	**Presentation by sponsors**
06:00 PM – 06:30 PM	**Award Ceremony and words from organizers**
06:30 PM – 07:00 PM	**Concluding Remarks by panel members**
07:30 PM – 09:30 PM **Dinner at Padma Vihar**	

Abstracts of Invited Talks

Fundamentals and applications of Density Functional Theory

Biplab Sanyal

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In this lecture, I will present the fundamentals of Density Functional Theory (DFT). The successes and failures of DFT with standard approximations of exchange and correlation will be discussed. Some advanced methods to go beyond the standard approximations will be covered. For all these aspects, applications of DFT will be highlighted.

Density Functional Theory across different Length Scales: Quantum and Classical

Swapan K Ghosh

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Concepts have been introduced in chemistry and physics from time to time for various interpretive and predictive purposes. One of the concepts that has played a major role in the conceptual as well as theoretical and computational developments covering all the length scales of interest is the concept of density (single-particle density, to be more precise). This encompasses the (i) electron density in the short (microscopic) length scale, useful for understanding chemical binding in molecules and solids as well as reactivity, (ii) particle number density in the intermediate (mesoscopic) length scale, useful for the investigation of soft matter systems and (iii) property density in the large (macroscopic) length scale that considers materials as a continuous medium.

In spite of the differences in the nature of the density variables used at different length scales, the corresponding theoretical frameworks involving energy density functionals, the so called Density Functional Theory (DFT) have been found to possess an underlying unified structure, covering quantum as well as classical systems. Within this broad framework, theoretical formalisms and computational algorithms, have attracted a great deal of attention in recent years.

In this context, the objective of the talk would be to first introduce the concept of density and the relevant energy density functionals across different length scales. As illustrative examples, the main emphasis will be applications of DFT for classical systems using particle number density as basic variable, while highlighting the similarities and dissimilarities with DFT of quantum systems, which uses electron density as the basic variable. The applicability to systems with length scale in the nano domain where the bridging of quantum and classical DFT will be desirable will also be highlighted. The formulation of DFT for time-dependent systems as well as DFT in parameter space will also be outlined.

An introduction to spin-orbit driven emergent phases.

Indra Dasgupta

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Spin–orbit coupling (SOC) is a relativistic effect, which may be thought of as an interaction between the intrinsic spin moment of an electron and the magnetic field generated in the rest frame of the electron due to its orbital motion around the positively charged nucleus. We shall illustrate that the combined effect of electron correlations and SOC leads to novel J_{eff}=1/2 Mott Insulators, bond-directional dependent exchange interactions important for the realization of Kitaev spin liquids and the possibility of Magnon Chern Insulators in honeycomb systems. [1], [2], [3].
In addition, we shall show emergence of Rashba and Dresselhaus spin–orbit interactions due to a gradient of electrostatic potential in non-centrosymmetric systems. Rashba-Dresselhaus systems exhibit characteristic spin textures important for spintronics research [4], [5] [6].

[1] Subhadeep Bandyopadhyay *et. al.* Physical Review B **105**, 184430 (2022)
[2] Atasi Chakraborty *et. al.* Physical Review B **104**, 115106 (2021)
[3] S Kundu *et. al.* Physical Review Letters **125**, 267202 (2020)
[4] S Bandyopadhyay and I Dasgupta, Phys Rev B **103**, 014105 (2021)

[5] S Bandyopadhyay, A Paul, and I Dasgupta, Phys Rev B **101**, 014109 (2020)
[6] Kunal Dutta, S Bandyopadhyay and I Dasgupta Phys Rev B **108**, 245146 (2023)

Ab initio Molecular dynamics

D G Kanhere

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I plan to give a bird's eye view of important aspects of molecular dynamics covering following topics. Intuitive view of dynamics of interacting particles: N interacting particles, free or in a box of volume V.Born Oppenheimer approximation Statistical Mechanics, ensembles, averages, measurements: Canonical and microcanonical Constant Volume, Constant pressure simulations. How to maintain temperature, Thermostats Numerical solution of equations of motion, velocity verlet, leap frog, time steps and time scale of simulations, Interatomic potentials and their importance, Total energy by density functional method, Hellman Feynman theorem and computation of forces. Plane waves verses localized basis, A quick glance at Car Parrinello method. Modern Machine learning methods for interatomic potentials with application to melting of sodium and aluminum clusters.
All this in one hour!

Berry phase in quantum physics of solids with some case studies

G.P. Das

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Adiabatic evolution of quantum systems leading to new property of a Bloch state, the Berry curvature, have become ubiquitous in quantum physics. It ignited the search for topological properties of electrons in solids via the so-called Berry phase, that is intimately linked with a "geometric phase" or a "Pancharatnam phase" [1,2]. It plays a central role in the theory of electron bands in crystalline materials, and has been extensively used to explain a large variety of phenomena e.g. various (quantum, anomalous, thermal, spin) Hall effects, electric polarization, orbital magnetization and topological insulators and Weyl semimetals [3,4]. In this talk, I shall give a bref pedagogic overview of the conceptual and mathematical foundation of Berry phase and Berry curvature, starting from the basics of geometric phase. I shall then take up some case studies on magnetic Weyl semimetals [5], that breaks either inversion symmetry or time reversal symmetry or both.

[1] M.V. Berry, Proc. R. Soc. Lond. A. Math. Phys. Sci. 392, 45–57 (1984).
[2] F. Wilczek and A. Shapere, Geometric Phasis in Physics, Advanced Series in Mathematical Physics Vol. 5, World Scientific (1989).
[3] Di Xiao et al, Rev. Mod. Phys. 82, 1959 (2010)
[4] D. Vanderbilt, Berry Phases in Electronic Structure Theory, Cambridge University Press (2018).
[5] A. Roy Karmakar, S. Nandy, A. Taraphder, and G. P. Das, Phys. Rev. B 106, 245133 (2022)), A. Roy Karmakar, A. Taraphder and G. P. Das, arXiv:2308.00045 (2024)

Exploring electronic structure through electron spectroscopy

Kalobaran Maiti*

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Electron spectroscopy, a technique based on photoelectric effect, directly probes the electronic structure of a material that derives the material properties. This is an ideal technique to reveal underlying physics of material properties such as superconductivity, magnetism, topological phases of matter etc. I will discuss the basics of the technique and its applications to solve complex problems. Some of the examples are unusual density wave states/giant anomalous
transport in an insulator due to localized electrons at the Fermi level. [1]Impurities and/or vacancies in a material can lead to ferromagnetism with high transition temperature even in a non-magnetic material.[2] We exploited the polarization of the pump pulse in a time-resolved measurement to selectively excite electrons of different orbital character in Fe-based systems and discover that one can selectively heat electrons of a particular character without affecting other electrons.[3,4] This method provides a way to disentangle parameters responsible for exoticity in a material. We discovered a kink in the Dirac bands due to proximity to correlated states.[5]

References:

[1] Maiti, K. et al., Origin of charge density wave formation in insulators from a high-resolution photoemission study of $BaIrO_3$, Phys. Rev. Lett. 95, 016404 (2005).
[2] Maiti, K., Medicherla, V.R.R., Patil, S. and Singh, R.S. Revelation of the role of impurities and conduction electron density in the high-resolution photoemission study of ferromagnetic hexaborides, Phys. Rev. Lett. 99, 266401 (2007).
[3] Adhikary, G. et al., Orbital-dependent electron dynamics in Fe-pnictide superconductors, Phys. Rev. B 98, 205142 (2018).
[4] Adhikary, G. et al., Orbital selective dynamics in Fe-pnictides triggered by polarized pump pulse excitations, Europhysics Letters 136, 17002 (2021).
[5] Datta, Sawani et al., Evidence of electron correlation induced kink in Dirac bands in a non-symmorphic Kondo lattice system, $CeAgSb_2$, Nanoscale 16, 13861 (2024).

At Cross Purposes: Spin-Crossover Systems on Metal Substrates

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Spin crossover systems contain magnetic atoms with partially occupied d-orbitals with two or more nearly degenerate states. The system can be switched between these states by external perturbations such as light, heat or an electric field. Together with experimental collaborators (the group of Vincent Repain at the University of Paris Cité and the group of Johannes Barth and Anthoula Papageorgiou at the Technical University Munich) we have investigated the magnetic properties of spin crossover systems deposited on various metal surfaces. Our density functional theory calculations show that the metal substrate plays an important role in determining the magnetic properties. Depending on the molecule-substrate interactions and the epitaxial strain imposed by the substrate, one can see various interesting phenomena, such as ordered mixed-spin states, and the isomerization of molecules. Of particular interest is the fact that we find one-dimensional coordination polymers in which the Fe atoms are in a ligand field where the symmetry is not octahedral, but planar, with different possible symmetries.

Computational Modelling of Transport Phenomena in a few Semiconductors

Swapan K Pati

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The Boltzmann transport equations for charge carriers and phonons have been developed along with first principles calculations to model and understand the transport processes in semiconductors, for their applications in advanced devices. Using this method, we have computed the thermoelectric efficiency in n-type Gd doped PbTe systems, which was synthesised and studied by an experimental group [1]. We have also computed thermoelectric efficiency in a few interesting and unique materials, namely, p-type SnO-PbO superlattice, n-type S and Te doped Ag_2Se systems and 9 Bi based half-Heusler compounds XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir) [2]. In the second part of my talk, I shall discuss the computational modelling for obtaining thermal conductivity in TlAgSe, which also have been synthesized and investigated experimentally [3]. I shall also discuss one of our recent attempts on finding the reasons behind the contradictory results from the theoretical calculations which predicted orders of magnitudes higher carrier mobility than what was observed experimentally in the transition metal di-chalcogenides (TMDC), $HfSe_2$ [4].

Reference:
1. M. Dutta, R. K. Biswas, S. K Pati, K. Biswas, ACS Ener. Lett. 6, 1625 (2021).
2. R. K Biswas, S. K Pati, ACS App. Ener. Mater. 4, 2081 (2021); R. K. Biswas, S. K Pati, Phys. Chem. Chem. Phys. (2024); S. Paul, S. Ghosal, S. K Pati, ACS App. Ener. Mater. (revision submitted, 2024).
3. R. Pathak, S. Paul, S. Das, A. Das, S. K Pati, K. Biswas, Angew. Chem. Int. Ed. (appeared online, 2024).
4. S. P. Keshri, S. K Pati, A. Medhi, J. Chem. Phys. 159, 144704 (2023).

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

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Novel properties such as piezoelectricity and valley physics arise at the nanoscale which are usually non-existent in the bulk form of the 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 SnNBr (h-NbN) monolayers [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) will also be unveiled [5]. Multifunctional low dimensional materials are also desired in several nanoscale applications. In this context, the conflux of tunable Rashba effect and piezoelectricity observed in flexible MgTe, CdTe, and ZnTe monolayers signify its super high prospects for self-powered flexible-piezo-spintronics [6]. Last but not least, intrinsic carrier mobility estimation in selected 2D materials will be presented, as mobility plays a crucial role in determining the performance of electronic devices [7].

References:

[1] M. K. Mohanta, A. De Sarkar, Phys. Rev. B, 102, 125414 (2020).
[2] P. Nandi, S. Sharma, A. De Sarkar, J. Appl. Phys. 135, 234302 (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] M. K. Mohanta, F. IS, A. Kishore, A. De Sarkar, ACS Appl. Mater. Interfaces, 13, 40872–40879 (2021).
[7] A. Arora, A. De Sarkar, Appl. Phys. Lett. 124, 082101 (2024).

Theoretical Prediction of ZrHfCoNiSnSb High Entropy Half Heusler Alloy with Low Lattice Thermal Conductivity

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Thermoelectric materials, provide an alternative source of energy harvesting by converting waste heat to electrical energy through Seebeck effect. The efficiency of a thermoelectric device depends on a quantity called figure of merit (zT) that depends on the transport properties of the material. Higher the value of zT, more is the efficiency of the material to convert heat. To achieve a high value of figure of merit a material must posess large values of Seebeck coefficient and electrical conductivity and low values of thermal conductivity.

Amongst the ever growing family of thermoelectric materials, half Heusler (HH) alloys are potential candidates for thermoelectric applications at elevated temperatures because of their excellent electrical transport properties and superior mechanical and thermal stability.

However, the high lattice thermal conductivity exhibited by these materials lowers their figure of merit, thereby limiting their use in practical applications. One way to circumvent this problem is to design hHs with complex structures that results in scattering of the heat carrying acoustic phonons.

In this work, using density functional theory based calculations we have proposed a novel hH alloy, namely, ZrHfCoNiSnSb that can be prepared by mixing two stable hHs ZrNiSn and HfCoSb or HfNiSn and ZrCoSb. Our free energy calculations show that these compounds can be synthesized at temperatures greater than 500 K and are stabilized with respect to the parent compounds through enhanced configurational entropy due to the presence of disorder at the different crystallographic sites. A critical analysis of the nature of the chemical bonding shows that there is a mixture of covalent and ionic bonds, which results in hierarchial bonding in the lattice. A consequence of this is that the lattice becomes more anharmonic as is evident from the large spread in the Gruneissan parameter of the acoustic phonons. As a result the computed lattice thermal conductivity of this material at room temperature, considering only normal and Umklapp scattering of the acoustic phonons, is half of that observed in the parent compounds. Moreover, due to the large variation of masses in the atomic species and their disordered arrangement in the lattice the acoustic phonons are further scattered, thereby reducing the lattice conductivity to about 5 Wm-1K-1 at 300 K, which is six times less than that observed in ZrCoSb, one of the parent compounds.

Intriguing Role of spin-orbit coupling on magnetic chirality of systems with broken inversion symmetries: Two examples

Debjani Karmakar

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For systems with broken inversion symmetries, spin-orbit coupling is instrumental to insinuate the antisymmetric and anisotropic intersite exchange interactions. Such exchange interactions play a crucial role to stabilize the magnetic ground states with complex chiral properties, having overreaching consequences on strongly correlated exotic properties of the underlying system. In this talk, we address three such systems after incorporating the dynamical nature of electron correlation. The first one is the Kagome series of magnetic superconductors, AV_3Sb_5 (A = K, Rb, Cs), where the complex interplay of spin-orbit coupling and spontaneous symmetry breaking with the superconducting, magnetic and charge-ordered phases of the system gives rise to a chiral magnetic ground state, having abilities to resolve many experimental conflicts. The second system is the middle member of the Fe_nGeTe_2 (n = 1, 2, 3) series, Fe_4GeTe_2, where the experimentally obtained complicacies of the magnetic and magnetothermal phase-diagram, encompassing multiple complex phases, are explained in the light of its calculated chiral magnetic properties. The third system is a heterostructure of transition metal dichalcogenide monolayer with 80:20 Permalloy, where with gradual increase of the spin-orbit coupling along MoS_2 - $MoSe_2$ - WS_2 - WSe_2, the system acquire a spin-spiral ground state.

Hole-doped two-dimensional magnets

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The cryogenic ordering temperatures of current two-dimensional magnets present a major challenge to their technological applications. This lecture will explore strategies to enhance magnetic properties, focusing on carrier-doping, particularly hole-doping. We will explore how microscopic magnetic interactions can be engineered to adjust the ordering temperature, using prime examples such as vander Waals magnets, including chromium trihalides and ditelluride. Additionally, we will discuss fascinating electronic and magnetic phase transitions in ultrathin nanosheets of ruthenates and iridates, where electron correlation, spin-orbit coupling, and kinetic energy compete to shape magnetic properties. The results presented are based on first-principles calculations coupled with Monte Carlo simulations, utilizing Heisenberg-Kitaev spin models.

Spin-Orbit Coupling in Ferroaxial Materials: Driving the Fourth Ferroic Order and Hidden Spin Polarization

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The spin-orbit interaction in condensed matter systems gives rise to a wide range of electronic, magnetic, and transport properties, from jeff=1/2 Mott insulators and magnetic skyrmions to hidden magnetic orders, along with fascinating geometric properties of Bloch bands and spin textures in reciprocal space, resulting in unconventional charge and spin transport. In this talk, I will focus on how spin-orbit interaction drives the emergence of the fourth type of ferroic order parameter—the electric toroidal dipole moment—completing
the set of known ferroics: ferromagnets, ferroelectrics, and ferrotoroidics. The electric toroidal dipole is the electric counterpart of the magnetic toroidal moment, defined both by the vortices of local dipoles and the cross product of orbital and spin angular momenta. The electric toroidal dipole moment has recently gained attention in the context of ferroaxial materials, which undergo a structural transition from a non-ferroaxial to a ferroaxial phase, characterized by a pure rotational mode, as the temperature decreases. Using examples of prototypical ferroaxial oxides with order-disorder and displacive transitions, I will highlight the crucial role of spin-orbit coupling in generating a non-zero atomic-site electric toroidal dipole moment, establishing it as the order parameter for these transitions. Additionally, I will discuss the hidden spin polarization in the band structure, which arises from the interplay of spin-orbit interaction and local inversion-symmetry-breaking sub-units, which also lead to vortices of local electric dipole moments.

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Sayantika Bhowal and Nicola A. Spaldin, “Electric toroidal dipole order and hidden spin polarization in ferroaxial materials”, arXiv 2407.08369 (2024).

Probing Magnetic & Defect structures in Oxides/Mixed Oxides of U, Pu, Am and Np through DFT

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Actinide oxides play an important role in a nuclear fuel cycle. On the one hand, UO_2 and PuO_2 and their mixed oxides (MOX) $(U,Pu)O_2$ serve as fuels in nuclear reactors; while on the other hand, burning of nuclear fuel generates a significant amount of minor actinides (MA), e.g., (isotopes of) Np, Am, Cm, etc. with half-lives running upto million of years. One way of disposing these long-lived radioactive MA is to transmute them by using them along with the fuel in a fast reactor. This involves formation of MOX of these actinides. The study of these MOX is particularly challenging due to complex magnetic structures of its end members, e.g., in $(U,Np)O_2$ MOX, UO_2 exhibits 3-k transverse magnetic structure and NpO_2 exhibit 3-k longitudinal magnetic structure. The talk will discuss the magnetic structures of $(U,Np)O_2$ MOX. Another important aspect of these actinide oxides is their non-stoichiometry ($AnO_{2\pm x}$). The deviation from stoichiometry governs the efficiency of burning of the fuel. Therefore the point defects and the non-stoichiometry in these oxides have been a subject of intense interest. This talk will also focus on stability and electronic properties of $PuO_{2\pm x}$ and vacancy-ordered structures in PuO_{2-x} and AmO_{2-x}.

Non-volatile electrically switchable half-metallicity in multiferroic TMDC-MXene heterostructures

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Rational control of Van der Walls ferromagnets to accomplish better performances in nanodevices can be done by electrical control which enables switching between magnetic states. For sustenance of this approach, the electrical control need to be non-volatile that is one which does not require persistent electrical control. One proven strategy to obtain non-volatile coupling
of electric and magnetic properties is construction of heterostructures. An heterostructure comprising of a ferroelectric and a ferromagnetic material can lead to non-volatile switching between magnetic states upon switching polarisation of the ferroelectric component in the heterostructure. In this work, we demonstrate this through bi-layer and tri-layer TMDC-MXene heterostructures.

Strong orbital-selective spin-orbital-phonon coupling in $CrVO_4$

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Coupling of charge, orbital, spin, and lattice degrees of freedom (d.o.f.) are essential to realizing various functional properties such as ferroelectricity, magnetoelectric effect, metal-insulator transition, superconductivity, and charge-density-wave (CDW). However, the relative contribution of the competing orders to controlling the desired behavior is challenging to decipher. A detailed experimental and theoretical mapping of electron, electron-spin, and lattice susceptibility is necessary to decipher the governing mechanism(s). In this talk, I will focus on the coupling of orbital degree of freedom with a spin exchange, i.e., Kugel-Khomskii-type interaction (KK) in $CrVO_4$ [1]. In general, KK-type interactions lead to deviation in experimental observables of coupled Hamiltonian near or below the magnetic transition. Using phonon, electron, and magnon spectroscopy experiments, we report anomalous changes in lattice parameters, electronic states, spin dynamics, and phonons at four times the Neel transition temperature (TN) in $CrVO_4$. The temperature is significantly higher than other d-orbital compounds, such as manganites and vanadates, where effects are limited to near or below TN. The experimental observations are rationalized using first-principles and Green's function-based phonon and spin simulations that show unprecedentedly strong KK-type interactions via a super-exchange process and an orbital-selective spin-phonon coupling coefficient at least double the magnitude previously reported for strongly coupled spin-phonon systems.

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Spin-orbit coupling and its dependence on magnetic symmetry applied to the enigmatic case Mn_3Sn

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Although weaker than exchange interactions the spin-orbit coupling plays important roles for magnetic states. However, historically these roles have mainly been studied for collinear states, leading to knowledges that cannot always be transferred to non-collinear states. In this presentation the symmetry of magnetic states will be briefly discussed for the most general case and how it influences both physics usually attributed to spin-orbit coupling as well as alter the effects of spin orbit coupling.

This kind of approach will be exemplified by results for some simple non-collinear magnets but mainly by results for the hexagonal co-planar magnet Mn_3Sn, which is mainly antiferromagnetic but with a weak ferromagnetic component. These magnetic materials will be theoretically studied through electronic structure calculations that are capable of handling non-collinear states. The results that will mainly be discussed are the variations of total energies and calculation of the pair exchange interactions for these magnetic states.

Some non-trivial results are that the spin-orbit coupling is inter-mixed with the effects from the non-collinear state, which for instance leads to the fact that, in opposition to existing arguments in literature, the weak ferromagnetic state of Mn3Sn originates from Dzyaloshinskii-Moriya interactions due to spin-orbit coupling, although perhaps in a non-trivial fashion.

Examining the ground state of the Slater insulator $NaOsO_3$

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Metal insulator transitions (MIT) have been widely studied in condensed matter physics as a suitable platform to understand the effects of correlations between electrons. In the Mott Hubbard picture, such transitions, driven by electron electron interactions, are usually accompanied by structural distortions. However, Slater put forward a different scenario where electron localization is caused by emergent antiferromagnetic ordering that opens up a band gap. There is no role for structural distortions in this transition. However, finding a material realization of a Slater insulator has been difficult as most materials that show a MIT have also been found to go through structural changes and symmetry lowering. NaOsO3 was considered to be an exception to this when it was found that the MIT in this material is also accompanied by a long-range, collinear G-type antiferromagnetic (AFM) ordering setting in. Although $NaOsO_3$ is usually accepted as an example of Slater insulator, some studies have put forward the idea of spin-orbit driven Lifshitz transition being responsible for the MIT in NaOsO3 I will discuss aspects of the ground state found in $NaOsO_3$ and the phase diagram that one finds under pressure.

Spin U(1) quasi-symmetry in materials with a quantized spin Hall effect

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Quasi-symmetry is an approximate symmetry of the Hamiltonian that holds under first-order perturbations but may break down in higher-order terms, potentially leading to a small hybridization gap between states with different characters, such as valley, orbital, or spin. Spin U(1) quasi-symmetry thus refers to the conservation of the S_z spin component at low energies, with minor corrections from higher-order spin-mixing terms at higher energies. In this talk, I will introduce the spin U(1) quasi-symmetry and demonstrate its presence in group Va monolayers with puckered lattices [1]. I will show how phosphorene and group Va monolayers realize atomically thin obstructed atomic insulators and transition to a state with significant spin-Berry curvature and a record-high quantized spin Hall effect. Through model Hamiltonian analysis, I will highlight the role of spin U(1) quasi-symmetry in realizing the double quantum spin Hall effect, supported by our calculations of spin-filtered edge states and spin Hall conductivity.

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Non-Linear Hall Effect in Flatlands and Chiral Crystals

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In recent years, it has been discovered that inversion symmetry broken systems can exhibit non-linear Hall effects even under time-reversal symmetric conditions [1]. The underlying quantum objects leading to this phenomena are the moments of the Berry curvature, termed the Berry curvature multipoles. This opens up avenues for exploring fundamental physics and possible applications [2,3]. However, despite such promise, the Berry curvature multipole induced non-linear Hall effect has been experimentally realized only in a handful of materials. It is, therefore, of vital importance to find materials with large and controllable Berry curvature multipoles.

In this talk, I will give examples from our work where such a controllable Berry curvature dipole has been predicted. First, we propose a giant non-linear Hall effect in the elemental buckled honeycomb lattices -- silicene, germanene, and stanene [4]. We show that the Berry curvature dipole is tunable by a transverse electric field which breaks inversion symmetry. We demonstrate that the electric field induced topological phase transitions are associated with a giant Berry curvature dipole near the critical field. Next, I will present chiral systems as promising platforms to study the non-linear Hall effects [5]. We use state-of-the-art first-principles computations, in conjunction with symmetry analyses, to explore a variety of chiral material classes. We demonstrate that the two enantiomeric pairs exhibit an opposite sign of the Berry curvature dipole, which may enable their identification via a non-linear Hall response.

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Spin-spiral magnetism in Honeycomb lattice of $CaMn_2P_2$ – A First-principles and Monte Carlo perspective

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Recently the Mn-based 122 type have been studied intensely owing to their close stoichiometric 122-type relationship to high-Tc iron pnictides and also as a new family of magnetically frustrated materials. In this context, we have theoretically studied the electronic structure and magnetism of antiferromagnetic insulator $CaMn_2P_2$ which adopt the trigonal structure containing corrugated Mn honeycomb layers.

In this talk, we will discuss our recent results on this system based on density functional theory + Hubbard U (DFT+U) approach and spin-dynamics simulations. Our results suggest that the observed spin-spiral ground state could be understood in terms of a simple Heisenberg Hamiltonian that include the 1^{st} and 2^{nd} nearest neighbour magnetic couplings (J_1 and J_2). Further, we proposed a phase diagram as a function of the ratio of J_2/J_1 that demonstrate the possibility of achieving a number of magnetic ground states with different spin-spiral propagation vectors (q-vector). We showed that in practical these states could be realized by simply applying tensile strain along crystallographic a and b-directions.

Controlling Hall response in epitaxial Mn_3Sn thin films

Shouvik Chatterjee

Non-collinear antiferromagnet Mn_3Sn has been shown to exhibit large anomalous Hall effect at room temperature and is a promising material system for spintronics applications[1-5]. However, so far anomalous Hall effect has only been observed with magnetic field lying within the Kagome plane. Here we show that it is possible to engineer canting of Mn moments out of the Kagome plane due to anisotropic in-plane strain in epitaxial Mn_3Sn thin films synthesized on tantalum buffer layers. This breaks both mirror and time-reversal symmetries that allows non-zero anomalous Hall conductivity with magnetic field applied perpendicular to the Kagome plane, which we observe in our thin films. In addition, we show that interfacial Dzyaloshinskii-Moriya interaction in Mn_3Sn/Ta bilayers can stabilize skyrmions leading to large topological Hall effect, appearance of which can be tuned by designing artificial heterostructures involving Mn_3Sn and heavy metal layers. Furthermore, both the anomalous and topological Hall effects can be tuned by application of electric current with modest current densities of ~1.8×10^{10} A/m^2. Our results establish the potential of realizing novel functionalities in Mn_3Sn by thin film engineering.

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Experiment, computation, and a possible quantum critical point in SmN

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The observation of a superconducting ground state of samarium nitride below 4 K is surprising in the light of it's semiconducting and ferromagnetic nature [1]. We investigate this unconventional superconductivity in SmN in the context of the breakdown of order between two magnetic phases. Nitrogen vacancy doped $SmN_{1-\delta}$, is a semiconductor which lies in the intermediary between ferromagnetic SmN and anti-ferromagnetic Sm metal. To explore the origin of unconventional superconductivity in SmN, we have undertaken a mixed experimental and computational study on $SmN_{1-\delta}$ films doped to cover a wide range of conductivities.

We show that the DFT+U band structure of SmN represents the physical material over a wide range of nitrogen vacancy doping, and that electrical transport is mediated though in-gap defect states, which project strongly onto majority spin Sm 4f states. We have tracked the superconducting and magnetic transitions of SmN and found that the most robust superconductivity is near the breakdown of magnetic order, at the boundary between the FM and AFM phases of SmN and Sm metal [2]. Our measurements point to the location of a quantum critical point in the SmN-Sm phase diagram and, coupled with anomalous Hall measurements of SmN [3, 4] provide an indication that the observed superconductivity is of unconventional S = 1 (spin-triplet) type.

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A refinement based approach for extracting electronic band structure information and its application in thermoelectric materials and devices

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Investigation of electronic band structure (EBS) plays a significant role in the advancement of thermoelectric materials and devices. Sophisticated experiments and theoretical calculations are usually required to obtain EBS information which represents a bottleneck in studying the vast number of thermoelectric materials. In this work, a refinement based approach, referred as multi-band refinement technique (MBRT)[1], for analyzing EBS of thermoelectric (TE) materials will be discussed. A least square minimization based approach is adopted for extracting EBS information, with the input being experimental electrical properties and an electronic structure model. In the presentation, the methodology and the validation of the technique using standard materials will be presented. In addition, the applicability of MBRT for analyzing the EBS of TE materials and utility in development of high efficiency TE devices will be discussed based on specific examples.

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Phonon thermal transport in low- and high-thermal conductivity solids

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Understanding phonon thermal transport physics in semiconductors is crucial for applications such as thermoelectricity, nuclear reactors, heat dissipation, data storage, etc. Conventionally, the thermal transport in crystalline semiconductors is described using Boltzmann Transport Equation with three-phonon intrinsic phonon-phonon scattering. Recently, this description of phonons needs to be revised to explain thermal transport in technologically relevant low- and high-thermal conductivity solids. In this talk, I will present some of our group efforts on methodology development to account for the relevant higher-order thermal transport physics for these materials. I will show results for two material systems, one with ultra-low thermal conductivity where temperature-dependent sampling of the potential energy surface, phonon renormalization due to anharmonicity, four-phonon scattering, and multi-channel thermal transport are all necessary, and the second system where all available methodologies fail, and the obtained thermal conductivity from state-of-the-art calculations is off from the experimental measurements by a factor of 3-5. [1-2]

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Nano-ring to Nano-barrel: Structural Evolution of CuO Clusters

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Monoclinic CuO is anomalous both structurally as well as electronically in the 3d transition metal oxide series. It deviates substantially from the trends of other monoxides (rock-salt structure) with lower atomic number.
One of the most fundamental applications of cluster science is to understand the evolution of materials at the sub-nanometer scale. In this presentation I shall discuss the atomic and electronic structures of (CuO)n clusters for n=1 to 12 using the plane wave based pseudo- potential approach under DFT formalism. The total energy calculations were carried out using LDA+U and hybrid functional approach along with spin-orbit coupling term. Two standout features in the structure evolution are; (i) upto heptamer, CuO clusters favor planar nano-ring structure and from octamer onwards they adopt three-dimensional motif with $(CuO)^{9}$ and $(CuO)^{12}$ forming a barrel shaped layered structure, (ii) $(CuO)^{4}$ planar ring structure acts as a building block to grow larger clusters in particular, $(CuO)^{8}$ and $(CuO)^{12}$ clusters. The correlation between the atomic structure and bonding has been established by detailed analysis of the energy states spectrum of these clusters. The results showed interesting competition between the bond strength of Cu-O (d-p) and Cu-Cu (d-d) governs the growth pattern from 2D-planar nano-ring to 3D-layered structure.

Beyond d-band center to identify the catalyst for oxygen evolution reaction

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Descriptors obtained through computational studies play important role in designing a catalyst for several catalytic reactions. A good descriptor can explain the catalytic activity and used to design new materials with selectivity. The d-band center is a well-known descriptor used for various reactions [1], however it fails to give significant correlation where the electronic environment is slightly for a same metal. Using Density Functional Theory (DFT), single atom catalysts embedded on two types of graphene nanoribbons for pristine and doped cases are used to check the oxygen evolution reaction activity. From these systems, possible d-band and p-band based descriptors were individually tested and proved no correlation with OER activity [2]. The approach of using multi-descriptor instead of single descriptor is proposed to address the peculiar descriptor problem and can be extended to other electrocatalytic reactions. The d-band frontier and the d-band occupancy scaled by width corrected band center together correlates with OER activity for same metal site under varying electronic environment. 432 active sites tested for OER activity using DFT and 105 possible descriptors are individually assessed for activity correlation and optimized using PCA and 8 machine learning algorithms.

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Polarization Coupled Magnetization Switching in Oxide Perovskites

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A key criterion for multiferroic materials is the ability to achieve combined switching of polarization and magnetization. This can be facilitated by inherent structural distortions and their coupling. In this talk, I will present two examples that demonstrate how structural modes play a crucial role in controlling polarization-magnetization switching.

First [1], I will discuss an improper ferroelectric hexagonal ABO_3 system, specifically $Lu_{1-x}Hf_xFeO_3$ (h-LHFO), where heavy electron doping in $LuFeO_3$ (h-LFO) induces spin-disproportionation in the Fe sublattices. Particularly for x = 1/2 and 2/3, this results in robust, room-temperature, out-of-plane, collinear ferrimagnetism, stabilized by a Jahn–Teller metal-to-insulator transition. Additionally, I will present heterostructures combining h-LHFO with a ferroelectric/ferromagnetic (FE/FM) monolayer MnSTe (h-2D), where skyrmions are stabilized without an external magnetic field. The chirality of these skyrmions is controlled by an external electric field via the polarization of h-LHFO, opening new possibilities for magnetoelectric applications.

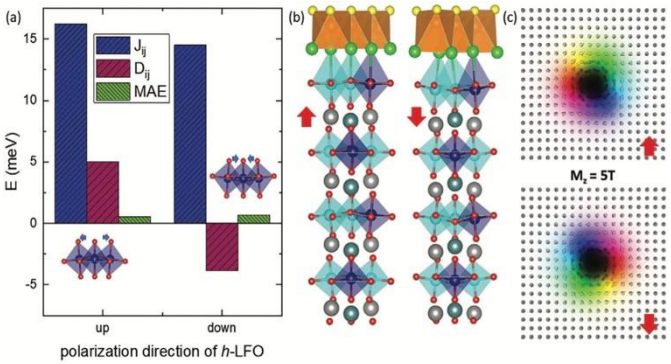

Figure: Polarization - Magnetization Coupling in electrondoped h-LHFO

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

Acknowledgments

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Coupling of the Structure and Magnetism to Spin Splitting in Hybrid Organic-Inorganic Perovskites

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The ability to couple structural, electric and magnetic degrees of freedom to materials properties is of tremendous scientific and technological importance. For example, coupling between structural and electron spin degrees of freedom is promising for applications in spintronics. Spin–orbit interactions in solids give origin to the so-called Rashba and Dresselhaus effects, which originate from structural inversion asymmetry and bulk inversion asymmetry, respectively [1]. Spin splitting leads to spin-momentum locking, which manifests in the existence of spin polarizations in momentum space or spin textures. In ferroelectrics, spin textures could couple to the electric polarization, which is known as ferroelectricity Rashba effects cofunctionality. Such coexistence allows for the control of spin-momentum locking by the external electric field [2-3]. Structural degrees of freedom are typically associated with ionic positions and lattice vectors and can be manipulated through temperature and external fields. Ferroics usually offer great opportunities for structural
manipulations, as they have a tendency to undergo phase transitions and often couple to electric fields. Magnetic degrees of freedom are usually associated with localized spins and may be either disordered or ordered. More subtle effect of spin splitting has been predicted from group theoretical analysis in antiferromagnetic (AFM) materials. Remarkably, some AFM materials can exhibit spin splitting even in the absence of spin–orbit interactions [2-3].
With the help of first-principles simulations, we find spin splitting in both conduction and valence bands of $[NH_2NH_3]Co(HCOO)_3$ induced by spin−orbit interactions, which can reach up to 14 meV. The direction of the associated antiferromagnetic order parameter is strongly coupled with spin splitting in the centrosymmetric phase, allowing for the creation and annihilation of spin splitting through the application of a magnetic field. Furthermore, the structural phase transition to the experimentally observed polar Pna21 phase completely
changes the aforementioned spin splitting and its coupling to magnetic degrees of freedom. This reveals that in $[NH2NH_3]Co(HCOO)_3$, the structure and magnetism are strongly coupled to spin splitting and can be manipulated through electric and

magnetic fields [1]. We believe that our findings offer an important step toward a fundamental understanding and practical applications of materials with coupled properties.

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Realizing Friedel oscillation in the orbital chanel: Valley driven physics of $NbSe_2$ with a magnetic impurity

B. R. K. Nanda, IIT Madras

Due to the coupled spin-valley physics, monolayer 2D transition metal dichalcogenides (TMDs) show many unusual electronic and transport properties. In this talk, we will show that a magnetic impurity in the metallic TMDs such as the $2H{-}NbSe_2$ induces a large orbital polarization in its neighborhood with a Friedel type oscillation, in addition to the usual spin polarization. We study the orbital polarization, hitherto unexplored for any impurity system, using the impurity Green's function approach as well as tight-binding and density functional methods. Concrete results are presented for the Mn substitutional impurity in $NbSe_2$ from density-functional calculations. The orbital polarization here is due to the orbital moment imbalance between the K/K' valleys, which is driven by the impurity-induced spin imbalance. Our work demonstrates the Friedel oscillation for the first time in the orbital channel.

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Data-Driven Discovery of Quantum Compatible Deep Centres in Semiconductors

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Deep centres in semiconductors present a promising avenue for addressing several longstanding challenges in the design of qubits, the fundamental units of quantum information processing. These defects introduce isolated bound electronic states deep within the material's band-gap, engineered to possess atom-like discrete energy levels. Exhibiting high coherence times, operational fidelity, and scalability with current fabrication technologies, they are strong contenders for future quantum technologies.

While a few quantum-compatible defects have been identified, notably in colour centres within diamond and silicon, the discovery of novel host materials with superior quantum coherence properties remains elusive. A key obstacle is the incomplete understanding of the structure–activity relationships that a host material must exhibit to support such defects. Developing this holistic understanding is currently beyond the reach of modern computational condensed matter simulations. Traditional approaches, such as *ab initio* searches, are resource-intensive and frequently yield results by chance.

In this work, we propose data-driven modelling as an efficient alternative for identifying suitable host materials. By exploring the feature space defined by machine-learnable representations of physical properties that govern the formation of deep centres, we construct machine learning models to capture the key influences on quantum compatibility. Our comparative analysis of these models demonstrates that a semi-empirical, holistic framework can be established, providing valuable insights into the structure–activity relationships required for host materials to support quantum-compatible defects.

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Strategic role played by the SOC in emerging magnetic and topological phases in oxides and alloys

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The role of the spin orbit coupling turns out to be one of the most crucial energy scales in emerging novel quantum phases across the electronic, magnetic and topological phases of matter. The current presentation based on how SOC plays the strategic role in dictating the J eff states in the iridates and topological crossover from insulator to Weyl semi metallic phases in the chalcopyrites.
It is common notion that for the iridates the SOC energy scales is the dominating factor in deriving Jeff states which eventually leads to the SOC enhanced Mott insulator over the conventional correlated Mott insulators. However, recently there are examples of iridates where the possibility of realization of Jeff state is not only determined by the SOC, rather competition with the other energy scales involved in the systems. In the presentation such low dimensional quantum magnet belonging to the iridate family will be discussed, where the unique balance of the SOC, band width, electronic configuration will dictate the weather one will get a correlated Mott insulator or SOC coupled Mott Insulator.
Along with that, we know SOC is very crucial to drive topological non trivial states either topological insulator or Weyl semimetal by breaking the symmetry. However, SOC can be also very important to do crossover from topological insulator to Weyl semi metallic phases in the same materials. Chalcopyrites alloys with time reversal symmetry will be one of the ideal platforms to transition from two different topological phases just by tuning the SOC strength. Interestingly, SOC coupled with the hybridization effect drives such interesting
topological crossover.

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Generation of efficient spin currents in topological and altermagnetic materials

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Generating efficient spin currents is crucial for the development of non-volatile memory technologies, and the band structure of materials plays a key role in this process [1]. Spin-orbit coupling can generate significant spin-Hall currents with Rashba-type symmetry under non-equilibrium conditions driven by either an electric current or a thermal gradient [1]. I will present our findings on electrically driven spin currents in the Dirac nodal line semimetal IrO_2 [2] and thermally driven spin currents in the topological insulator Bi_2Se_3 [3]. These spin-Hall currents are sufficiently large to switch both 2D and 3D perpendicular magnetic materials [4]. Following this, I will introduce a novel method of spin-current generation using "tilted spin currents" in altermagnets [5], a newly discovered class of magnetic materials [6]. This approach could provide an efficient means for controlling perpendicular magnets, potentially enabling high-density memory applications [6].

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Abstracts of Poster Presentations

A1. C3N-based buckled dumbbell-like morphologies - New Age Topological Thermoelectrics?

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Two-dimensional carbon nitride materials have been the center of attention for their diverse usage in energy harvesting, environmental remediation and nanoelectronic applications. A broad range of utilities with decent synthetic plausibility have made this family a sweet spot to dive into, whereas the underlying analytical aspects are yet to have prominence. Recently, using the machinaries of first principles, we reported a family of six different structures C3NX [J. Phys. Chem. C 127 (2023) 18001] with a unique dumbbell-shaped morphology, functionalizing the recently synthesized monolayer of C3N [Adv. Mat. 29 (2017) 1605625]. We have critically explored the underlying non-trivial topological phases of the semimetallic Dumbbell C3NX sheets and nanoribbons. Spin-orbit coupling (SOC) induced gap across the Fermi level, its subsequent tuning via an external electric field, portrayal of band inversion from the Berry curvature distribution and the evaluation of Z2 topological index using the Wannier charge center (WCC) firmly establishes the traces of topological footprint. Fascinating features of these quasi-1D systems are observed utilizing the Su-Schrieffer-Heeger (SSH) model where different twisted phases reveal distinct topological signatures even in a low atomic mass system like DB C4N. The `light-heavy' admixture of primary band valleys added to the heavier secondary valley convergence entertains ultrahigh carrier mobilities with large Seebeck coefficients. Higher weighted mobility added to substantial anharmonic scattering induces ultralow lattice thermal conductivity that imparts an impressive thermoelectric quality factor. Large room temperature power factors at optimum carrier concentrations lead to a maximum thermoelectric figure of merit of 0.80 (and 0.94 at 900 K) with decent conversion efficiency. These findings critically address the future prospect of waste heat management abilities of these new topologically non-trivial dumbbell-like geometries.

A2. Density Functional Studies on Li-Based Anti-Perovskite Materials for Solid State Battery Applications

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Rechargeable Li-ion batteries with high energy density and ensured safety are regarded as next-generation energy storage devices. Traditional Li-ion batteries use liquid electrolytes which are toxic and flammable1. So replacing liquid with solid electrolytes promises to be safer2. In this work we made the first principle studies on the anti-perovskite materials Li3OX (X = Br, Cl) for calculating its electronic band structure, the density of states, and effective mass using GGA-PBE and GLLB-SC3 exchange-correlation functionals. All the calculations are done using an open-source Python tool called GPAW and the Atomic Simulation Environment (ASE) modules, which utilize the Projected Augmented Wave (PAW) method. Before the property calculations, we optimize the structural parameters using the Broyden- Fletcher-Goldfarb-Shanno (BFGS) optimization method. The structural optimization was done using the energy cut-off of 900eV with 7×7×7 k-mesh and force convergence of 0.01eV/Å.

From the electronic band structures, we found that both the materials possess wide band gaps (>5eV using GLLB-SC and >4 using GGA-PBE) which shows that both materials can have a wide electrochemical stability window, which is a major property that a solid-state electrolyte material should have. From the density of states of both the materials, we noticed that Li s and p-orbitals have main contributions in the conduction band which indicates the diffusion of Li ions in the materials, which is critical for ionic conductivity. We also find the effective mass of holes and electrons in different high-symmetry points to understand the mobility of the electrons. Our results show that Li3OX (X = Br, Cl) materials have the potential to be used as solid-state electrolytes for solid-state battery applications.

A3. Designing layered oxides as cathodes for sodium-ion batteries: A density functional theory-based modelling

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Sodium-ion batteries (SIB) have acquired significant attention due to its natural abundance and low cost. Transition metal oxides with layered structures have been reported to be one of the promising electrode materials for SIBs [1]. Both P2 and O3-type sodium layered oxides+ (NaxTMO2, TM = different 3d transition metals) have been identified as cathodes for SIBs with faster Na diffusion and high-rate kinetics. However, low capacity at the initial stage of cycling limits their application. To overcome this issue, the strategy of dual doping of 3d transition metals (TM) with equal concentration has been employed. For instance, it has been found that the P2-NaxFe0.5Mn0.5O2 cathode exhibits a high discharge capacity of 190 mAh/g at a rate of 0.07 C [2]. In this work, we have enumerated a series of 3d TM doped cathode compositions, considering the parent P2-NaxFe0.5Mn0.5O2 compound as a backbone structure. Na0.67TM10.5TM20.5O2 where, (TM1, TM2) ε {(Ti, Cr), (Ti, Fe), (V, Fe)} and Na0.67TM10.5TM20.5O1.944F0.056 where, (TM1, TM2) ε {(Ti, Cr), (Ti, V), (Ti, Fe), (Ti, Ni)} has been identified by the first principles density functional theory (DFT) calculations, which results in an average voltage between 2.8 to 4.4 V. We further assessed the phase stability, electronic structure, magnetic property and dynamic stability of each of these non-stoichiometric compounds using DFT and ab initio molecular dynamics (AIMD) simulations. Additionally, the magnetic moments of the 3d TMs as well as their valence states have been estimated by examining the t2g–eg resolved densities of states for each TM in the systems. The combination of the above mentioned electronic properties suggests that these compounds are promising candidates for enhancing the performance of sodium-ion batteries. Our approach could significantly accelerate the discovery of novel cathodes and provide valuable insights for the study of intercalating materials.

A4. Ab-initio calculation of Lattice Thermal Conductivity of Janus Graphene

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Unlike other two-dimensional Janus materials such as MoSSe which exhibit different properties on either side of their atomic planes owing to the presence of multiple elements, different adatoms on both sides or stacked heterojunctions, Janus graphene presents an 'intrinsic' symmetry breaking to account for the effect. Thermoelectric (TE) materials with a high thermoelectric figure of merit (ZT) are an effective way to reduce energy consumption while protecting the environment. Maximizing the efficiency of thermoelectric materials requires a low value of lattice thermal conductivity (κlat). Through this paper, we aim to study the phonon transport in the newly discovered 2D material, Janus graphene, within the framework of the Peierls-Boltzmann Transport Equation (PBTE). The optimum combination required for a high value of ZT is observed to be unique to semiconductors. In semiconductors, thermal conductivity is predominantly due to contribution from lattice owing to low charge carrier concentration. The bandgap of the material calculated through the PBE GGA approximation, confirms it to be a semiconductor. With the increasing emphasis on use of 2D materials for micro/nanoelectronic applications with the advantage of device miniaturization, exploring a potent material like Janus graphene could be crucial in the design of TE devices.

A5. First principle study of thermoelectric properties of Nb_2Co_2InSb and Nb_2Co_2GaSb double half-Heuslers

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Valence electron count (VEC) 18 half-Heusler (hH) alloys are promising candidates for thermoelectric applications at high temperatures due to their excellent Seebeck coefficient, mechanical robustness, and thermal stability. However, their high lattice thermal conductivity (kL) poses a significant challenge for thermoelectric efficiency. Introduction of mass disorder at lattice sites can be an effective strategy to reduce the kL by scattering of heat carrying phonons. NbCoSn is an example of a half-Heusler alloy with a low figure of merit (zT) of just 0.05[1], despite its high power factor of 2.1 mW/mK2 at room temperature. This low zT is primarily attributed to its lattice thermal conductivity, which has been experimentally measured to be 13.25 W/mK[1] and theoretically predicted to be 18 W/mK[2] at room temperature. In this project, we investigated the thermoelectric properties of different structural phases of Nb2Co2InSb and Nb2Co2GaSb, which can be viewed as variants of NbCoSn where Sn atoms are replaced by In/Ga and Sb atoms. Our study included two ordered structures and two Special Quasirandom Structures (SQSs). According to our calculations, all of these phases are dynamically stable, as indicated by the absence of imaginary modes in the phonon spectra. The relative energetics analysis reveals that, for Nb2Co2InSb, the ordered structure is the most stable one while for Nb2Co2GaSb, the 2×2×2 SQS structure is the most stable configuration. Using the Debye-Callaway model[3], we calculated kL, finding it to range between 5.5 W/mK and 6.9 W/mK (4.7-5.8 W/mK) at room temperature for the different phases of Nb2Co2InSb (Nb2Co2GaSb). We note that the values of kL for these double half-Heuslers are less than half of that observed in ternary NbCoSn. This reduction in lattice thermal conductivity leads to a zT of 1.1 for n-type and 1.42 for p-type in one of the SQS phases of Nb2Co2InSb at 1000K. For the ordered phases of Nb2Co2GaSb at 1000K, the zT values are 1.7 and 2.0 for n-type and 1.1 and 1.3 for p-type, respectively. Hence our calculations predict that these can be used for both p-type and n-type thermoelectric material.

A6. Multifunctional $La_{1-x}Sr_xMnO_3$ Perovskite for Enhanced Energy Storage and Conversion in Supercapacitors, Zn-Air Batteries, and Catalytic Applications

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The rapid advancement of technology, particularly in the fields of portable electronics, electric vehicles, and renewable energy, has intensified the need for efficient, sustainable, and versatile energy storage and conversion systems. Supercapacitors1 and Zn-air batteries2 are pivotal for high-performance energy storage, offering rapid charge-discharge cycles and long-term stability, essential for next-generation portable devices and electric vehicles. Simultaneously, catalytic processes like urea oxidation reaction and water splitting are at the forefront of clean energy production, playing a critical role in hydrogen generation and the conversion of waste into valuable resources3. By critically analyzing recent progress in replacing noble metals with non-precious perovskite-based alternatives, so the researcher's efforts integrating these domains into a single multifunctional material. We examine the impact of strontium doping on the electronic structure, magnetic properties, and spin polarization of La1−xSrxMnO3 (LSM) through experimental and computational studies, where the findings reveal that strontium substitution, significantly improve electrical conductivity, magnetic ordering, and catalytic performance. These advancements position La1−xSrxMnO3 as a promising candidate for supercapacitors, Zn-air batteries, urea oxidation reaction, and water splitting applications. This work presents material design for multifunctional, offering a comprehensive approach to the development of advanced energy technologies that are both efficient and sustainable.

A7. Effect of AFM Ordering on Thermoelectric Responses of Mg_3X_2 (X: C, Si, Ge) Monolayers: A DFT Insight

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Two-dimensional materials have gained a lot of attention in the last few decades due to their potential applications in thermoelectric and nano-electronic devices [1,2]. This study systematically presents the mechanical, electronic, and thermoelectric characteristics of two-dimensional honeycomb-Kagome Mg3X2 (X: C, Si, Ge) structures in the framework of Density Functional Theory (DFT) computations and by solving semiclassical Boltzmann transport equation. The geometrical stability of these structures is validated by phonon diagram and molecular dynamics simulations. Following the elastic constants, we have inferred that all the systems are mechanically stable and brittle in nature. Lower values of Debye temperature of all structures suggest that Mg3X2 monolayers should have lower values of lattice thermal conductivity compared to graphene. Electronic structure calculations indicate that these materials are semimetallic in their nonmagnetic (NM) phase. All the structures display remarkably low lattice thermal conductivity (0.9-1.5 W/mK) due to a large scattering factor and higher anharmonicity. The presence of sharp density of states (DOS) peaks close to the Fermi level, arising from nearly flat and dispersionless band in the antiferromagnetic (AFM) arrangement, is poised to enhance the Seebeck coefficient, thereby potentially boosting the thermoelectric performance. The estimated values of thermoelectric figure of merit (ZT) are around 0.78 and 0.67 for Mg3Si2 and Mg3Ge2 structure respectively in AFM phase at T = 700 K. These outcomes of our findings suggest that Mg3X2 monolayers exhibit substantial promise for thermoelectric device application.

A8. Recent progress in device fabrication using Mg_3Sb_2-Mg_3Bi_2 solid solution

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The Mg3Sb2-Mg3Bi2 solid solution system has become a standout candidate for thermoelectric energy conversion, especially in the mid-temperature range, due to its impressive potential[1]. Recent advancements in device fabrication have been all about fine-tuning these materials to boost their thermoelectric performance and ensure they can withstand practical use. By refining synthesis techniques, exploring different doping strategies, and applying nanostructuring methods, researchers have managed to significantly improve their power output and lower thermal conductivity.

Advanced sintering methods, like spark plasma sintering (SPS), have been crucial in producing high-quality bulk materials with closely controlled grain boundaries, essential for making durable and reliable thermoelectric devices. Furthermore, efforts to create single-leg thermoelectric modules and segmented devices, which combine Mg3Sb2-Mg3Bi2 solid solutions with other materials, are showing real promise for practical applications[2]. This work aims to capture the latest trends in fabrication techniques, address the ongoing challenges of material stability, and enhance device-level performance, ultimately paving the way for more efficient thermoelectric devices powered by the Mg3Sb2-Mg3Bi2 system.

A9. Identification of C_3N/Silicene heterostructure as anode materials for Li-ion battery and its origin

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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.

B1. Phonon-Driven Spin Wave Modulation in Nickel Oxide

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Recent advancements in terahertz (THz) pulse generation techniques,such as difference frequency generation and optical parametric amplification [1] have enabled the precise control of lattice vibrations or phonons in materials, opening new avenues for manipulating their magnetic properties. Examples include inducing a net magnetic moment due to the splitting of crystal field by phonon mode in antiferromagnetic CoF2 [2]. Our study investigates the effect of phonon-induced perturbations on exchange interaction (J) and spin waves in Nickel Oxide (NiO), a promising antiferromagnetic material for spintronics applications. Experimental techniques like inelastic neutron scattering measurements allow us to study the spin dynamics but lack the time resolution to measure J with perturbations. We employ Green's function based approach to obtain the orbital resolved J [3]. Subsequently, the mode-specific renormalization of J and spin wave with perturbation is determined. Our findings reveal a quadratic dependence of J on atomic perturbations, contrary to the commonly assumed linear relationship. This quadratic variation of J stems from the changes in Ni-O-Ni orbital overlap i.e., via d3z2−1 − pz −d3z2−1 orbitals. The J and spin waves exhibit approximately 2% renormalization under phonon perturbations. These results provide a quantitative understanding of how phonon-driven lattice distortions drives the magnetic interactions in NiO. Our work demonstrates the mode resolved renormalization of J and spin waves, offering potential pathways for controlling antiferromagnetic order in spintronics devices.

B2. Ab *initio* & Monte Carlo study of electronic and magnetic properties of 2D frustrated triangular lattice compound $CsTbSe_2$

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Rare-earth compounds with spins arranged in a frustrated triangular lattice are known for their highly unusual ground state properties. In this context, systems like YbMgGaO4, CsNdSe2, and TbInO3 have been identified both theoretically and experimentally as spin-liquid materials. Motivated by these intriguing properties, we have theoretically investigated the electronic and magnetic characteristics of a less explored rare-earth material, CsTbSe2, where Tb ions are organized in a triangular lattice within two-dimensional (2D) hexagonal layers. Using density functional theory (DFT) + Hubbard 'U' method and including spin-orbit coupling (SOC), we thoroughly examined its ground state properties. Our calculations reveal that CsTbSe2 is a SOC-driven insulator with a 1.80 eV energy gap. For magnetic properties, we evaluated the exchange coupling strengths among neighboring ions and discovered that the Tb ions form a frustrated triangular antiferromagnetic arrangement with minimal interaction between the Tb-hexagonal layers along the c-axis. We also implemented Monte Carlo algorithms to carry out spin dynamics simulations and obtained temperature dependence of magnetization and specific heat, suggesting no sign of long range order. Thus, our findings indicate that CsTbSe2 is a highly frustrated 2D magnet with no long range order and an insulating ground state, potentially making it an excellent candidate for antiferromagnetic spin-liquid or for exhibiting incommensurate magnetic structures.

B3. Magnetism of the s = 1/2 frustrated Heisenberg trimer spin chains

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In this work, we have investigated the spin s = 1/2 frustrated J1−J1−J2 trimerized Heisenberg quantum spin chains with frustration introduced through NNN antiferromagnetic exchang

e interaction J3, in the presence of magnetic field using density matrix renormalization method, where J1 and J2 are the ferromagnetic and antiferromagnetic exchange interaction constants. Ground state magnetic phase diagram consisting of different phases and phenomena of 1/3 magnetization plateau in the magnetization process are studied for the competing exchange constant coupling ratios γ, κ, where γ=J2/J1, and κ=J3/J1. The critical coupling parameter γc for the onset of 1/3 magnetization plateau is found to be γc ≃ 0.30 through energy level crossing analysis. The occurrence of 1/3 plateau is also seen through energy-gap in the excitation spectra of the system. Frustration (κ≠ 0) decreases the critical coupling parameter γc. The spatial profile of magnetization and spin-spin correlation in different phases of the magnetic phase diagram are calculated, and spin-spin correlation decays as power law $r^{-\eta}$ with $\eta < 1$. Further, the melting of the 1/3 magnetization plateau state owing to thermal fluctuations, and other thermodynamic properties such as specific heat and susceptibility are also studied.

B4. The Weyl semimetallic behavior of quaternary Heusler compound FeRhCrSi

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Theoretical prediction of half metallicity, ferromagnetism and spin gapless behaviour of Heusler compounds play a significant role in understanding and designing new materials for various spintronic applications. Heusler alloys show a stable half metallic state with a high Curie temperature and have compatible lattice structures with existing spintronic devices. These systems show variety of spintronic as well as topological properties with respect to different elemental composition and structure. We have performed spin polarized density functional theory calculations for the quaternary Heusler alloy FeRhCrSi. The density of states and band dispersion show a half metallic ferromagnetic state with a total magnetic moment of 3μB/formula unit. The band dispersion with and without spin-orbit coupling reveal spin semi metallic as well as a Weyl semi metallic behavior in FeRhCrSi. The presence of Weyl nodes is further confirmed from the source and sink type of flux in normalized Berry curvature, from tight binding model studies. A finite Berry curvature is present in the system, which gives rise to a large anomalous hall conductivity of about 530 S/cm at the Fermi level.

B5. First-principles study of robust half-metallic ferromagnetism and electronic structure of the Heusler compounds $Co_{2-x}Cr_xMnGe$

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Half-metallic ferromagnets (HMFs) are among the most promising materials in the field of spintronics because of their distinct band structure, which consists of two subbands: one with semiconductor-like behavior and the other with metallic features. Using density functional theory-based calculations, we have carried out in-depth studies to predict the effects of Co replacement by Cr on electronic structure as well as the magnetic properties of Co2-xCrxMnGe with $0 \leq x \leq 1$. The results show that the alloys are stable in the ferromagnetic phase with half-metallic nature and are found to be dynamically stable based on their phonon frequencies. The origin of ferromagnetism can be explained by Ruderman-Kittel-Kasuya-Yosida (RKKY), like exchange interaction. All alloys have high Curie temperatures, which scaled linearly with the total magnetic moment, thereby facilitating applications at room temperature and above. The electronic properties have undergone a transition from half-metallic to semi-metallic character for higher doping concentration (x=0.75, x=1.0). The calculated total magnetic moments are found to decrease with increasing doping concentration, which is consistent with the Slater-Pauling rule. All the substances under study have a high value of spin polarisation, indicating their potential for use in spintronics applications.

B6. Magnetic Weyl semimetallic phase in Simple Cubic System

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Weyl nodes emerges from the dirac like dispersion when TRS or IS is broken , splits into Weyl points which can be understood as source and sink monopole of berry curvature in momentum space giving rise to weyl semimetals(WSMs)[1]. When these weyl nodes are close to the Fermi level, the materials can give rise to new exotic quantum phenomena such as large intrinsic anamalous hall effect and Anomalous Nernest effect (ANE), which can be useful for building electronic devices[2]. In this work, we employ first principles calculation to find magentic Weyl semimetal in simple cubic crystal structure that intrinsically have broken time reversal symmetry and have opposite chirality Weyl nodes between Γ to X and Γ to M direction at kz=0. The unique properties of MWSMs, such as the Anomalous Hall effect arises from the interplay between the nontrivial topology of the electronic structure and the magnetic orders. These materials also show promise for applications in spintronics and quantum computing due to their intrinsic magnetism and the enhanced Berry curvature. However, unambiguous experimental confirmation of MWSMs remains challenging, and further research is needed to fully understand the rich physics and potential applications of these materials. The exploration of MWSMs opens up new avenues for investigating the interplay between topology and magnetism in condensed matter systems [3].

B7. A Comparative Study of Structural, Electronic, and Geometric Properties of TMDs (MX_2 and MXY)

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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.

B8. First principles studies on functional mode couplings in oxide superlattices

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Our research investigates the functional mode couplings in multiferroic materials with perovskite oxide superlattices, focusing on nickelates and ferrites, which are crucial for technological applications due to their unique electronic and magnetic properties [1]. In particular, the hybrid improper ferroelectric mechanism in oxide superlattices (ABO3) m/(A'BO3) n, (where m and n = 1,2 and 3) induces microscopic polarization and also can tune the electronic structure and can tailor metal to insulator transition. Specifically, LaNiO3/CaNiO3 superlattices showed a ferromagnetic polar ground state with a half-metallic phase which is crucial for spintronics, memory storage, and memory transport [2]. On the other hand ferrite side, superlattices like BiFeO3/LaFeO3 and BiFeO3/CaFeO3 are valued for their robust magnetic properties and potential in spintronic devices. The BiFeO3/CaFeO3 superlattice, in particular, is noted for its strong magnetoelectric coupling and potential to stabilize exotic magnetic phases under strain. Utilizing first-principles calculations, we explore the structural, electronic, magnetic properties, and strain effects on BiFeO3/CaFeO3 and LaNiO3/CaNiO3 superlattices. In addition to the primary order parameters, rotation (a0a0c+) and tilt (a-a-c0) distortions along a0a0c+ and a-a-c0 and antiferroelectric distortion, we have discovered a polar charge disproportionation mode (QCD) in (1/1) superlattice [3]. Our findings show that refining functional mode couplings makes the system much more stable and possible to get enhanced ferroelectricity, magnetoelectric coupling, and tunable electronic band topologies. These insights provide a pathway for designing multifunctional materials with tailored properties, paving the way for next-generation devices in electronics, spintronics, and energy conversion.

C1. Utilization of Ti-based 2D-MXenes as HER Catalyst: A Computational Investigation

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The industrialized economy and growing population have led to a surge in energy, particularly in ecologically sound and sustainable energy sources. Hydrogen has emerged as an optimistic solution to green energy storage1 and conversion challenges. The water-splitting-based Hydrogen Evolution Reaction (HER) is cost-effective and eco-friendly, with precious metal-based electro-catalysts like platinum (Pt) and ruthenium (Ru) demonstrating high efficiency and stability. Nevertheless, limited resources and increasing costs have impeded the demand for these electro-catalysts. Non-precious metal (NPM)-based electro-catalysts for HER, such as MXenes (MnXn+1, M = transition metal, X = C or N), provide a more efficient option. These catalysts are advantageous due to their abundance, stability, cost- effectiveness, and exceptional electrical conductivity, which enhances their overall catalytic efficiency.2 Extensive study on Ti-based MXenes like Ti3C2 has been conducted since 2011. Our work investigates the capability of Ti-based MXenes as electro-catalysts for the adsorption of hydrogen in the process of sustainable hydrogen production. Zirconium (Zr)-doped MXenes, namely (Ti.93Zr.07)3C2 and (Ti.93Zr.07)3CN, exhibit significant catalytic efficacy that is on par with conventional precious metal catalysts. Density Functional Theory (DFT)1 calculations were used to analyze the Gibb's free energy of hydrogen adsorption in Ti-based MXenes. We decided to use single hydrogen (H) coverage on bare MXenes in order to examine how the specific composition and structure of pristine MXenes can affect their catalytic activity for HER.

C2. Origin of Room Temperature Incommensurate Multiple Charge-Density-Wave in $NbTe_4$

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Transition-metal chalcogenides exhibit multiple phases of matter ranging from charge-density-wave (CDW) and superconductors to topological insulators (semimetals). In particular, transition-metal tetra telluride MTe4 (M = Nb, Ta) adopts a structure different from other tetrachalcogenide chains due to the diffusive nature and high covalent character of tellurium valence electrons. Although sulfides and selenides, including NbS2, NbSe2, and NbSe3, have been investigated in detail for their competition between CDW and superconductivity, tellurides have not been explored until recently. The partially filled dz2 orbital of quasi-one-dimensional NbTe4 results in a Fermi surface consisting of two nearly planar sections responsible for forming CDW. To elucidate the origin of CDW and to identify the Fermi surface nesting (FSN) wave vectors, qCDW, we calculate the Lindhard response function, $\chi 0(q, \omega)$ in the entire Brillouin zone. Here, the divergence in the $\mathrm{Im}\{\chi 0\}$ gives the FSN wave vector, and the divergence in $\mathrm{Re}\{\chi 0\}$ confirms the presence of electronic instability that is responsible for CDW generation. From the divergence in calculated $\mathrm{Re}\{\chi 0\}$, we identify incommensurate qCDW, which are consistent with CDW measurements at room temperature. We also find a divergence of $\mathrm{Im}\{\chi 0\}$ at the same qCDW, thus confirming that CDW is driven by FSN. To verify the robustness of CDW, we recalculate $\chi 0$ under phonon perturbation but do not find any change in qCDW; however, qCDW changes significantly by shifting the Fermi level, highlighting the sensitivity of the system to doping.

C3. Hydrogen Adsorption over Hexagonal Zinc Oxide Monolayer: A Combined DFT and Kinetic Monte- Carlo Study

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One of the main challenges faced during the use of hydrogen (H2) gas as a clean energy fuel is the lack of an appropriate storage material. In the present study, two theoretical methods: van der Waals density functional theory (vdW-DFT) and kinetic Monte-Carlo (kMC) simulation have been combined to predict on the adsorption and evolution of H2 molecules over a hexagonal zinc oxide (ZnO) monolayer [1]. H2 molecules can attach to the ZnO monolayer surface via a weak physisorption process with a maximum adsorption energy of around 60 meV. The lateral repulsion present between the H2 molecules controls the maximum number of gas molecules that can be packed over the substrate. The output of the DFT calculations has been fed to a kMC code to describe the adsorption, desorption, and diffusion dynamics of the H2 molecules over the ZnO substrate. The kMC calculations indicate that the H2 adsorption is favorable at a low temperature and high pressure. Further, the adsorption of H2 molecule over ZnO monolayer results in the increase of the band gap value, subsequently changing the conductivity of the system. Thus, this present work highlights the suitability of using a ZnO monolayer for the storage and sensing of H2 gas molecules.

C4. MXene-Based Lateral Heterojunctions for High-Performance FETs

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Identifying low-contact resistance 2D-2D metal-semiconductor contacts is crucial for minimizing power dissipation and improving the overall performance of field-effect transistors (FETs). We investigate the potential of MXene-based lateral heterojunction for low-resistance FETs. By systematically exploring the electronic properties of sixteen metallic and five semiconducting MXenes, we identified Ta2CO2-Ti2CO2, Nb2CO2-Ti2CO2, and Zr2CF2-Sc2CF2 as promising candidates with low n-type Schottky barrier heights. Non-equilibrium Green's function simulations further confirm the superior I-V characteristics of Ta2CO2-Ti2CO2, attributed to its minimal contact resistance and suppressed metal-induced gap states. To further enhance the performance of these contacts, we created alloys of Ta2CO2 by replacing Ta with Ti, demonstrating that Ta2xTixCO2 further minimizes contact resistance. These results demonstrate the potential of MXene-based FETs to meet the stringent performance requirements outlined in the International Roadmap for Devices and Systems (IRDS).

C5. Electronic descriptor to identify Cu based FCC-FCT alloy nanoparticles towards C_2 product over C1 product on (111) plane

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The product distribution in electrochemical reduction of CO2 (CO2ER) towards different 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. Obtaining C2 products (double carbon products) possessing higher energy density and more industrial values than C1 products (single C product) in CO2ER is greatly worthwhile but remains a challenge. Cu is a unique metal which can reduce CO2 into C2 products but the selectivity towards final product remains as a challenge. C2 product formation consists of several intermediates, key interposes and multipole electron-proton transfer on any plane. In general, bulk Cu in (100) plane favor C2 production while its (111) plane promotes C1 product formation. Conversely, (111) plane of Cu nanoparticle (Cu NP) favor C1 or C2 products depending on the size, shape, active site of the active plane. Introducing new metal atom by forming alloys can alter the electronic property of the catalysts to influence the CO2ER towards ethanol as C2 product. Moreover, finding any descriptor to predict ethanol formation as C2 product in (111) plane is highly demanding. Here we report the Cu NP based FCC-FCT alloys to selectively promote the ethanol product formation on (111) plane via *CO-*CO dimerization. Finally, two different fundamental descriptors are studied to explain and predict the possibility of ethanol formation in CO2ER. 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 CO2ER towards ethanol production.

C6. Stone-Wales Decorated Phagraphene: A Promising Material for Supercapacitor Electrodes and Thermal Transport Applications

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In this new era of instrumental wonders, the modifications of physical properties of two-dimensional carbon allotropes by defects or doping is quite easy. This serves as an excellent choice from industrial perspectives due to its low cost and stability. Hence the importance of experimentally synthesized graphene allotropes is increasing day by day. In recent year, the experimental realization of non-hexagonal phagraphene nanoribbon dictates its huge possibility in real life applications. Here we demonstrates, how phagraphene can be modified to perform different purposes by introducing Stone-Wales defects into the structure, using density functional theory calculations and machine learning approaches. The structural stability in terms of dynamical, thermal and mechanical properties has been established for this structure. Graphene like formation energy, dense atomic packing and sp2 hybridization narrates the structural integrity of the system. Significant modifications of electronic properties (metallic in nature) due to Stone-Wales defects and increased porosity of the structure indicate its suitability as supercacitor electrodes. Large amount of quantum capacitance with applied voltage indicate that the structure can be used as electrodes in asymmetric supercapacitors. Besides, lattice thermal conductivity of the structure has been calculated using machine learning approaches to explore its possibility as multipurpose applications. Good electrical conductivity and thermal conductivity strengthen its potential in transport applications also.

C7. Tuning of Band Topology and Topological Hall Effect in Skyrmion Crystals via Spin-orbit Coupling

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In recent years, magnetic skyrmions have attracted significant attention due to their role in unconventional electron transport driven by topology. One such property is the topological Hall effect (THE), which is the transport of electronic charge along the transverse direction. Here, using the many-body model Hamiltonian on a two-dimensional (2D) skyrmion crystal, we study THE under various spin-orbit couplings (SOC) like Rashba, Dresselhaus, and Weyl. We find that at an optimal SOC strength, a nearly uniform emergent magnetic field distribution is achieved at which subband dispersions and quantization plateaus of THE closely resemble the Landau levels and plateaus of quantum Hall effect in 2D crystal under a uniform magnetic field, respectively. Moreover, varying SOC alters band topology that enables transition between ordinary and Chern insulating states. Also, it changes the Chern number from negative to positive, which results in a flip of the edge current direction. Interestingly, varying SOC also reverses the sign of THE at a critical point. Since Rashba and Dresselhaus SOC can be tuned by electric fields, these results could pave the way for future quantum devices and create new avenues for controlled charge transport in skyrmions, sparking intrigue and excitement in the field of condensed matter physics and materials science.

C8. New High-Pressure Phases of Titanite-Type CaTiSiO5 Predicted from First-Principles

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Titanite-type CaTiSiO5 is one of the common accessory minerals in igneous, metamorphic, sedimentary, and ultra-high-pressure rocks. It is largely known due to its importance as a petrogenic indicator, as versatile host for rare earth elements (REE), and as a U−Pb geochronometer for dating geological events. Determination of the high-pressure crystal-chemical behavior of titanite type silicate minerals is crucial to comprehending the crystalline materials in deep-earth geospheres. It exists in monoclinic structure (monoclinic-I, SG- P21/c) at ambient conditions; whereas at high temperature (HT) and/or high pressure (HP), it undergoes a monoclinic-I (P21/c) → monoclinic-II (C2/c) structural phase transition. However, apart from the monoclinic structure types, several titanite minerals are also well known in triclinic structure type (SG - P-1). As there are intricacies related with structural polymorphs at ambient as well as HP, it is highly expected to discover possible structural candidates within a certain pressure range. Here, we have used evolutionary algorithms to predict thermodynamically favourable structures at ambient (0 GPa) and HP (10 – 50 GPa). At 0 GPa, we have found monoclinic structures are most favorable which are also experimentally known. Futhermore, two new structural phase transitions are proposed: one is displacive type monoclinic-II (C2/c) → triclinic (P-1) phase transition and other one is reconstructive type triclinic (P-1) → orthorhombic (Pnma) phase transition at 10 and 18 Gpa, respectively. All the predcted structures are dynamically as well mechanically stable which is confirmed by calculating phonons and elastic properties. We have also performed ab-initio molecular dynamics simulations (AIMD) for further understanding the contribution of temperature on the structural phase transition.

C9. Phonon-assisted control of magnonic and electronic band splitting

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We demonstrate the ability to control non-relativistic magnonic splitting and spin splitting in the electronic band structure by manipulating phonon modes. Using MnF2 as a model system, known for its non-relativistic spin splitting in electronic bands, we uncover a similar d-wave splitting in magnon modes of specific handedness. Our results reveal a correlation between magnonic and electronic splittings, showing that the magnitude and sign of energy splitting in both magnon and electronic bands of MnF2 can be controlled by phonon modes. These findings offer valuable insights into the interaction of charge, spin, and lattice degrees of freedom in spin-split antiferromagnets and open avenues for phonon-driven magnonic applications in such materials.

C10. Coexistence of Giant Rashba Splitting, Multiple Band Inversion, and Multiple Dirac Surface States in 3D Topological Insulator XSnBi (X=Rb, Cs)

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Composite quantum compounds (CQCs) have emerged as a key tool for examining the interactions between two different physical phenomena. Some of these CQCs that have lately received a lot of community attention are topological superconductors and axion insulators, among others. Despite being two distinct quantum phenomena, Rashba spin physics and topological non-triviality can coexist in a CQC platform. In this work, we have conducted ab initio calculations to identify materials that exhibit both giant Rashba splitting and topological nontrivial states within a single crystalline system, referred to as intrinsic Composite Quantum Compounds (CQCs). We have specifically explored two materials, RbSnBi and CsSnBi, which have been found to be strong topological insulators. These materials also demonstrate a substantial Rashba splitting energy in their valence bands, with values of 133 meV and 228 meV, respectively. The Rashba coefficient (α R) for RbSnBi is 4.26 eV Å, while CsSnBi exhibits the largest αR among previously reported topological materials, at 6.4 eV Å for its valence bands. These remarkable values of α R highlight the unique characteristics of these materials. The coexistence of Rashba spin physics and topological non-triviality in RbSnBi and CsSnBi has the potential to unveil novel physical phenomena. Furthermore, for both of these materials, the topological insulating state is associated with the presence of multiple band inversions and multiple Dirac surface states. This research paves the way for further exploration and understanding of these intriguing intrinsic CQCs.

Abstracts of Oral Presentations

O1. Ab initio Study of Magnetic Properties in 2D Metallic Magnets: A Case Study of the FenGeTe$_2$ Family and FeNbTe$_2$

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The Fe n GeTe$_2$ family of 2D ferromagnets exhibits near-room-temperature Curie transitions, making them promising candidates for spintronic applications. These materials consist of a metallic FenGe layer sandwiched between two Te layers, separated by van der Waals (vdW) gaps. However, the underlying physics driving their complex magnetic behavior remains poorly understood due to their intricate structural composition. In this study, we employed ab initio methods to investigate the magnetic properties of the Fe n GeTe$_2$ family. Our results reveal that a unique structural reconstruction may explain several open questions regarding Fe$_5$GeTe$_2$. Additionally, FeNbTe$_2$, a recently synthesized 2D magnet, has shown intriguing magnetic properties, although theoretical understanding of its magnetic interactions remains incomplete. Using density functional theory (DFT), we explored the exchange mechanisms and magnetic anisotropy in both systems, contributing to a deeper understanding of their magnetic phenomena.

O2. Anisotropic Magnetoresistance of Gadolinium Nitride

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The lanthanide nitrides (LnN) are a series of intrinsic ferromagnetic semiconductors and as such are the subject of increasing interest in both fundamental and applied fields [1]. The successful application of this rare confluence of electronic and magnetic ground states requires a full understanding of both. Gadolinium Nitride, the central member of the series, provides a clear starting point, and significant effort has been placed into understanding its properties thus far [2,3,4,5]. The simple crystal and magnetic structure of ferromagnetic GdN also provides a good testing ground for magnetic and spintronic computational methods before extension to other LnN or other systems. But, while the electron wavefunctions (and thus the properties of the LnN) can be calculated using Density Functional Theory (DFT), there are many predictions which lack experimental validation and many experimental results that lack theoretical description, particularly those relating to electron transport. Here, we provide an experimental link between calculations and the physical material, showing that the shape of the Fermi surface of Gadolinium Nitride matches that predicted from DFT. In particular we find that the magnetoconductivity tensor, derived using the Boltzmann transport equation in the relaxation time approximation on the electron wavefunctions taken from DFT calculations, reproduces the structure and field dependence of the experimentally measured anisotropic magnetoresistance (AMR). This correspondence validates the computational work and motivates the use of parameters derived from the band structure in the design of realistic devices.

O3. Unravelling the Rashba-Dresselhaus effect and spin switching in ferroelectric AIO 3 (A=K, Rb, Cs, Tl) perovskites

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Harnessing the Spin-orbit coupling (SOC) driven manifestations in electronic structure for device application comprises one of the challenging fields in spintronics application. One such avenue to achieve this is via Rashba-Dresselhaus (RD) effect, which leads to the splitting of spin states at the band edges in momentum space enabling the creation of separate spin channels for spin current control. In some multifunctional perovskite materials, the RD effect coexists with ferroelectricity, where ferroelectric (FE) phase transitions can induce spin chirality reversal, presenting opportunities for spin-FET development. We explore the effect of A cation (A= K, Rb, Cs, Tl) in spin-FET application of AIO3 compounds via investigating the RD effect and FE properties. Our results demonstrate that smaller A-cation size leads to higher RD spin splitting, with KIO3 exhibiting the most promising performance. Out of the four compounds studied, three of them show RD spin splitting ≥ 1 eVÅ at the conduction band. Furthermore, we observe that FE phase transitions in all these compounds can influence the spin chirality. The FE switching barriers of all four compounds are below 1 eV/atom. KIO3 has the lowest barrier of 193 meV/atom. These findings highlight the potential of AIO3 compounds for spin-FET applications and suggest avenues for further optimization.

O4. Coexistence of Altermagnetism and Weyl Fermions in GdAlSi

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Spintronics has emerged at the forefront of technological applications in current times and is set to play a major role alongside conventional electronics. The discovery of topological phases of matter with robust and symmetry-protected electronic states further offers exciting spintronic applications. Very recently, a fundamentally new type of collinear magnetic order similar to a collinear antiferromagnet, but showing non-relativistic spin-splitting, has been proposed theoretically and subsequently verified by experiments. This new order, dubbed “Altermagnetism”, shows promise for the upcoming field of antiferromagnetic spintronics. In this work, we show the coexistence of non-trivial topology and altermagnetism in a single crystalline material GdAlSi. Our ab-initio calculations show GdAlSi to have a collinear antiferromagnetic ground state with momentum-dependent non-relativistic spin-splitting which is a consequence of crystalline symmetries. Further investigations reveal GdAlSi to be a topologically non-trivial Weyl semimetal hosting exotic and robust spin-polarized surface states known as Fermi arcs. Second-harmonic generation and magnetization measurements confirm the non-centrosymmetric crystal structure and antiferromagnetic nature of GdAlSi respectively whereas angle-resolved photoemission spectroscopy reveals the presence of Fermi arc-like features. Such unprecedented coexistence of altermagnetic order and Weyl Physics in a single material could pave the way for future spintronic device applications.

O5. Electronic and Thermoelectric properties of 1- quintuple layer chalcogenides- A DFT Study

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Thermoelectric (TE) materials are of great interest to the scientific community due to their potential application in clean and renewable energy sectors. TE materials are advantageous as they can directly convert the largely unused thermal energy to the electrical energy with nominal cost to the environment. Among the various TE materials, chalcogenides has drawn attention due to the narrow band gap and outstanding thermoelectric performance. The discovery of graphene has prompted the researchers to think of 2- dimensional materials in various fields, including thermoelectrics. The low dimensional structures can probably show better thermoelectric performance due to the increased boundary scattering of phonons, which reduces the lattice thermal conductivity

In this work, we have selected four monolayer chalcogenides, including the tellurium as well as selenium based and investigated their electronic and thermoelectric performances. The DFT calculations (utilizing PAW pseudopotentials with the QUANTUM ESPRESSO (QE) package [1-2]) were employed to calculate the electronic properties whereas semi-classical Boltzmann transport theory (using BOLTZTRAP code [3]) was utilized to calculate the thermoelectric performance of Sb2Te3 , Bi2Se3 , BiSbSe3 and BiSbTe3 monolayers. Calculation of electronic properties revealed all the monolayers to be of indirect band gap type with the BiSbSe 3 QL to have the narrowest band gap (0.19 eV) among the others. Whereas, the widest band gap of 0.69 eV was obtained for BiSbTe 3 QL. A decreasing trend in Seebeck coefficient was observed with carrier concentration for all the monolayers. The BiSbTe3 QL showed highest and BiSbSe 3 monolayer showed the lowest Seebeck coefficient among others. The trend was explained by positioning of Fermi energy level in band structure of the monolayers. The electrical conductivity (σ/τ) showed increasing trend with carrier concentration for all the materials with the highest value obtained for Sb2Te3 QL. This was explained from the value of indirect band gap of the materials. The power factor (PF) of the materials showed maxima at a particular carrier concentration with highest value of 3.1×10^{11} $WK^{-2}m^{-1}s^{-1}$ obtained for Sb2T3 QL. The BiSbTe3 and Bi2Se3 monolayers showed low PF values among others. The highest value of figure of merit, ZT (1.00 corresponding to carrier concentration of 6.24×10^{19} e/cm3) was obtained for Sb2Te3 QL with a relatively smaller value of 0.60-0.64 obtained for BiSbSe3 and BiSbTe3 monolayers.

O6. First-Principles Study of Titanite-Type $CaTiSiO_5$ Under Pressure

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The titanite-type $CaTiSiO_5$ is widely recognized for its significance as a petrogenic indicator, a versatile host for rare earth elements (REE), and as a U-Pb geochronometer for dating geological events. Further, it is also a promising wasteform for the high level nuclear wastes. In ambient conditions, it exhibits a monoclinic structure (monoclinic-I, SG-$P2_1/c$). However, it shows phase transitions from the monoclinic-I (P21/c) phase to a monoclinic-II (C2/c) structure at higher temperature. In addition to these monoclinic forms, some titanite minerals are also well known for having a triclinic structure (SG-Pī). In this work, we have studied this phase under pressure ranging from 0-50 GPa. In this study, we have identified two new structural polymorphs at higher pressures using an evolutionary algorithm. Further analysis of their structural, elastic, and dynamical stability has revealed the pressure-dependent stability regions of these new polymorphs.

Evolutionary algorithms as implemented in USPEX package [1] was used for prediction of the crystal structures at high pressures. The structures at high pressure, initially, screened using USPEX package interfaces with classical force field. The structures which energies are within 2eV to the most stable structure are then optimized using density functional theory based calculations as implemented in VASP. PAW potentials [2] were used in all the calculations. The symmetry of the structures were analysed using VASPKIT software[3].

We have found $P2_1/c \rightarrow C2/c$ phase transition around 8 GPa by using DFT-PBE exchange-correlation functional however, no phase transition is observed in case of DFT-LDA functional. From the crystal structure prediction, we have predicted two new phases; one is triclinic (SG-*P*ī) at 10 GPa and another one is orthorhombic (SG-*Pnma*) at 20 GPa. The predicted triclinic structure resembles those structural prototypes found in other titanite minerals. In our calculations, both triclinic and orthorhombic structures are mechanically and dynamically stable. The orthorhombic structures which is quenchable at 0 GPa, possesses a novel topological rearrangement of SiO_6 and TiO_6 octahedra that has not been observed in any of the HP structural prototypes of silicate minerals.

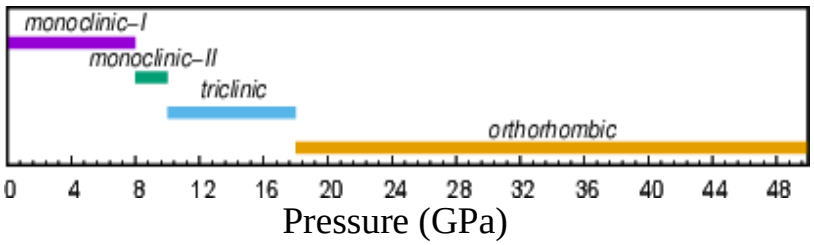

Figure 1: Stability region of different high pressure phases of titanite type $CaTiSiO_5$

High pressure crystal structures are predicted for $CaTiSiO_5$ composition. The new predicted triclinic and orthorhombic structures are mechanically and dynamically stable.

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O7. Pressure Induced electronic and magnetic transition in antiferromagnetic NiS: A combined DFT+U and Monte-Carlo study

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Employing first-principle density functional theory + Hubbard U (DFT+U) approach and classical Monte-Carlo simulations, we investigated the lowest energy electronic structure in hexagonal NiS which exhibits a semi-metallic antiferromagnetic ground state at ambient condition. We derived a spin model Hamiltonians consisting of Heisenberg exchange interactions (Jij) up to the third nearest neighbours, Dzyaloshinskii–Moriya interactions (DMI), and single ion anisotropy (K). Our calculations show that the 3rd nearest neighbour (NN) and 1st NN Jij are strongly antiferromagnetic, while the 2nd NN Jij is weak ferromagnetic. Further the effect of spin-orbit coupling (SOC) is also found to be significant, leading to a finite DMI and K. The classical Monte-Carlo result nicely capture the experimental specific heat, magnetic susceptibility etc, giving credence to our derived spin-model. The application of external pressure is demonstrated to be an effective tool to exhibit electronic and magnetic transition in NiS. We found that tensile stress gives rise to a metal-insulator transition, while compressive stress provides the ways to collapse local magnetic moment on Ni site. The dominant exchange couplings are calculated for various values of pressure and the route for enhancing transition temperature is proposed based on Monte-Carlo study. Our results are expected to enrich the understanding of electronic structure and magnetism in NiS.

O8. Effect of spin-orbit coupling on the thermoelectric power factor of CoBi-based half-Heusler compounds

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Among the diverse array of thermoelectric (TE) materials explored previously, half-Heusler compounds have emerged as up-and-coming candidates for mid to high-temperature TE power generation due to their large power factors and robust thermal and mechanical properties. However, these materials typically exhibit relatively high lattice thermal conductivity (κ_L), typically >10W/m-K for pristine compounds [1]. Consequently, the figure of merit (zT), of state-of-the-art half-Heusler remains relatively low compared to other established material systems. Hence, ongoing efforts are focused on enhancing zT by reducing κ_L without significantly compromising the power factor, for instance, by introducing mass disorder into the lattice.

A recent study highlights the discovery of p-type ZrCoBi-based half-Heusler compounds with a remarkable zT of approximately 1.42 at 973 K [2]. This outstanding performance is attributed to its distinctive band structure, which provides a high band degeneracy (N_v) of around 10 arising from the valence band extrema (VBM). The bands at the L and Γ points in k-space exhibit a slight energy difference of approximately 0.06 eV, with the bands at L being at a higher energy level than those at Γ, all contributing to transport. Additionally, this compound exhibits low thermal conductivity, benefiting from its low mean sound velocity (v_m) of around 2800 m/s. In contrast, its iso-electronic counterpart, TiCoBi, lacks a similar band structure, with bands at the Γ (E_Γ) point being at higher energy levels than those at L (E_L), resulting in suppressed transport properties compared to ZrCoBi.

This study explores the possibility of band convergence in the solid solution of ZrCoBi ($E_L > E_\Gamma$) and TiCoBi ($E_\Gamma > E_L$) which holds great promise for enhancing the thermoelectric performance of half-Heusler compounds. Theoretical investigation using density functional theory (DFT) is used to provide insights into the solid solution ($Ti,ZrCo_2Bi_2$) compounds' electronic structure, and band convergence. Bismuth being a heavy, element spin-orbit coupling is used in the calculations. Due to the splitting of the band at the extrema, the power factor of the solid solution is found to deteriorate as compared to ZrCoBi. Although band convergence was achieved for ($Ti,ZrCo_2Bi_2$), the splitting of degeneracy due to SOC resulted in a reduction of power factor. Thus, the improvement in the figure of merit for this compound lies solely in the reduction of lattice thermal conductivity. Thus, this work highlights the significance of selecting suitable dopants to enable the design of

solid solutions with enhanced power factors, paving the way for the development of next-generation thermoelectric materials for power generation applications at mid to high temperatures.

O9. Unraveling Rashba effect through spin-texture evolution in unidimensional-confined halide-perovskite under compression

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In this work, we envisage an evolution paradigm in a promising noncentrosymmetric one-dimensional zigzag chain structure, (3AMP)BiI_5 [where AMP indicates (aminomethyl)piperidinium], through rigorous electronic structure calculations based on density functional theory (DFT). The electronic and optical properties along with the Rashba splitting and spin texture are systematically observed within the thermodynamic limit under compression equivalent to 9.6 GPa in this promising halide perovskite. Our study successfully reveals the intriguing transition of the electronic band structure from an indirect to a direct band gap phenomenon under compression in addition to an interesting redshift in the optical absorption spectra. To accurately describe the spin polarization both in plane and out of plane, we explore a three-dimensional Rashba model. The in-plane spin texture is found to arise from the octahedral distortion along the b direction. The fundamental interplay between structural distortions and the Rashba splitting in the considered one-dimensional system under the influence of compression along with the evolution of spin texture could hold great potential for the pursuit of sustainable energy.

O10. Machine Learning and Atomistic Simulations for Predicting Ferroelectric Switching in Hybrid Improper Ferroelectric Double Perovskites Oxides

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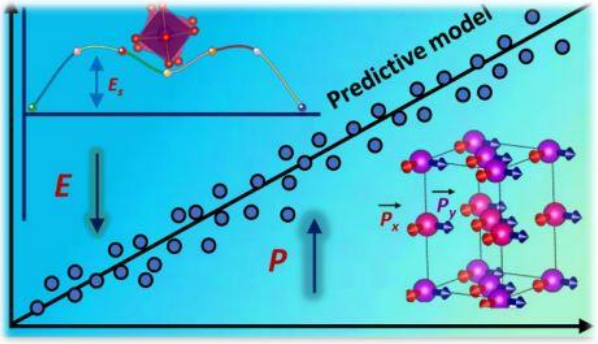
The computational design of suitable multiferroic double perovskite oxides requires finding materials that exhibit sizable polarization, magnetization, and coupling between them. Oxides with the chemical formula of AA′BB′O6 with building blocks of ABO3 single perovskite oxides in centrosymmetric Pnma symmetry are strong candidates that have been reported to satisfy such criteria. The system lowers to non-centrosymmetric, polar P21 symmetry if A/A′ layered and B/B′ rocksalt cation orderings are imposed. A detailed compositional search over a variety of chemical spaces followed by evaluating their polarization may lead to the identification of more of these compounds with ferroelectric ordering. The standard density functional theory practices to estimate polarization within the Berry phase formalism require the systems to be perfectly insulating. In this work, we introduce a predictive learning strategy based on importance sampling to build a series of machine learning models using results from first-principles simulations to predict polarization and the corresponding switching barrier. The geometry-driven features associated with charge states and cationic radii are crucial for predicting switching barriers, supported by key structural mode-based order parameters. These modes help make accurate predictions of polarization components using machine learning models. Our models identify double perovskite oxides with high polarizations and low switching barriers, highlighting promising candidates for future spintronic device applications.



O11. Investigating magneto-caloric effect and exchange interaction in NdMnO3 Perovskite: A computational study

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In this study, we investigate the magnetic characteristics and magnetocaloric effect of NdMnO3 perovskite in order to comprehend its potential applications in magnetic refrigeration and spintronics. We analyse the electrical density of states and band structure of this perovskite utilising density functional theory (DFT) calculations with generalized gradient approximation, revealing its behaviour as a ferromagnetic half-metal material. Following that, using Monte Carlo simulations based on the Heisenberg model with nearest and next-nearest neighbour interactions, we investigate various magnetic parameters including magnetization, susceptibility, specific heat, internal energy and the Curie temperature (TC). This helps to establish the thermal magnetic entropy profiles with temperature and external magnetic field for the material, and hence quantify the adiabatic temperature change. We also investigate the subtle interplay between crystal field effects and exchange interactions involving Mn-Mn, Nd-Nd, and Nd-Mn magnetic atoms. Additionally, we examine the relative cooling power (RCP) across different magnetic field strengths, shedding light on the magnetocaloric potential of NdMnO3 under various conditions. The collective insights obtained from our computational study shows NdMnO3 perovskite as a viable option for use in spintronics and magnetic refrigeration. We underline the significance of magnetic anisotropy in determining the magnetocaloric behaviour of this material, opening the door for the development and enhancement of effective cooling systems based on perovskite oxides.