QMAT-2024

7th Annual Conference

on

Quantum Condensed Matter

ABSTRACT BOOK

December 20 - 23, 2024

Venue: Indian Institute of Technology Guwahati

This conference abstract book is compiled and implemented in Latex by :

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Timetable

Program Schedule

QMAT 2024

Organized by IIT Guwahati, 20th -23rd December 2024

Day 0, 20th Dec 2024 (Friday):

Time	Events
11:00-12:00	Registration
12:00-13:45	Lunch
14:15-14:50	Inauguration
15:00-16:00	Public Lecture (Mandar M. Deshmukh, TIFR Mumbai, India)
16:00-16:30	High Tea
16:30-19:00	Registration Continued
19:00-onwards	Dinner

Day 1, 21st Dec 2024 (Saturday):

Day 1: Parallel Session-1	*Session Chair:* Rajdeep Sensarma	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast & Registration	
9:00 – 9:30	Diptiman sen	Kinetically constrained models showing Hilbert space fragmentation
9:30 – 10:00	Ajit C Balram	Static structure factor and the dispersion of the Girvin-MacDonald-Platzman density-mode for fractional quantum Hall fluids on the Haldane sphere
10:00 – 10:15	Manodip Routh	Emergent Quadrupolar Order in the Spin-1/2 Kitaev-Heisenberg Model
10:15 – 10:30	Ankit Gill	Speed Limits and Scrambling in Krylov Space
10:30 -11:00	Tea/Coffee	
Day 1: Parallel Session-1	*Session Chair: Diptiman Sen*	
11:00 – 11:30	Sumilan Banerjee	Measurement-Induced Superconductor-Insulator Transition in Weakly Monitored Josephson Junction Arrays

11:30 – 12:00	Rajdeep Sensarma	Phase Transitions in Twisted Bilayer Graphene
12:00 – 12:15	Subhasis Shit	Reducing the vortex entanglement via Pb substitution in the charge reservoirs of Bi-2212 superconductor
12:15-12:30	Jagannath Sutradhar	Singlet, triplet, and mixed all-to-all pairing states emerging from incoherent fermions
12:30 – 14:00	Lunch	
Day 1: Parallel Session-1	*Session Chair: Mandar M. Deshmukh*	
14:00 – 14:30	Satyajit Banerjee	Exploration of emergent rich strongly correlated state in SmB_6 and a comparison of this system with a conventional topological insulator Bi_2Se_3
14:30 -15:00	Ravi Prakash Singh	Superconducting Natural Heterostructures: A Novel Platform for Unconventional Superconductivity
15:00 -15:15	Shubham Patel	Electron-phonon coupling, critical temperatures and gaps in $NbSe_2/MoS_2$ Ising Superconductors
15:15 -15:30	Souvik Banerjee	Unconventional vortex states in the Chevrel phase superconductor $PbMo_6Se_8$
15:30 – 16:00	Tea/Coffee	
Day 1: Parallel Session-1	*Session Chair: Satyajit Banerjee*	
16:00-16:30	Sudeep Kumar Ghosh	Origin of Sign change in Thermopower of Strained Sr_2RuO_4
16:30 – 17:00	Mintu Mondal	Exceptionally slow and long-range critical fluctuations anticipate the singularity in second order phase transition
17:00- 17:15	Supriya Ghosal	Bi based half-Heusler alloys: Potential candidates for thermoelectric applications
17:15- 17:30	Sorav Karan	Robust and Thermally Stable Pinning Mechanisms Behind the High Jc State of HTSC-TMC NPs Nanocomposites
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	

19.00 onwards	Banquet Dinner

Day 1: Parallel Session-2	*Session Chair:* Vidya Kochat	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast & Registration	
9:00 – 9:30	Debraj Choudhury	Tuning dielectric responses and polar-instabilities in orthorhombic rare-earth chromates
9:30 – 10:00	Tamalika Banerjee	Large Tunneling magnetoresistance in all-oxide magnetic tunnel junctions with perpendicular magnetic anisotropy
10:00 – 10:15	Sudipta Chakrabarty	Optically enhanced negative differential resistance in reduced graphene oxide coated silicon nanorods
10:15 – 10:30	Mouli Roy Chowdhury	Frustration driven low-temperature spin-glass behavior and short-range correlations in tri-cation spinel
10:30 -11:00	Tea/Coffee	
Day 1: Parallel Session-2	*Session Chair: Tamalika Banerjee*	
11:00 – 11:30	Ashis Kumar Nandy	Tailoring Topological Phases and Anomalous Hall Effect in Noncollinear Antiferromagnets
11:30 – 12:00	Biplab Sanyal	Complex magnetism and spin transport in two-dimensional magnets
12:00 – 12:15	Simrandeep Kaur	Controlling the Particle-hole symmetry in fractional Quantum Hall state in ABA trilayer graphene.
12:15 – 12:30	Mijanur Islam	Electron-phonon coupling induced topological phase transition in an a-T_3 Haldane-Holstein model
12:30 – 14:00:	Lunch	
Day 1: Parallel Session-2	*Session Chair:* Tulika Maitra	
14:00 – 14:30	Vidya Kochat	Broken symmetry quantum Hall states, layer hybridization and screening effects in

		twisted bilayer graphene at intermediate angles
14:30 -15:00	Kausik Majumdar	Exciton-Exciton Interaction in a Moiré Superlattice: Repulsive or Attractive?
15:00 -15:15	Hilol Biswas	Various phases of a discrete time crystal in driven central spin model
15:15 -15:30	Simrandeep Kaur	Controlling the Particle-hole symmetry in fractional Quantum Hall state in ABA trilayer graphene.
15:15 – 16:00:	Tea/Coffee	
Day 1: Parallel Session-2	*Session Chair:* Chandra Shkehar Yadav	
16:00-16:30	Anindya Das	Thermopower probing emergent local moments in magic-angle twisted bilayer graphene
16:30 – 17:00	Atindra Nath Pal	Nontrivial transport in driven by charge-density-wave in 1T-TaS_2
17:00- 17:15	Ajit Kumar Dash	Utilizing low energy electron beam irradiation for ultrasharp single photon emitter generation in monolayer transition metal dichalcogenides
17:15- 17:30	Ajay Pratap Singh Rana	Spin caloritronics and magneto-thermoelectric effect in two-dimensional magnetic materials
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	
19.00 pm onwards	Banquet Dinner	

Day 1: Parallel Session-3	*Session Chair:* Anindya Das	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast & Registration	
9:00 – 9:30	Chandan Bera	Electron and phonon transport properties in two-dimensional magnetic materials
9:30 – 10:00	Prasana Kumar Sahoo	Engineering Excitons in 2D Lateral Heterostructures and Devices

10:00 – 10:15	Nikhil Malviya	Experimental Extraction of Phonon Scattering Lifetimes in vdW Materials Using Transient Grating
10:15 – 10:30	Manvi Verma	Digital Twin Enabled Understanding and Modulation of Nucleation Density for Optimized 2D Material Synthesis
10:30 -11:00	Tea/Coffee	
Day 1: Parallel Session-3	*Session Chair:* Anamitra Mukherjee	
11:00 – 11:30	Angom Dilip Kumar Singh	Topological entanglement entropy from exact diagonalization
11:30 – 12:00	Amal Medhi	Convolutional restricted Boltzmann machine correlated variational wave function for the Hubbard model on a square lattice
12:00 – 12:15	Kuntal Bhattacharyya	Topological phase transition through electron-phonon interaction in an alpha-T3 quantum spin Hall insulator
12:15 – 12:30	Anirban Das	Generation of Macroscopic Entanglement via Quantum Annealing
12:30 – 14:00:	Lunch	
Day 1: Parallel Session-3	*Session Chair:* Biplab Sanyal	
14:00 – 14:30	Anjan Barman	Ultrafast Magnetization Dynamics in 2D Material/Ferromagnet Heterostructures
14:30 -15:00	Swapan K Pati	Computational Modeling of Materials for Energy Storage and Generation
15:00 -15:15	Sk Kalimuddin	Free Sliding Charge Density Wave: A Dynamical Critical Phenomenon
15:15 -15:30	Sagnik Chaudhuri	Stability of Emergent Conservation Laws in Periodically Driven Quantum Systems
15:30 – 16:00:	Tea/Coffee	
Day 1: Parallel Session-3	*Session Chair:* Arnab Sen	
16:00-16:30	Vijay Shenoy	Edge Theories of Fractonic Systems
16:30 – 17:00	Anamitra Mukherjee	Spin-excitations of low-dimensional cuprates beyond linear response

17:00- 17:15	Ramita Sarkar	A maximum concurrence criteria to investigate absolutely maximally entangled states
17:15- 17:30	Tista Banerjee	Entanglement transitions and role of emergent symmetry in non-Hermitian integrable Floquet systems
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	
19.00 onwards	Banquet Dinner	

Day 2, 22nd Dec 2024 (Sunday):

Day 2: Parallel Session-1	*Session Chair:* Arijit Saha	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Tanmoy Das	Fractional, Entangled and Quasi Orbitals
9:30 – 10:00	*Arnab das*	Unprotected Emergent Conservation Laws in Interacting Quantum Matter
10:00 – 10:15	Nilanjan Roy	Superlattice induced electron percolation within a single Landau level
10:15 – 10:30	Saikat Mondal	Percolation transition in a topological phase
10:30 -11:00:	Tea/Coffee	
Day 2: Parallel Session-1	*Session Chair:* Tanmoy Das	
11:00 – 11:30	Arijit Saha	Distinguishing between topological Majorana and trivial zero modes via transport and shot noise study in an altermagnet heterostructure
11:30 – 12:00	Soumya Bera	Many-body localization dynamics
12:00 – 12:15	Subhamita Sengupta	Inverse Melting in A Pinned Vortex Liquid
12:15 – 12:30	Pooja Saini	Revival of the Hofstadter butterfly in the Presence of various disorders and Correlation Strength
12:30 – 14:00:	Lunch	
Day 2: Parallel	*Session Chair:* Ravi Prakash Singh	

Session-1		
14:00 – 14:30	Ajaya Kumar Nayak	Non-coplanar magnetic structure driven Large Anomalous Hall Effect in electron doped Mn_3Sn
14:30 -15:00	Kalpataru Pradhan	Strain-driven magnetic reorientation in transition metal oxides
15:00 -15:15	Mantu Modak	Unusual magnetic properties of $TbRu_2Ge_2$ compound
15:15 -15:30	Arun B	2D broadband FMR data acquisition with Vector Network Analyzer and Determination of Asymptotic Lande g-Factor
15:30 – 16:00:	Tea/Coffee	
Day 2: Parallel Session-1	*Session Chair:* Pratap Roychaudhuri	
16:00-16:30	Mandar M Deshmukh	High temperature Josephson diode
16:30 – 17:00	Chandra Sekhar Yadav	Signature of point nodal superconductivity in the Dirac semimetal PdTe
17:00- 17:15	Debika Debnath	Diode effect in quantum dot-based Josephson junction
17:15- 17:30	Somak Basistha	Linear and Non-Linear response in the mixed state of superconducting NbN and a-MoGe thin films using a low-frequency two-coil mutual inductance technique
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	
19.00 pm onwards:	Dinner	

Day 2: Parallel Session-2	*Session Chair: Sudip Chakraborty*	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Indra Dasgupta	Spin-orbit driven emergent phases in quantum materials
9:30 – 10:00	Amrita	In search of spin orbit driven ferroelectric

	Bhattacharya	Rashba swtitches in Perovskite oxides
10:00 – 10:15	Dipanwita Bhattacharjee	Influence of band convergence on the thermoelectric transport properties of CoBi-based half-Heusler alloys
10:15 – 10:30	Ankita Bhattacharya	Electric field induced second-order anomalous Hall transport in unconventional Rashba system
10:30 -11:00:	Tea/Coffee	
Day 2: Parallel Session-2	*Session Chair*: Indra Dasgupta	
11:00 – 11:30	Arnab Sen	Fate of many-body localization in an Abelian lattice gauge theory
11:30 – 12:00	Uday Narayan Maiti	TBA
12:00 – 12:30	Sudip Chakraborty	Computational Roadmap of Emerging Materials: Implications of Piezochromism and Rashba Physics
12:30 – 12:45	Subhajyoti Pal	Theoretical analysis of multi-spin Excitations in 2D Antiferromagnet probed by Resonant Inelastic X-ray Scattering (RIXS)
12:45 – 14:00:	Lunch	
Day 2: Parallel Session-2	*Session Chair*: Surajit Saha	
14:00 – 14:30	Aveek Bid	Universality of quantum phase transitions in the integer and fractional quantum Hall regimes
14:30 -15:00	Binoy K. Hazra	Multifunctional properties of non-collinear antiferromagnet Mn_3Sn
15:00 -15:15	Snehasish Sen	Theory of Polar Skyrmions in Layered Structure of Ferroelectric Perovskites
15:15 -15:30	Shaili Sett	Impact of antiferroelectric moiré domains on a graphene field-effect transistor
15:30 – 16:00:	Tea/Coffee	
Day 2: Parallel Session-2	*Session Chair*: Swapan K Pati	

16:00-16:30	Bahadur Singh	Spin U(1) quasi-symmetry and quantized spin Hall effect in puckered lattice materials
16:30 – 17:00	Mukul Kabir	Reversible Quantum Phases in Magnetic Topological Insulators
17:00-17:30	Souvik Paul	Trends in magnetic interactions of transition-metal trilayers under electric fields
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	
19.00 pm onwards:	Dinner	

Day 2: Parallel Session-3	*Session Chair:* Kalpataru Pradhan	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Ramesh Chandra Nath	Field induced magnetic transition in the double trillium lattice antiferromagnet $KBaCr_2(PO_4)_3$
9:30 – 10:00	Surajit Saha	Tuning the robust magnetic properties in MPS_3 (M= Mn, Fe, and Ni)
10:00 – 10:15	Amit Vashist	Magnetic phase transitions in an antiferromagnetic topological insulator probed by nanomechanical resonators
10:15 – 10:30	Suraj S. Hegde	Emergent topology and its signatures in dissipative dynamics of topological condensed matter.
10:30 -11:00:	Tea/Coffee	
Day 2: Parallel Session-3	*Session Chair: Sumilan Banerjee*	
11:00 – 11:30	Sudhansu S Mandal	Solution of a Spin-1/2 Trimer Chain and Experimentally Verifiable Quantities
11:30 – 12:00	V Ravi Chandra	Spin wave interactions in the pyrochlore Heisenberg model with Dzyaloshinskii-Moriya terms
12:00 – 12:15	Biplab Pal	Engineering flux-controlled flat bands and topological states in a Stagome lattice
12:15 – 12:30	Kuldeep Suthar	Non-Hermitian Many-Body Localization and

		Skin Effect
12:30 – 14:00:	Lunch	
Day 2: Parallel Session-3	*Session Chair:* Sudeep Kumar Ghosh	
14:00 – 14:30	Kush Saha	Frequency-selective amplification of nonlinear response in strongly correlated bosons
14:30 -15:00	Auditya Sharma	Interplay of external drive and long-range hopping in the PLRBM model.
15:00 -15:15	Deepak Gaur	Non-Equilibrium Dynamics of Ultracold Bosonic Gases: Insights from Cluster Mean Field Theory
15:15 -15:30	Naba Prakash Nayak	Weak topological insulator phase in two-dimensional chiral symmetry class and universality of Anderson transition in chiral class
15:30 – 16:00:	Tea/Coffee	
Day 2: Parallel Session-3	*Session Chair:* Kush Saha	
16:00-16:30	Rejish Nath	Commensurate supersolids and re-entrant transitions in an extended Bose-Hubbard ladder
16:30 – 17:00	Sreejith Ganesh Jaya	Full distribution of local observables in an exactly solvable current carrying steady state of a driven XXZ chain
17:00- 17:15	Mainak Pal	Scar-induced imbalance and anomalous mid-spectrum zero modes in Rydberg ladders with staggered detuning
17:15- 17:30	Rajat Sharma	Temperature-induced supersolidity in spin-orbit-coupled Bose gases
17:30-18:00	Tea/Coffee	
17:30-19:00	Poster presentation/Scientific Discussions	
19.00 pm onwards:	Dinner	

Day 3, 23/12/24 (Monday):

Day 3:	*Session Chair:* Sreejith Ganesh Jaya

Parallel Session-1		
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Nayana Shah	Systematically compactifying the two-channel Kondo model: fermions to bosons and back in a consistent way
9:30 – 10:00	Awadhesh Narayan	Non-Linear Hall Effect in Flatlands and Chiral Crystals
10:00 – 10:30	Arti Garg	Trade-off relations between quantum coherence and measure of many-body localization
10:30 – 10:45	Koushik Dey	Negative Capacitance for Stabilizing the Logic State in a Tunnel Field-Effect Transistor
10:45 -11:00:	Tea/Coffee	
Day 3: Parallel Session-1	*Session Chair:* Amrita Bhattacharya	
11:00 – 11:30	Nitesh Kumar	Goniopolarity in an Altermagnetic System
11:30 – 12:00	Thirupathaiah Setti	$Sn_{0.06}Cr_3Te_4$: A Skyrmion Superconductor
12:00 – 12:15	Nayana Devaraj	Interplay of altermagnetism and pressure in hexagonal and orthorhombic MnTe
12:15 – 12:30	Krishnendu Patra	*Origin of Multiple Lifshitz Transitions in Weyl Semimetal RhSi*
12:30-12:45	Vinod Ashokan	Many body correlation effects in electron-electron quantum bi-wire systems
12:45 – 14:00:	Lunch Break	
Day 3: Parallel Session-1	*Session Chair:* Nayana Shah	
14:00 – 14:30	Akshay Singh	Dynamics of Moire Excitons and Quantifying Interfaces in 2D Heterostructure
14:30 -15:00	Tapan Mishra	Signatures of non-trivial doublon formation using a quantum computer
15:00-15:30	Malleswararao Tangi	Chiral spin textures in Epitaxial Acentric Quantum materials
15:30-15:45	Saisab Bhowmik	Magnetism, Fermi surface reconstructions,

		and Chern insulators in twisted bilayer graphene
16:15-16:30	Tea/Coffee	
16:30-17:00	Concluding Ceremony	
19.00 pm onwards:	Dinner	

Day 3: Parallel Session-2	*Session Chair:* Angom Dilip Kumar Singh	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Pankaj Kumar Mishra	Structural and dynamics of ultra-dilute spin-orbit coupled quantum droplet
9:30 – 10:00	Ayan Khan	Liquids and Solids in Ultracold Atomic Gases
10:00 – 10:15	Swarup Kanti Sarkar	Interaction-induced spin-dependent localization of spin-1/2 Bose-Einstein condensates in a random disorder potential
10:15 – 10:30	Sonali Gangwar	Structure and dynamics of imbalanced quantum droplet in spin-orbit coupled Bose-Einstein condensates
10:30-10:45	Shawan K. Jha	Energy spectra and fluxes of 2D turbulent quantum droplet
10:45 -11:00:	Tea/Coffee	
Day 3: Parallel Session-2	*Session Chair:* Akshay Singh	
11:00 – 11:30	Pratap Raychaudhuri	Superconductivity in tungsten
11:30 – 12:00	Srijani Mallik	Exploring Rashba parameter and superconductivity in anisotropic $KTaO_3$ based two-dimensional electron gases
12:00 – 12:30	Satyabrata Patnaik	Experimental Manifestations of Topological Superconductivity
12:30-13:00	Navaneetha Krishnan Ravichandran	Data-driven discovery of unconventional heat flow regimes in common semiconductors
13:00 – 14:00	Lunch	
Day 3:	*Session Chair: Awadhesh Narayan*	

Parallel Session-2		
14:00 – 14:30	Sebabrata Mukherjee	Ultrafast Laser-inscribed Photonic Topological Materials
14:30 -15:00	Ashish Arora	Novel high-performance differential magneto-spectroscopy techniques: results and challenges
15:00 -15:30	Sudipto Chakrabarti	The interplay between magnetism and chemical binding
15:30-15:45	Debadrita Ghosh	Determining entanglement in spatial photonic qutrit pair generated via pump beam modulation technique.
15:45-16:00	Surajit Dutta	Visualizing isospin magnetic texture in rhombohedral tetralayer graphene
16:00-16:15	Aditi Chakrabarty	Absence of Wannier-Stark localization and skin effect in driven non-Hermitian systems
16:15-16:30	Tea/Coffee	
16:30-17:00	Concluding Ceremony	
19.00 onwards:	Dinner	

Day 3: Parallel Session-3	*Session Chair:* Nitesh Kumar	
Time	Speaker	Title of the talk
7:30-9:00	Breakfast	
9:00 – 9:30	Tulika Maitra	Emerging triferroicity and polar metallic state in two dimensional rare-earth halide based monolayers
9:30 – 10:00	Atikur Rahman	Effect of Defects and Strain on the Optoelectronic Properties of Monolayer TMDs
10:00 – 10:30	Ratnadwip Singha	Using crystallographic motifs to search for new quantum materials
10:30-10:45	Payal Wadhwa	Machine learning-aided study of surface reconstructions of Cu_2O (111) plane
10:45 -11:00:	Tea/Coffee	
Day 3: Parallel Session-3	*Session Chair:* Ramesh Chandra Nath	

11:00 – 11:30	Udit Khanna	Quantum Hall Phase Diagram in Bilayer Graphene
11:30 – 12:00	Subhra Sen Gupta	Chaos and Eigenstate Multifractality in Disordered Quantum Spin Systems and some Special Random Matrix Models
12:00 – 12:30	Bivas Dutta	1/2-quanta Thermal Conductance of an Isolated Quantum Hall Channel
12:30 – 12:45	Tuhin Maji	Interface Engineering of Ag@Au Nanohybrid for Ultra-strong Electron-phonon Coupling and Non-classical Electron Transport
12:45-13:00	Zainab Chowdhry	Investigation of magnetism in 2D material MoS_2
13:00 – 14:00:	Lunch	
Day 3: Parallel Session-1	*Session Chair:* Thirupathaiah Setti	
14:00 – 14:30	Pavan Nukala	Emergent functions via proximity coupling of Mott insulators with ferroelectrics
14:30 -15:00	Jhuma Sannigrahi	Unraveling the Magnetoelectric Coupling in $CaMn_7O_{12}$
15:00 -15:30	Saikat Bhaumik	Luminescent metal halide perovskite nanocrystals for various applications
15:30-15:45	Shalini Verma	Investigation of Structural, Magnetic, and Dielectric Behavior in Nd-Doped $Gd_3Fe_5O_{12}$ multiferroic samples
15:45-16:00	Akriti Singh	Investigating temperature-induced structural phase transition in Double Perovskite oxides
16:00-16:15	Arpita Deb Singha	Canonical spin-glass dynamics in distorted Kagom and Triangular lattices
16:15-16:30	Tea/Coffee	
16:30-17:00	Concluding Ceremony	
19:00 onwards	Dinner	

Saturday, 21st December, 2024

List of Abstracts – Talks

Day1 Parallel Session -1

Kinetically constrained models showing Hilbert space fragmentation

Diptiman Sen*
Indian Institute of Science, Bangalore

We will discuss some models where kinetic constraints in the Hamiltonian lead to a shattering of the Hilbert space into a large number of disconnected fragments. The Hilbert space fragmentation may be strong or weak depending on the ratio of the size of the largest fragment to the size of the full Hilbert space. Each fragment can be characterized in terms of a single irreducible string (IS), such that all the states of that fragment can be reached via the Hamiltonian starting from the IS. The number of states in a fragment can be obtained from the structure of the IS. The nature of the dynamics can be completely different in different fragments, being non-integrable in some fragments and integrable or even trivial in others. The different behaviors can be understood by studying a variety of quantities, such as the energy level spacing statistics, a plot of the half-chain entanglement versus the energy, the time-evolution of autocorrelation functions, and the Loschmidt echo. We will illustrate all these ideas using some one-dimensional lattice models with density-dependent hopping amplitudes between nearest-neighbor sites..

References

[1] S. Aditya, D. Dhar and D. Sen, Phys. Rev. B 110, 045418 (2024).
[2] M. Ganguli, S. Aditya and D. Sen, arXiv:2409.15943.

Static structure factor and the dispersion of the Girvin-MacDonald-Platzman density-mode for fractional quantum Hall fluids on the Haldane sphere

Rakesh K. Dora and Ajit C. Balram*

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Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India
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We study the neutral excitations in the bulk of the fractional quantum Hall (FQH) fluids generated by acting the Girvin-MacDonald-Platzman (GMP) density operator on the uniform ground state. Creating these density modulations atop the ground state costs energy since any density fluctuation in the FQH system has a gap stemming from the underlying inter-particle interactions. We calculate the GMP density-mode dispersion for many bosonic and fermionic FQH states on the Haldane sphere using the ground state static structure factor computed on the same geometry. Previously, this computation was carried out on the plane. Analogous to the GMP algebra of the lowest Landau level (LLL) projected density operators in the plane, we derive the algebra for the LLL-projected density operators on the sphere, which facilitates the computation of the density-mode dispersion. Contrary to previous results on the plane, we find that in the long-wavelength limit, the GMP mode does provide an accurate description of the dynamics of the primary Jain states.

Ref: Rakesh K. Dora and Ajit C. Balram, *Static structure factor and the dispersion of the Girvin-MacDonald-Platzman density-mode for fractional quantum Hall fluids on the Haldane sphere*, arXiv:2410.00165

Emergent Quadrupolar Order in the Spin-1/2 Kitaev-Heisenberg Model

Manodip Routh[1], Sayan Ghosh[1], Jeroen van den Brink[2,3,4], Satoshi Nishimoto[2,4], and Manoranjan Kumar[1]

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[3]W¨urzburg-Dresden Cluster of Excellence ct.qmat, Germany
[4]Department of Physics, Technical University Dresden, 01069 Dresden, Germany.

Motivated by the largely unexplored domain of multi-polar ordered spin states in the Kitaev-Heisenberg (KH) systems we investigate the ground state dynamics of the spin-1/2 KH model, focusing on quadrupolar (QP) order in 2-leg ladder and two-dimensional honeycomb lattice geometries. Employing exact diagonalization and density-matrix renormalization group methods, we analyze the QP order parameter and correlation functions. Our findings reveal a robust QP order across a wide range of the phase diagram, influenced by the interplay between Heisenberg and Kitaev interactions. Notably, we observe an enhancement of QP order near Kitaev quantum spin liquid (QSL) phases, despite the absence of long-range spin-spin correlations. This highlights a complex relationship between QP order and QSLs, offering new insights into quantum magnetism in low-dimensional systems. Our findings provide a rational explanation for the observed nonlinear magnetic susceptibility in α-$RuCl_3$.

Speed Limits and Scrambling in Krylov Space

Ankit Gill , Tapobrata Sarkar

We investigate the relationship between Krylov complexity and operator quantum speed limits (OQSLs) of the complexity operator and level repulsion in random/integrable matrices and many-body systems. An enhanced level-repulsion corresponds to increased OQSLs in random/integrable matrices. However, in many-body systems, the dynamics is more intricate due to the tensor product structure of the models. Initially, as the integrability-breaking parameter increases, the OQSL also increases, suggesting that breaking integrability allows for faster evolution of the complexity operator. At larger values of integrability-breaking, the OQSL decreases, suggesting a slowdown in the operator's evolution speed. Information-theoretic properties, such as scrambling, coherence and entanglement, of Krylov basis operators in many-body systems, are also investigated. The scrambling behaviour of these operators exhibits distinct patterns in integrable and chaotic cases. For systems exhibiting chaotic dynamics, the Krylov basis operators remain a reliable measure of these properties of the time-evolved operator at late times. However, in integrable systems, the Krylov operator's ability to capture the entanglement dynamics is less effective, especially during late times.

Measurement-Induced Superconductor-Insulator Transition in Weakly Monitored Josephson Junction Arrays

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In quantum many-body systems, ‘measurement-induced phase transitions’ (MIPT), have led to a new paradigm for dynamical phase transitions in recent years. I will discuss a model of continuously monitored or weakly measured arrays of Josephson junctions (JJAs) with feedback. Using a combination of a variational self-consistent harmonic approximation and analysis in the semiclassical limit, strong dissipation limit, and weak coupling perturbative renormalization group, I will show that the model undergoes re-entrant superconductor-insulator MIPTs in its long-time non-equilibrium steady state as a function of measurement strength and feedback strength. I will contrast the phase diagram of monitored JJA with the well-studied case of dissipative JJA.

Phase Transitions in Twisted Bilayer Graphene

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We study the normal state of twisted bilayer graphene in the carrier density range n/n_s =-2 and n/n_s =-3. We show that the system undergoes two phase transitions, from a inter-valley coherent (K-IVC) state to a valley polarized state to an anomalous quantum hall state as a function of carrier density. We calculate the phase diagram as a function of carrier density and interaction strength. The symmetries of the different phases force the bandwidth of the low energy bands to vary non-monotonically as a function of carrier density.

Reducing the vortex entanglement via Pb substitution in the charge reservoirs of Bi-2212 superconductor

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Abstract: Doping at the charge reservoirs of cuprate superconductors has been shown to markedly enhance various superconducting properties. In this present study, a comprehensive comparative analysis has been conducted on the vortex states and pinning potential (U) in $Bi_{2-x}Pb_xSr_2CaCu_2O_{8+\delta}$ (x = 0, 0.5) superconducting samples. Although the pinning potential at zero temperature (U_0) (estimated in the thermally activated flux flow (TAFF) model) decreases slightly upon doping, increased magnetic fields hardly affect U_0 for the doped sample unlike the undoped one. This observation suggests a lower degree of entanglement of vortex lines and reinforcement of plastic pinning by partial substitution of Pb ions in the Bi sites. Besides, high superconducting transition temperature (T_c) and high critical current density (J_c), higher stability in U_0 at high magnetic field is also required for the technological applications. At the vicinity of the vortex-glass state, the vortices may be frozen to the 2D vortex-glass state. In both samples, the estimated critical exponent (S) is smaller than 2.7, the lower limit of the 3D vortex-glass state. Notably, doping Pb to $Bi-2212$ superconductor results in a significant increase in the stability of U_0 at high magnetic fields, as well as the broadening of its pinned vortex-liquid region, while retaining a high T_c value and this aspect has technological importance. Finally, an interesting vortex-phase diagram featuring diverse vortex states has been constructed from the magneto-transport measurement, for both undoped and Pb-doped samples.

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

Jagannath Sutradhar, Jonathan Ruhman, Avraham Klein

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

Exploration of emergent rich strongly correlated state in SmB_6 and a comparison of this system with a conventional topological insulator Bi_2Se_3

Sayantan Ghosh, Sugata Paul, Tamoghna Chattoraj, Amit Jash, Zachary Fisk, **Satyajit S. Banerjee* (*IITK Dept of Physics; satyajit@iitk.ac.in)**

Abstract:
We present results of our recent investigations [1,2] on a detailed comparison sensitive pick-up response of SmB6 single crystal with that of a conventional topological insulator (TI), Bi2Se3 single crystal. Our studies identify the distinct onset of three distinct temperature regimes for SmB6. These temperature markers relate to the onset of Kondo localization in the system, followed by a regime with strengthening of correlations leading to what is predicted to be a a Kondo lattice with a Kondo gap and finally a third regime below the gap where we the see the emergence unusual new features in SmB6. This is the regime where we see the emergence of a high conducting surface state. This regime is explored in detail to reveal novel features of correlations in this surface state along with unique frequency dependence and non scalability of the data with varying drive. These features suggest that in SmB6 the presence of unique strongly correlated surface conductivity emerging just below the Kondo gap and we discuss its origin. Along with the above measurements through a combination of sensitive AC and DC excitation studies, we demonstrate that SmB6 exhibits Mott-like behaviour with disorder-induced sublinear frequency dependence of the electrical response at low temperatures. The study also reveals the presence of localized states, which contribute to non-linear current-voltage characteristics and strong correlations in the system. These insights are further supported by specific heat measurements, indicating an intricate interplay between localized Schottky anomalies and dissipationless states in the bulk. Our findings highlight the complex admixture of correlated bulk and surface phases in SmB6, offering new pathways to explore the physics of topological Kondo insulators. If time permits we will also discuss our recent results on high sensitivity transport current imaging to visualize the surface states to explore the topological states in these materials.

Ref.
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[2] Sayantan Ghosh, Sugata Paul, Tamoghna Chattoraj, Amit Jash, Zachary Fisk and S. S. Banerjee* (submitted 2024)

Superconducting Natural Heterostructures: A Novel Platform for Unconventional Superconductivity

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The recent discovery of unconventional superconductivity in twisted bilayer graphene has ignited a surge of interest in van der Waals (vdW) materials. This paradigm shift empowers us to engineer heterostructures with tailored electronic properties. Naturally stacked heterostructures, such as layered chalcogenides and misfit compounds, are particularly promising due to their intrinsic layered structures. This built-in adaptability allows for precise control over device functionality, potentially leading to simpler and more efficient devices. Superconducting natural heterostructures form a new class of superconducting compounds. By carefully combining layers, we can induce unconventional superconducting states with intriguing properties like time-reversal symmetry breaking and nematic order.

In this presentation, I will discuss recent findings on the unconventional superconducting characteristics of natural heterostructure superconductors.

Electron-phonon coupling, critical temperatures and gaps in $NbSe_2/MoS_2$ Ising Superconductors

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Utilizing Migdal-Eliashberg theory of superconductivity within the first-principles calculations, we work out the role of electron-phonon coupling (EPC) and anisotropic superconducting properties of a recently discovered 2D van der Waals heterostructure comprising a single layer of MoS2 and few layers of NbSe2. We find strong EPC and a softening of phonon modes in the lowest acoustic branch. While the single MoS2 layer does not actively contribute to the EPC, it significantly elevates the superconducting critical temperature Tc compared to monolayer NbSe2. This is attributed to the degradation of the charge-density wave (CDW) by the MoS2 layer. Notably, we observe a two-gap superconductivity in NbSe2/MoS2 and extend our study to three layers of NbSe2. A reduction in Tc with increasing thickness of NbSe2 is observed. Incorporation of spin-orbit coupling (SOC) suggests a possible mechanism for Ising superconductivity. We find that SOC reduces EPC while Tc is suppressed concomitantly by about 5K, leading to a closer estimate of the experimental Tc.

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Unconventional vortex states in the Chevrel phase superconductor $PbMo_6Se_8$?

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Abstract

We present a comprehensive investigation of superconducting properties in the Chevrel phase compound $PbMo_6Se_8$ by x-ray diffraction, dc magnetization, resistivity, heat capacity, and magnetic relaxation experiments. We determine a bulk superconducting transition temperature T_c of 3.8 K. Key superconducting parameters such as lower [$\mu_0 H_{c1}(0)$] and upper [$\mu_0 H_{c2}(0)$] critical fields, coherence length [$\xi_{GL}(0)$], penetration depth [$\lambda_{GL}(0)$], Ginzburg-Landau parameter (κ), Pauli paramagnetic field ($\mu_0 H_{str}^P$), and Maki parameter (α_M) are obtained. The BCS model provides a reasonable description of the heat-capacity data. An unconventional vortex state is evident from the investigation of the unusual fishtail effect and nonmonotonous magnetic field dependency of the vortex pinning energy obtained from the magnetic relaxation experiments, indicating a deviation from the ideal type II superconducting vortex, in $PbMo_6Se_8$. A detailed $\mu_0 H$-T phase diagram has been drawn illustrating a multiphase vortex crossover.

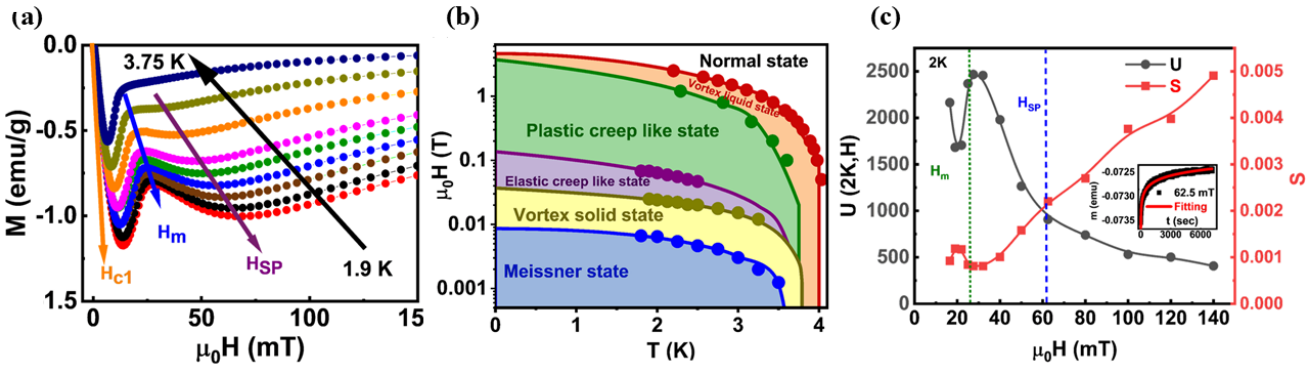

Fig. 1: *(a) Observation of 'fishtail effect' in isothermal magnetization associated with $\mu_0 H_{SP}$. (b) Multi-vortex phase crossover in the detailed $\mu_0 H - T$ phase diagram. (c) Unconventional vortex pinning is evident from the non-monotonous dependency of pinning potential U, on the external applied magnetic field $\mu_0 H$. The inset shows magnetic relaxation fitted with the Anderson model.*

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Origin of Sign change in Thermopower of Strained Sr_2RuO_4

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Exceptionally slow and long-range critical fluctuations anticipate the singularity in second order phase transition

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Second-order phase transitions are prevalent across various disciplines in the natural sciences. Traditionally, these transitions are understood through Ginzburg-Landau mean-field theory, which describes the thermodynamic properties near the critical points. While the order parameter fluctuations play a pivotal role in determining the critical properties of these systems, direct experimental investigations have been lacking.

In this talk, I will discuss our recent experimental investigation of order parameter fluctuations in a quasi-one-dimensional charge density wave (CDW) system., specifically (TaSe4)2I with infinitely long TaSe4 chains. The (TaSe4)2I single crystal undergoes CDW transition at around 263 K. We are able to directly measure the CDW order parameter fluctuations via the resistance fluctuation on account of their coupling to the dissipative normal carriers in pinned CDW state.

Our experimental findings reveal that the order parameter fluctuations are slow enough to persist in the thermodynamic limit and dominate the phase transition over a wide temperature window around the critical point. We observe that both the variance and the relaxation time of these fluctuations increase dramatically, and their behavior becomes noticeably non-Gaussian. These are classic signatures of "critical opalescence" and "critical slowing down," well-anticipated phenomena in a critical transition. Our study provides new insights into the critical behavior of electronic systems and contribute to a broader understanding of criticality across various disciplines in natural sciences.

Reference: Sk Kalimuddin et al, Phys. Rev. Lett. 132, 266504 (2024)

Bi based half-Heusler alloys: Potential candidates for thermoelectric applications

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The unique feature of thermoelectric (TE) materials such as conversion of waste heat into electricity projects them potential candidates for renewable energy harvesting process. During last 15 years, half-Heusler (HH) materials, owing to their exceptional mechanical strength, thermal stability and thermoelectric efficiency, becomes most promising TE materials for the mid to high temperature waste heat management. In this study, we have investigated thermoelectric characteristics of HH alloys XYBi (X: Ti, Zr, Hf; Y: Co, Rh, Ir). These HH alloys possess formation energy in between -0.36 to -0.74 eV/atom. Not only energetic stability, but also Born-Huang's criteria related to mechanical characteristics and absence of imaginary frequency in phonon spectra related to dynamical stability satisfied which dictates about feasibility for experimental design. Electronic band structure analysis based on Heyd-Scuseria-Ernzerhof (HSE06) functional including the effect of spin-orbit coupling suggest that except HfIrBi with semi-metallic nature, all other HH alloys exhibit semiconducting bandgap in between 0.62-1.25 eV. Transport properties are achieved by solving semi-classical Boltzmann transport equation in both electron and phonon aspects. Taking into consideration electro-acoustic phonon and electro-optical phonon scattering processes, these HH alloys generate thermoelectric figure of merit around 0.72-1.93 (0.56-1.98) for hole (electron) regime respectively. Among these HH alloys, it is also possible to generate thermoelectric conversion efficiency value up to 17% which enhances their possibility towards real world thermoelectric applications. Thus, a possible thermoelectric device with its n-type and p-type legs as HH alloys may shed light into thermoelectric device fabrications.

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Robust and Thermally Stable Pinning Mechanisms Behind the High J_c State of HTSC-TMC NPs Nanocomposites

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Abstract: We investigate the impact of the admixture of Co_2C nanopowder on the critical current density (J_c) of Bi-2223 high-temperature superconductor (HTSC). Our analysis of compacted composite pellets of Bi-2223 admixed Co_2C nanopowders, containing 0%, 0.05%, and 2% Co_2C by weight, identifies two distinct populations of Co_2C: intra-granular speckles (~30-40 nm) and inter-granular clusters (~0.1 μm). The analysis of $J_c(H)$ and pinning force ($F_p(H)$) identifies a temperature (T) dependent crossover field (H_{cr}). Across H_{cr}, the pinning mechanism transitions from a regime that is a mix of conventional and unconventional to one that is predominantly unconventional. Analysis below H_{cr} reveals that Co_2C clusters decorating the grain boundaries in Bi-2223 and Co_2C speckles lead to strong pinning features with unconventional field and temperature dependence. Magnetization relaxation measurements along with a three-dimensional pinning force analysis identify Co_2C clusters decorating the Bi-2223 grain boundaries as the predominant source of strong (unconventional) pinning characteristics which are stable against large thermal fluctuations in the high T regime. Our study shows vortex activation energies as high as 3000 meV retained in the high T regime between 70 to 80 K. The strong pinning force range due to Co_2C particles is estimated to be a few nanometers at 80 K. The superconducting ferromagnetic properties of the Josephson junctions at Co_2C-decorated grain boundaries contribute to these robust pinning features at high T. Our findings highlight the potential of transition metal carbide-HTSC nanocomposites to enhance the performance of HTSC materials, particularly in applications operating at elevated, liquid Nitrogen temperatures.

Day1 Parallel Session -2

Tuning dielectric responses and polar instabilities in some orthorhombic rare-earth chromates

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Rare-earth chromates exhibit varied functional properties. In this presentation, we shall discuss our experimental results towards understanding and tuning of low-temperature dielectric relaxations in some $RCrO_3$ to design an otherwise lossy-dielectric to become a candidate high-k dielectric material. Further, we shall discuss our experimental results towards designing a general route to achieve room-temperature ferroelectricity of structural origin in a range of rare-earth chromates.

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Large Tunneling magnetoresistance in all-oxide magnetic tunnel junctions with perpendicular magnetic anisotropy

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Present day spintronic devices utilize energy-efficient approaches for their operation, exploiting schemes such as electric current, spin transfer torque and spin orbit torque. The essential building block in such devices is the magnetic tunnel junction (MTJ) comprising of a complex metallic magnetic stack designed to obtain the required magnetic anisotropy and includes a thin insulating or ferroelectric layer as the tunneling barrier. The material and design aspects of such MTJs are well explored and today includes antiferromagnets as active elements, expanding computing primitives beyond spin to include orbitals and magnons for new applications. Complex oxides, endowed with a rich phase space and exploiting strong correlation effects and topology leading to emergent phenomena at their heterointerfaces are gaining prominence as an important material class in this regard. The versatility of these materials in creating epitaxial interfaces utilizing strain control, designing crystalline symmetry and tailoring spin-orbit coupling effects are less explored but essential for new generation of MTJ.

In this work we use well-characterized epitaxial interfaces of ferromagnetic SrRuO3 (SRO) electrodes with SrTiO3 (STO) as insulating barriers, tailored to obtain perpendicular magnetic anisotropy for studying spin-polarization tunneling. In recent works topological Hall effects, Weyl fermions and topological textures such as skyrmion bubbles were reported in SRO. We report, surprisingly large tunnelling magnetoresistance (TMR) and spin polarization across SRO/STO/SRO MTJs with different electrode thicknesses persisting up to high voltage bias and temperatures. Using density functional theory (DFT) calculations, we find the majority-spin states of SRO to decay in STO according to the Δ_1 band of STO, whereas the decay of the minority-spin states follows the Δ_5.This results in a high transmission in the parallel state due to a perfect correspondence between symmetry and spin while transmission in the anti-parallel state is reduced because spins cannot be transmitted between majority-spin Δ_1 states and minority-spin $\Delta_5$states. The calculated TMR is found to be 1800%, lower than the experimentally observed value. These new considerations that explains the experimental findings are a new direction for MTJ spintronic devices and relevant for applications beyond conventional MRAMs such as in new computing energy-efficient hardware.

Optically enhanced negative differential resistance in reduced graphene oxide coated silicon nanorods

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Silicon technology has made an irreversible impact on our daily life by improving the modern technology in almost every aspect of life such as computing, communication, energy and quantum technology [1]. However, the demand of miniaturization for faster data communication results in increase of temperature of the device leading the microelectronic technology towards a stagnancy until we can switch to photonic communication instead of electronic one. Silicon in bulk form exhibit poor optoelectronic properties due to its indirect band gap nature, however in nano-dimension quantum confinement of charge carriers resulting in widening of band gap. Consequently, the relaxation in *k*-selection rule for transition between the edges of conduction band and the valance band establishes nanocrystalline Si a potential candidate for photonic and photovoltaic applications. On the other hand, due to large surface to volume ratio Si nanocrystals get easily oxidized in ambient air and this oxide layer becomes favorable for photoluminescence but detrimental to charge transport and electroluminescence reducing the potential of Si nanocrystals for photonic communication [1-2]. This problem may be possible to overcome by capping the quantum structures of Si with a transparent thin and conducting material like graphene or reduced graphene oxide.

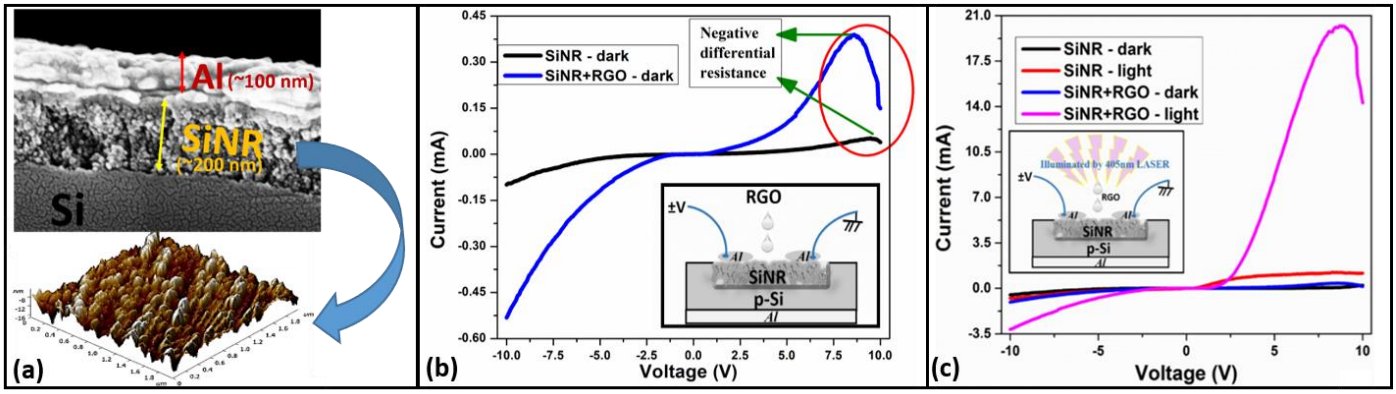

Fig. 1: (a) Cross-sectional FESEM image of the device with the 3D topographic AFM image of SiNRs; I-V characteristics of SiNR before and after addition of RGO (b) in dark and (c) under illumination with inset depicting the schematic device arrangements.

Motivated by the above aspects, in this work we have explored the effect of illumination on charge transport through an amine functionalized reduced graphene oxide (RGO) coated nanocrystalline Si layer containing Si nano-rods (SiNR). Si nano-rods (SiNR) prepared by well-known electrochemical etching process on a p-type electropolished bulk Si substrate are clearly visible in 3D topographic atomic force microscopic (AFM) image (Fig. 1(a)). RGO has been prepared by modified Hummer's method followed by the characterization through FTIR and Raman spectroscopy [2]. Metallic contact on the layer containing SiNRs has been established through deposition of Aluminium (Al) using thermal evaporation technique. Schematic cross-section of FESEM image of the device is shown in Fig. 1(a). I-V measurements have been performed between two Al contacts on the SiNR layer in dark and under illumination and this process is repeated by addition of RGO drop by drop between the electrodes on the SiNR layer as depicted in the schematic inset Fig. 1(b,c). The most salient feature is the negative differential resistance (NDR) obtained in the voltage regime ~8V like a tunnel diode already reported elsewhere in case of SiNR only [3]. The overall current including NDR through SiNR obtained in dark gets enhanced ~8 times after addition of RGO (Fig. 1(b)) whereas the photo-current after addition of RGO is ~20 times higher than that was before addition of RGO (Fig.1(c)). NDR has got enhanced a lot after addition of RGO under illumination. The conductivity is increasing with increasing amount of RGO. So, the addition of highly conducting RGO is enhancing the light assisted charge transport process indicating that this RGO coated SiNR composite has the potential to be used in the area of photoconduction as well as to have application in oscillators and amplifiers at microwave frequency for the obtained NDR.

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Frustration driven low-temperature spin-glass behavior and short-range correlations in tri-cation spinel

Mouli Roy-Chowdhury[1], Tapati Sarkar[2], Eun Sang Choi[3], Subhash Thota[1,*]

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ABSTRACT

Magnetically diluted compounds can be experimentally derived from conventional long-range ordered spinels like Co_3O_4 or Mn_3O_4 by site-specific elemental substitution at one or both of the cationic sites, tetrahedral (*A*) and octahedral (*B*), in the spinel lattice [1]. Such systems often provide an exciting platform to study magnetic frustration and random anisotropy leading to the loss of long-range magnetic order and emergence of exotic low-temperature phases like the spin-glass (SG) phase. In this work, we studied a doubly-diluted derivative of Mn_3O_4 exhibiting ferrimagnetic ordering, leading to a tri-cation spinel oxide: $ZnMnCoO_4$ (ZMCO). This system was synthesized using conventional solid-state synthesis techniques from binary transition metal oxides (ZnO, MnO_2, and Co_3O_4) as precursors. All of the *A*-sites in the 'parent' Mn_3O_4 lattice got replaced by nonmagnetic Zn^{2+}, while 50% of the *B*-sites got replaced by nonmagnetic Co^{3+} leaving the system with only one type of magnetic (Mn^{3+}) cations at the *B*-site.

Polycrystalline ZMCO crystallized in cubic symmetry belonging to the space group *Fd*-3*m* as confirmed by x-ray diffraction. Although it appears quite simple, however, their nature of magnetism is complex and quite intriguing. Temperature and field dependent DC and ac magnetic measurements established a 'hierarchically organized' cluster SG ground state. This was further confirmed by a non-exponential time evolution of isothermal remanent magnetization. The presence of only short-range ordering in the investigated system was demonstrated by the absence of a λ-shaped peak in the specific heat versus temperature data [2]. Differential DC magnetic susceptibility plots revealed another transition in the system above the cluster SG phase. Above the 'glassy' transition, ZMCO exhibited ferrimagnetic behavior (T_{FN} = 38 K) with short-range magnetic correlations. A field-induced transition was also observed. All these are represented on the *T*-*H* plane as shown in Fig. 1. Thus, site-specific elemental substitution can lead to magnetic frustration and short-range magnetic correlations.

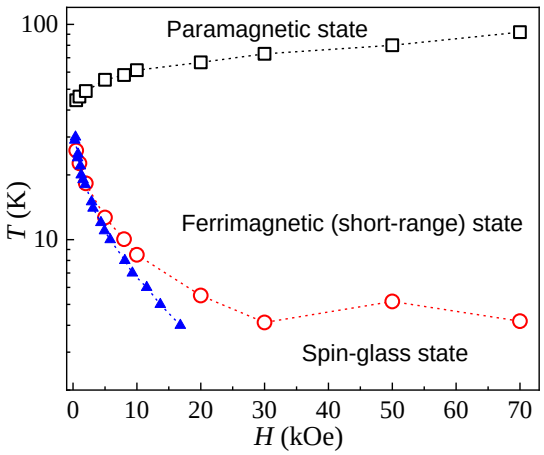

Fig 1. The phase diagram of ZMCO is mapped out on the *T*-*H* plane depicting the major phase transitions.

Keywords: Spinel oxides, Magnetic Frustration, Spin-glass.

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Tailoring Topological Phases and Anomalous Hall Effect in Noncollinear Antiferromagnets

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Noncollinear antiferromagnets (AFMs) have emerged as promising platforms for realizing novel topological phases and unconventional transport phenomena. In this work, we investigate the interplay between magnetic order and electronic topology in a class of planar noncollinear AFMs, Mn_3X (X=Sn, Ga, Ge) [1]. The magnetic order is characterized by a vector chirality **κ**, which can assume values of +1 or -1, and can be switched between these states. We demonstrate that a subtle rotation (staggered) of the magnetic moments can induce a topological phase transition from a nodal ring semimetal to a Weyl semimetal. This transition is accompanied by a significant enhancement in the anomalous Hall conductivity, which can be tuned by manipulating the magnetic orderFurthermore, we investigate the role of higher-order exchange interactions in stabilizing noncoplanar magnetic states in electron-doped Mn_3Sn [2].These noncoplanar configurations give rise to a large scalar spin chirality-induced anomalous Hall effect. Our findings highlight the potential of noncollinear AFMs for realizing multifunctional spintronic devices with tunable transport properties.

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Complex magnetism and spin transport in two-dimensional magnets

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In recent years, the realization of magnetic long-range order in atomically thin two-dimensional (2D) materials has shown a big potential in spintronic applications in ultrathin magnets due to the possibility of manipulation of magnetism by external fields, strain or proximity effects in van der Waals heterostructures. Specifically, the family of metallic magnets Fe_nGeTe_2 (n=3, 4, 5) has attracted a huge attention due to their high Curie temperatures and intriguing properties. In this talk, I will present results obtained by ab initio density functional theory, calculations of interatomic exchange interaction parameters and Monte Carlo simulations. A particular emphasis will be given on the systematic study of the electronic structure and magnetism of Fe_nGeTe_2 magnets along with some critical discussions on the importance of electron correlation with the aid of dynamical mean field theory, spin-orbit coupling and effects of transition metal doping. Finally, some results on the spin-polarized quantum transport will be shown for $PtTe_2/Fe_4GeTe_2/PtTe_2$ van der Waals heterostructures, especially on high tunnelling magnetoresistance.

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Controlling the Particle-hole symmetry in fractional Quantum Hall state in ABA trilayer graphene.

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Abstract:

In this talk, I will present a detailed experimental study of the particle-hole (PH) symmetry of the the abelian and a putative non-abelian Fractional Quantum Hall (FQH) state about half filling in a multiband system. Specifically, we focus on the lowest Landau level of the monolayer-like band of Bernal stacked trilayer graphene (TLG). In pristine TLG, the excitation energy gaps, Lande g factor, effective mass, and disorder broadening of the FQH states is the same as their hole-conjugate counterpart. This precise PH symmetry stems from the lattice mirror symmetry that precludes Landau-level mixing. Introducing a non-zero displacement field D disrupts this mirror symmetry, facilitating the interaction and hybridization between the $N_M = 0$ of monolayer-like and $N_B = 2$ bilayer-like Landau levels. This band hybridization eventually leads to a violation of the particle-hole symmetry of the FQH states. We find the one-third and two-fifth FQH states to be more robust against Landau level mixing than their hole-conjugate states, which agrees with theoretical predictions [1]. The Landau level mixing parameter κ is found to increase sharply with D. Our research identifies an external factor that can be manipulated to adjust the particle-hole symmetry in FQH states.

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Electron-phonon coupling induced topological phase transition in an α-T_3 Haldane-Holstein model

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We present impelling evidence of topological phase transitions induced by electron-phonon (e-ph) coupling in an α-T_3 Haldane-Holstein model that facilitates smooth tunability between graphene ($\alpha = 0$) and a dice lattice ($\alpha = 1$). The e-ph coupling has been incorporated via the Lang-Firsov transformation which adequately captures the polaron physics in the high frequency (anti-adiabatic) regime, and yields an effective Hamiltonian through zero phonon averaging at $T = 0$. While exploring the signature of phase transitions driven by polaron and its interplay with the parameter α, we identify two regions based on the values of α, namely, the low to intermediate range ($0 < \alpha \leq 0.6$) and larger values of α ($0.6 < \alpha < 1$), where the topological transitions host distinct behaviour. There exists a single critical e-ph coupling strength for the former, below which the system behaves as a topological insulator characterized by edge modes, finite Chern number, and Hall conductivity, with all of them vanishing above this value, and the system undergoes a spectral gap closing transition. Further, the critical coupling strength depends upon α. For the latter case ($0.6 < \alpha < 1$), the scenario is more interesting where there are two critical values of the e-ph coupling at which trivial-topological-trivial and topological-topological-trivial phase transitions occur. Our study shows a significant difference with regard to the well-known unique transition occurring at $\alpha = 0.5$ (or at 0.7) in the absence of the e-ph coupling, and thus underscores the importance of interaction effects on topological phase transitions.

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Broken symmetry quantum Hall states, layer hybridization and screening effects in twisted bilayer graphene at intermediate angles

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ABSTRACT

Twisted bilayer graphene (TBLG) at intermediate twist angles ($3^0 < \theta < 8^0$), forms a bilayer two-dimensional electron/hole gas system with sub-nm layer separation, in which the momentum mismatch between the Dirac cones of individual layers leads to a breakdown of interlayer coherence. This removes the layer degree of freedom from the spin and valley degrees of freedom of individual layers resulting in eight-fold degeneracy in the Landau levels (LL). Here, we discuss the role of charge imbalance, layer hybridization and broken symmetries in the Quantum Hall (QH) states of twisted bilayer graphene with intermediate twist angle. The longitudinal magnetoresistance (R_{xx}) minima and the corresponding QH plateaus were observed at total filling factors, ν_{tot}, similar to Bernal-stacked BLG, but with magnetic field, B-dependent LL crossings at large ν_{tot}, where the QH sequence changes. This is attributed to the charge carrier imbalance between the top and bottom layers arising from partial screening of the gate field (V_G) where the filling of LLs of each layer is determined by the compressibility of the bottom layer and the charging energy of the top layer. At low filling factors the broken symmetry QH states were observed where the spin, valley and layer degeneracies are broken, with a QH insulator state emerging at $\nu_{tot} = 0$. In addition to these, a notable B-dependent hysteresis emerged in the R_{xx} - V_G sweeps which can be understood as charge localization in individual layers manifesting in asymmetric charge distribution between the layers. These results provide a comprehensive understanding of layer hybridization, screening and charge localization in the QH states of twisted bilayer graphene at intermediate twist angles.

Exciton-Exciton Interaction in a Moiré Superlattice: Repulsive or Attractive?

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A twisted hetero-bilayer hosts a special type of excitons – the inter-layer excitons – where the constituent electrons and holes are spatially located in two different layers due to a type-II heterojunction. Such excitons exhibit an in-plane transition dipole and an out-of-plane permanent dipole moment – allowing a strong tunability through external stimulus. These excitons exhibit intricate moiré superlattice effects when trapped in a periodic array of potential wells resulting from the moiré effect in the hetero-bilayer.

In this talk, I shall show our experimental efforts in understanding the inter-exciton interaction by cleverly enhancing the local exciton density even at a low optical power through exciton funneling in a strained WS_2/WSe_2 moiré superlattice. While interaction among inter-layer excitons is usually perceived as repulsive in nature, I shall show evidence of a switching from repulsive to attractive interaction owing to the anisotropic dielectric screening. Such attractive interaction has intriguing implications such as stabilization of moiré biexciton and other higher order excitonic complexes.

Various phases of discrete time crystal in driven central spin model

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Abstract: We propose and characterize a driving protocol for an interacting central spin system to establish a perfect period doubling time crystal phase at certain values of interaction strength for any initial state and any system size. The nature of the time crystal depends on the odd-even parity of the number of satellite spins. Alongside the numerical simulation, we provide an analytical explanation for this behavior. Then we explore the sensing capability of this system to measure the interaction between the central spin and the satellite spins. The time crystal phase shows enhanced sensitivity as we see the Quantum Fisher Information scales as N^2 (N being the system size). Along with this, we find some period 12 and period 24 time crystal at some finely tuned values of interaction strength.

Thermopower probing emergent local moments in magic-angle twisted bilayer graphene

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Abstract: Recent experiments on magic-angle twisted bilayer graphene (MATBLG) have revealed the formation of flatbands, suggesting that correlation effects are likely to dominate in this system. Yet, a global transport measurement showing distinct signatures of strong correlations like local moments arising from the flatbands is missing. Utilizing thermopower as a sensitive global transport probe for measuring entropy, we unveil the presence of emergent local moments through their impact on entropy. Remarkably, in addition to sign changes at the Dirac point ($\nu = 0$) and full band filling ($\nu = \pm 4$), the thermopower of MATBLG demonstrates additional sign changes at the location, $\nu_{cross} \sim \pm 1$, which do not vary with temperature from 5K to ~ 60K. This is in contrast to sensitive temperature dependent crossing points seen in our study on twisted bilayer graphene devices with weaker correlations. Further, we have investigated the effect of magnetic field (B) on the thermopower, both B∥ and B⊥. Our results show a 30% and 50% reduction, respectively, that is consistent with suppression seen in the layered oxide due to the partial polarization of the spin entropy. The observed robust crossing points, together with suppression in a magnetic field, cannot be explained solely from the contributions of band fermions; instead, our data is consistent with the dominant contribution arising from the entropy of the emergent localized moments of a strongly correlated flatband.

Nontrivial transport in driven by charge-density-wave in 1T-TaS_2

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The interplay between charge density wave (CDW) formation and electron correlations can lead to the emergence of novel topological phases in materials. In this talk I will focus on a well-known CDW systems,1T-TaS_2. In quasi-2D 1T-TaS_2, below approximately 150 K, the system transitions from a nearly commensurate (NC) to a commensurate (C) CDW phase. Here, we show that the NC-CDW to C-CDW phase transition is marked by the emergence of a finite planar Hall and nonlinear Hall effect, alongside sign changes in the ordinary Hall and thermoelectric signals, indicating the reconstruction of the Fermi surface in the C-CDW phase. Our theoretical calculations suggest that the C-CDW phase, stabilized by specific layer stacking, breaks both mirror and inversion symmetries. This leads to finite Berry curvature and a substantial Berry curvature dipole, giving rise to the observed planar Hall and nonlinear Hall effect. Our study highlights the nontrivial topological properties of 1T-TaS_2 and opens new possibilities for developing innovative topological sensors. Finally, I will show new experimental data at lower temperatures (below 30 K). We observe the emergence of topological Hall effect below ~ 10 K, followed by a sign change in the planar Hall signal ~ 15 K, suggesting another phase transition driven by unusual spin textures. Thus, we provide emergence of different quantum phases driven by electron correlation and layer stacking in the CDW phase of 1T-TaS_2.

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Utilizing low energy electron beam irradiation for ultrasharp single photon emitter generation in monolayer transition metal dichalcogenides

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Single photon emitters (SPEs) hosted by two dimensional (2D) materials are building blocks of modern quantum technologies including quantum computing and quantum communication. In this aspect, defect and strain engineering of 2D transition metal dichalcogenides (TMDs) can create deterministically placed bound exciton manifolds ideal for quantum applications [1].

Atomically thin MoS_2 is the most extensively studied TMD. Despite wide range of defect and strain engineering techniques utilized elsewhere, helium ion beam irradiation is the only successful method employed for single photon generation in MoS_2 [2]. An alternative is the use of electron beam irradiation, which has lower momentum than the ion beam, and is expected to minimize surrounding lattice damage and improve SPE performance. In our earlier work, we demonstrated that ultralow energy electron beam irradiation can be used to create defects in monolayer MoS_2 [3]. Now, we demonstrate formation of ultrasharp defect bound exciton manifolds in hBN-encapsulated MoS_2 by low energy electron irradiation [4]. The ultrasharp (< 1 meV) defect bound excitons show very low spectral jittering (< 200 μeV), ideal for quantum technologies. Magneto-optics experiments suggest that the sharp peaks originate from sulfur vacancies and their complexes. Further, the defect emission is circularly polarized at finite magnetic fields which is indicative of the spin nature of defects. Finally, deterministic defect creation with high spatial resolution (~ 50 nm) was demonstrated by localized electron irradiation. In summary, we utilized ultra-low energy electron beam for the first time for localized SPE generation in monolayer MoS_2. These ultrasharp, stable SPEs have potential applications in photonics and quantum technologies. This work will also motivate studies on the defect creation mechanisms at ultralow energy electron irradiation.

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Spin caloritronics and magneto-thermoelectric effect in two-dimensional magnetic materials

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Category: Oral

Keywords: Thermoelectric, Anomalous Nernst effect, Spin Seebeck effect, Spin-phonon coupling.

Spin caloritronics and magneto-thermoelectric effect in two-dimensional materials can convert waste heat into beneficial electrical power in devices. In our recent work, density functional theory (DFT), combined with the semi-classical Boltzmann transport equation, is used to investigate conventional thermoelectric (TE) effects, the Spin-Seebeck Effect (SSE), and the Anomalous Nernst Effect (ANE). Our research reveals a high Spin Seebeck coefficient near the Fermi level at room temperature, underscoring the strong suitability of these materials for spin caloritronics applications. We also focus on understanding the role of spin-phonon coupling, which critically influences the thermoelectric performance of these monolayers. We will also discuss the figure of merit of conventional TE, Spin-Seebeck Effect, and Anomalous Nernst Effect (ANE) for the 2D materials and the possibility of further improving these figures of merit.

Electron and phonon transport properties in two-dimensional magnetic materials

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A basic understanding of the transport properties of phonons and electrons in two-dimensional materials is vital for designing new devices. In this talk, I will focus on the calculation of thermal and electron transport in two-dimensional magnetic materials using the Density functional theory and the Boltzmann transport equation. I will also discuss the different scattering mechanisms contributing to the transport properties of these materials.

Engineering Excitons in 2D Lateral Heterostructures and Devices

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Atomically thin semiconductors such as transition metal dichalcogenides (TMDs) have opened a new field with exotic physical properties and exciting potential applications.[1-4] There are enormous possibilities in combining diverse 2D materials for the unique design of efficient optoelectronic and quantum devices.[1] Among these, lateral heterostructures, which can only be fabricated through direct growth, present unique opportunities for engineering the formation, confinement, and transport of electrons, holes, exciton, phonon, and polariton.[4-8] We have developed a novel approach for directly fabricating seamless TMD lateral heterostructures and superlattices with controlled 1D interfaces, alloying, and spatial modulation using chemical vapor deposition.[4-6] Electrical transport measurements revealed diode behaviour across the 2D lateral junctions, promising for electroluminescence at room temperature. Temperature-dependent photoluminescence from neutral exciton, trion, and quantum emitters provides a better understanding of the optical properties of these as-grown 2D lateral heterostructures.[8] We demonstrate unique electro-optical properties using an n-p-n lateral heterostructure, including tunable photoconductance achieved through controlled exciton and trion generation via resonant excitation. Our findings provide a significant step forward in understanding and harnessing excitonic properties of 2D lateral heterostructures, paving the way for future innovations in 2D quantum materials and multimodal optoelectronic devices.

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Experimental Extraction of Phonon Scattering Lifetimes in vdW Materials Using Transient Grating

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As electronic devices continue to miniaturize, managing high heat flux becomes increasingly challenging. The latest advancements in enhancing heat dissipation are centered on utilizing ultrahigh thermal conductivity materials like boron arsenide and boron nitride, which provide passive and energy-efficient solutions for the thermal management of these electronic devices. Here we use a **first-principles theory-guided experimental approach** to investigate the ability of low-dimensional van der Waals (vdW) materials like graphite and layered MoS_2 in effectively dissipating heat.

In these semiconducting materials, phonons, which are the quanta of lattice vibrations, are the dominant heat carriers and the resistance to heat flow is caused by the scattering of phonons. Using an ultrafast non-contact optical pump-probe technique called the transient grating (TG) [1,2], along with guidance from the first-principles solution of the governing equation for phonon transport - the Peierls-Boltzmann equation [3], we show that higher-order scattering among four-phonons dramatically reduces the thermal conductivity of the vdW materials. By **harnessing the capability of the TG technique in extracting mode-specific phonon properties** such as phonon scattering lifetimes [2], we identify those individual phonon modes that are the most strongly affected by four-phonon scattering, thus opening up pathways for phonon transport engineering in these materials.

In the TG experiment, two short pulsed pump lasers interfere onto the sample, forming a spatially sinusoidal intensity profile, which is absorbed by the sample as a spatially sinusoidal temperature profile with a well-defined grating period Λ. We probe the decay of this instantaneously set up temperature profile using a probe laser beam. These temporal thermal decay measurements of the sinusoidal temperature profile at different grating periods, combined with the results from the first-principles calculations, give us information about the mode-specific phonon lifetimes, as demonstrated in the previous works of one of the co-authors [2].

We use the TG to probe the phonon lifetimes for van der Waals materials like graphite and layered MoS_2. Our experimental measurements highlight the **significant contribution of four-phonon scattering** to thermal resistance in these materials around and beyond room temperature, predominantly from low frequency acoustic phonons. By comparing our experimental measurements of phonon lifetimes with the first-principles predictions, we conclude that the momentum-conserving **Normal scattering processes among phonons dominate the total phonon scattering rates** at low phonon frequencies in many of the studied vdW materials, particularly around and below room temperature. Interestingly, we find that four-phonon Normal scattering rates are much stronger than the three-phonon Umklapp (momentum-dissipating) scattering rates, which is quite unusual compared to several other materials studied earlier [4]. The comparison of our experimental measurements with first-principles predictions also reveals **strong anharmonic renormalization of phonon frequencies** in several of the vdW materials, even at room temperature, thus significantly affecting their thermal conductivities. Our experimental findings, with insights from predictive first-principles calculations, shed light on the fundamental nature of phonon-phonon interactions in layered and low-dimensional materials.

This work is supported by the Prime Minister's Research Fellowship (02-01036) and the Science and Engineering Research Board's Core Research Grant No. CRG/2020/006166 and the Mathematical Research Impact Centric Support Grant No. MTR/2022/001043.

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Digital Twin Enabled Understanding and Modulation of Nucleation Density for Optimized 2D Material Synthesis

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Controllable synthesis of superior quality, single crystalline 2D materials is crucial for semiconductor and optoelectronic applications[1]. Chemical Vapor Deposition (CVD) is the leading technique for scalable synthesis of 2D materials[2], including semiconducting Transition Metal Dichalcogenides (TMDs). A key requirement for large-scale 2D-TMD growth is the control of nucleation density[2], but synthesis approaches for achieving this are rather limited. Further, CVD studies rarely rely on coupled mass, fluid, and heat transport profiles to infer the effect of process parameters on obtained growth, or to model process modifications for a desired outcome.

We have created a hyper-realistic multiphysics computational fluid dynamics (CFD) model, acting as a digital-twin of our CVD system[3]. We experimentally reveal the remarkable influence of a confined-space substrate holder on carrier gas velocity and 2D-TMD nucleation, leading to Molybdenum Disulfide (MoS_2) monolayers. Interestingly, significant modifications in the carrier gas flow near the substrate alter the precursor delivery. Thus, precursor flux, which is a function of the gas velocity, precursor concentration, and concentration gradient, emerges as the critical parameter controlling nucleation. The non-trivial effect of space confinement on suppressing nucleation is experimentally verified by scanning electron microscopy and supported by analytical calculations. The digital twin also makes an important prediction regarding a large time-lag between the set temperature and reactor growth temperature. This time lag is nearly impossible to observe experimentally and has immense implications on synthesis. Our work offers novel ways to control 2D material growth governed by precursor flux, revealed by a combined quantitative temperature and transport model. The digital-twin is independent of specific reactive species involved, and may be applied generally to controlled, large scale synthesis of 2D materials via CVD.

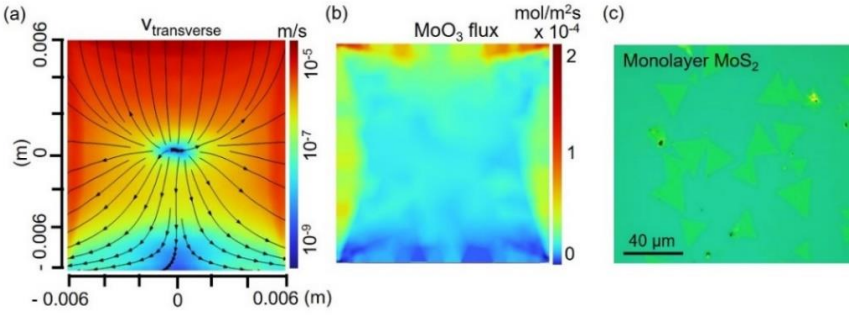

Figure 1. (a) Transverse component of the carrier gas velocity at the space confined substrate. Lines on the substrate denote gas flow streamlines. (b) Transition metal precursor flux at the substrate for a space confined substrate, plotted for 5 minutes after growth starts. Note the low flux at bottom of the substrate (c) Optical microscopy images of CVD-grown monolayer MoS_2 on similarly confined SiO_2/Si substrate.

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Topological entanglement entropy from exact diagonalization

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We have developed a new method of exact diagonalization ideal for 2D lattice systems using a heirarchy of wavefunctions. The heirarchy ranges from single-site to a cluster of rows. In short, starting from single-site Fock states, we construct the basis set in terms of row states and multirow states. This simplifies the application of constraints and calculation of the Hamiltonian matrix. The wavefunction obtained from the method is suitable for systematic partitioning required to obtain reduced density matrices and calculate different measures of entanglement. Using the method, we identify the fractional quantum Hall states of bosons in optical lattices and calculate the topological entanglement entropy.

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Convolutional restricted Boltzmann machine correlated variational wave function for the Hubbard model on a square lattice

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Abstract

The neural-network quantum states (NQS) wave functions have recently been shown to be highly accurate in representing the ground states of several quantum many-body systems. These wave functions constructed based on artificial neural networks have a large number of variational degrees of freedom and are highly unbiased. The NQS wave functions offer the possibility of removing the main drawback of biased results in the otherwise powerful variational method to study many-body physics. Though there have been several studies of NQS wave functions for bosonic systems, their applications to fermionic systems have been few. The main reason has been the failure of NQS wave functions to capture the complicated sign structure of fermionic wave functions. In this talk, I will present our recent work (Phys Rev B 110, 125125 (2024)) on a novel convolutional restricted Boltzmann machine (CRBM) correlated variational wave function for the two-dimensional (2D) fermionic Hubbard model. The wave function is shown to be highly accurate. It outperforms some of the best known Jastrow-type variational wave functions in terms of energy. Moreover, the number of variational parameters in the wave function does not grow automatically with the system size and is computationally much more efficient compared to other neural network wave functions. I will present the detailed results for the half-filled 2D Hubbard model obtained by using this wave function.
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Topological phase transition through electron-phonon interaction in an α-T_3 quantum spin Hall insulator

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We study the phenomenon of topological phase transitions induced by electron-phonon (e-ph) coupling in an α-T_3 Kane-Mele-Holstein model that presents smooth tunability between graphene ($\alpha = 0$) and a dice lattice ($\alpha = 1$). The e-ph coupling has been incorporated via the Lang-Firsov transformation, which adequately captures the polaron physics in the high frequency (anti-adiabatic) regime and yields an effective Hamiltonian of the system through zero phonon averaging at $T = 0$. While investigating the phase transition driven by polaron and its interplay with the parameter α, we identify two regions based on the values of α, namely, the low to intermediate range ($0 < \alpha \leq 0.5$) and larger values of α ($0.6 \leq \alpha < 1$) where the topological transitions show distinct behaviour. There exists a single critical e-ph coupling strength for the former, below which the system behaves as a topological insulator characterized by helical edge modes and evolution of the Wannier charge centres ($\mathbb{Z}_2$ invariant), with all of them vanishing above this value, and the system undergoes a spectral gap closing transition. Further, the critical coupling strength depends upon α. In addition to that, we find that the system hosts a semi-metallic point (gapless bulk) for $\alpha = 0.52$ in the absence of e-ph coupling, which closely resemblances the well-known unique transition occurring at $\alpha = 1/2$ (or at $1/\sqrt{2}$). For the latter case ($0.6 \leq \alpha < 1$), the scenario is more interesting where there are two critical values of the e-ph coupling at which a trivial-topological-trivial phase transition occurs accompanied by the (dis)appearance of helical edge modes and $\mathbb{Z}_2$ invariant. We also observe the evidence of higher (second) order topological insulator (HOTI) phases in our system induced by an in-plane magnetic field, which are characterized by the existence of corner modes. Interestingly, these corner modes are wiped out beyond a particular strength of e-ph coupling (albeit different for different α), referring to a HOTI-trivial phase transition mediated through the e-ph coupling. Our study thus underscores the importance of interaction effects on the topological phase transitions.

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Generation of Macroscopic Entanglement via Quantum Annealing

Anirban Das

Abstract: We propose a general protocol to create macroscopically entangled states by reaching the lowest energy degenerate eigenspace of some target Hamiltonian, starting from the ground state of some simple Hamiltonian, via quantum annealing. Starting from a symmetric phase and ramping towards symmetry broken phase, the time complexity is dominated by the smallest energy gap in the path of evolution. If the adiabaticity can be maintained throughout the dynamics, and no symmetry breaking field (which breaks the symmetry explicitly) is allowed at any point, we reach in a linear superposition of macroscopically distant states present in degenerate manifold, and as an effect of that useful macroscopic entanglement is generated. However Energy gap between these nearly degenerate states can be exponentially small in system size, and the cost of the process can be exponentially large in system size. We show that one can preserve useful entanglement by sacrificing the intent to reach the actual ground state, but necessarily reach the nearly degenerate ground state sector, and cost becomes polynomial in system size. As an application to this protocol we prepare various states like GHZ state, W state, linear cluster states by designing various target Hamiltonian and characterize the amount of entanglement by the speed of the unitary ramp evolution.

Ultrafast Magnetization Dynamics in 2D Material/Ferromagnet Heterostructures

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The 2D material/ferromagnet interface promises a plethora of new science and technology. They will form important building blocks for new-generation spintronics due to their unique spin transport, spin-orbit coupling and interface hybridization, providing new opportunities for the spin-based device fabrication [1]. For ultra-high speed spintronics applications, it is essential to have a deep insight about the magnetization dynamics occuring over nanosecond to femtosecond timescale. The optimization of these devices demands understanding and possible control of ultrafast demagnetization, Gilbert damping as well as spin-wave propagation.

We discuss here the ultrafast spin dynamics occurring over femtosecond to nanosecond timescale measured by an all-optical time-resolved magneto-optical Kerr effect technique [2] in single layer graphene (SLG)/CoFeB thin film heterostructures with varying CoFeB thickness and compared it with reference CoFeB thin films without SLG underlayer. The modulation of Gilbert damping with CoFeB layer thickness is extensively modelled to extract the spin-mixing conductance for SLG/CoFeB interface and isolate the contribution of two-magnon scattering from spin pumping. In SLG/CoFeB, we establish an inverse relationship between the ultrafast demagnetization time and the Gilbert damping parameter dominated by the interfacial spin accumulation and pure spin current transport [3].

The interfacial Dzyaloshinskii Moriya interaction (iDMI) is crucial for stabilizing chiral spin textures, which are important for future spintronic devices. Here, we will present direct evidence of iDMI in graphene, MoS_2, WS_2/ferromagnet heterostructures from the asymmetry in spin-wave dispersion using Brillouin light scattering (BLS) technique. Linear scaling of iDMI with the inverse of ferromagnetic layer thicknesses affirms purely interfacial origin of iDMI. We study the roles of defect induced extrinsic spin-orbit coupling and Rashba spin-orbit coupling, as well as atomic layer thickness in determining the iDMI by extensive experiment and analyses [4-7].

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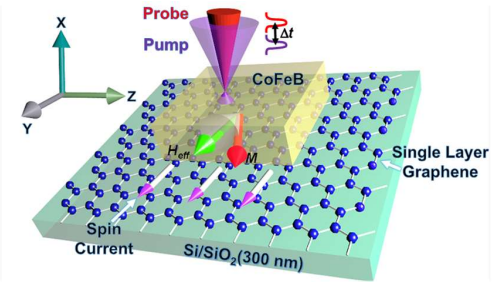

Fig. 1. Schematic of spin current driven ultrafast spin dynamics in SLG/CoFeB heterostructure.

Computational Modeling of Materials for Energy Storage and Generation

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I shall discuss modeling of a few materials for their applications in energy storage and generation purposes. Basically, I shall speak on four topics, namely, materials for (a) hydrogen generation by electrochemical splitting of water, (b) oxygen evolution and reduction reactions, (c) generating electricity from heat through Seebeck effect and (d) design of the cathode and electrolyte for a better Li ion rechargeable battery. For electrochemical hydrogen generation from water, we have modelled the SiPF-tetrazine covalent organic framework (COF) which exhibits superior HER catalytic activity with ΔG_{H^*} values being close to zero [1]. I shall discuss the bifunctional electrocatalytic activity of transition metal (Co/Rh/Ir) and N co-doped graphene (G) system with varying N concentrations using first principles calculations. The TM-N_4@G systems are found to be highly efficient bifunctional electrocatalysts and we find ΔG_{OH}* to be a good descriptor in designing superior bifunctional electrocatalysts [2]. I shall also discuss on modelling p-type SnO- PbO superlattice and n-type S and Te doped Ag_2Se systems for finding their thermoelectric efficiency at 700K and at room temperature, respectively [3]. Finally, I shall discuss our efforts in designing a spinel-based material which can be used as an efficient high voltage cathode for Li ion battery [4].

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Free Sliding Charge Density Wave: A Dynamical Critical Phenomenon

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Critical slowing-down in highly non-equilibrium settings, where the timescale of traversing the phase boundary becomes comparable to the timescale of dynamical fluctuations is less understood compared to equilibrium critical transitions. Pinning has long been discussed as profoundly affecting the dynamics of an incommensurate charge density wave (CDW), which would otherwise slide through the lattice without resistance. $(TaSe_4)_2I$ is a well-studied paradigmatic quasi-one-dimensional compound long-known to have a charge-density wave (CDW) transition around 263 K wherein we studied the critical fluctuations in its pinned state [1]. We present the slow dynamics of CDWs investigated through measurements of non-equilibrium electron transport and infer threshold fields of the collective CDW motion from non-linear conductance measurements.

We experimentally establish that this electric field-driven de-pinning transition, unlike in other CDW compounds such as TaS_2, is non-hysteretic with no change in phase. The onset of the sliding motion of CDWs were also identified from the large growth in noise variance. Furthermore, dynamical slowing down is captured in the characteristic relaxation time of the conductance auto-correlation function. The growing correlation lengths were indirectly inferred from the growth of the non-Gaussian character of the fluctuations. Non-equilibrium dynamics of CDWs reveal the complexity of systems far from equilibrium conditions, with profound insights into their underlying mechanisms and behaviors [2].

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Stability of Emergent Conservation Laws in Periodically Driven Quantum Systems

Sagnik Chaudhuri

According to Floquet ETH, a generic non-integrable periodically driven (Floquet) quantum system is predicted to heat up in an unbounded fashion, with no obvious conservation law to contain this heating. It has been shown in previous studies that if such a system is subjected to strong periodic driving, then such unbounded heating can be avoided due to the emergence of a set of approximate global conservation laws that are not present in the undriven system. These conservation laws emerge only when the strength of the driving field crosses a particular threshold. This phenomenon is referred to as Dynamical Freezing. In this talk, we present evidence to show that although these emergent conservation laws are approximate, they are perpetually stable. We show that these approximate conservation laws are stable up to exponential timescales. This stability is shown starting from all x-basis states and also from thermal mixed states. It is seen that even at exponentially long times, the overlap of the time-evolved state with states outside its own conservation sector is negligibly small. As a consequence of this conservation up to exponentially long times, for some particular initial states (e.g., $|\uparrow\downarrow\uparrow\downarrow \ ...\rangle$ and $|\uparrow\uparrow\downarrow\downarrow \ ...\rangle$), we see the phenomenon of Super-Oscillations - periodic oscillations (with an exponentially long time period where the period scales exponentially with system size) of entanglement entropy, fidelity and overlaps with other basis states in the same conservation sector. This stability of the conservation laws up to exponentially long times indicates that what we are observing is not a prethermal phenomenon. Rather, the approximate conservation laws are perpetually stable.

Edge Theories of Fractonic Systems

Vijay B. Shenoy, IISc Bengaluru

I will begin with a brief review of fractonic phases. We adopt a field theoretical framework with second-rank gauge fields with a Chern-Simons action parametrized by an integer level k, where point charges are immobile, dipoles move only along lines perpendicular to their moment, and quadrupoles (and higher multipoles) are freely mobile. The theory realizes a dipolar Hall state whose transport coefficient is determined by the level k. We demonstrate that a non-trivial statistical phase (determined by the level k) between two bulk excitations is obtained only in two cases: a point quadrupole braids around an immobile point charge or two non-orthogonal dipoles braid around. By studying the gauge anomaly of the theory in a system with an edge, I will demonstrate that *two* distinct types of edge excitations are necessary to cancel the anomaly. After deriving a novel type of current algebra satisfied by these excitations, I will show that one of them is a fractonic mode with immobile charges and longitudinal dipoles, and the second one is a non-fractonic mode with transverse dipoles. Further, exploring the stability of the edge modes by studying the allowed local tunneling between two such edges. I will show t that edge reconstruction is generically possible. In addition to providing clarifying theoretical insights connecting the transport properties, quantum statistics of bulk excitations, and the properties of edge excitations, this work offers a route to characterize the properties of fractonic systems by the study of their edge excitations in future experiments

Spin-excitations of low-dimensional cuprates beyond linear response

Resonant inelastic X-ray spectroscopy (RIXS) has emerged as an essential tool for measuring spin and charge correlators of strongly correlated materials. RIXS is a photon in-photon out process. In RIXS, an X-ray photon whose energy is resonant to the energy difference between a core-level and a conduction band excites a core electron to a specific conduction band, leaving behind a core hole. The final state involves the inelastic process of absorption of energy, momentum, and angular momentum by the material and emission of lower energy photons. The scattering cross-section, up to atomic-form-factors, contains information on the charge and spin dynamics of the material beyond linear response, second order in the Fermi-golden rule.
I will briefly discuss a perturbation expansion of the RIXS experimental cross-section in the inverse lifetime of the core hole. I will use linear spin wave theory and exact diagonalization to show how three-magnon-excitations can explain experimental observations for undoped cuprate compound La_2CuO_4 [1]. I will also present predictions for the RIXS cross-section of fractionalized spin-excitations for one-dimensional cuprate spin-trimer chain $Na_2Cu_3Ge_4O_{12}$ using Lanczos and density matrix renormalization group [2].

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A maximum concurrence criteria to investigate absolutely maximally entangled states

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Abstract

We have proposed a simple method to find the maximal entanglement of pure states by providing the criteria of maximal concurrence, which is the identification of entanglement. Based on this approach, we have discovered many Absolutely Maximally Entangled pure states for some qubits systems (3,5... etc.). Absolutely Maximally Entangled (AME) states are maximally entangled in all possible bipartition. We have shown that any state having an odd number of coefficients of its subsystems will not satisfy the criteria of absolutely maximal entanglement. Furthermore, We obtain the maximal Genuine Multipartite Entangled states using our maximal concurrence criteria.

Entanglement transitions and role of emergent symmetry in non-Hermitian integrable Floquet systems

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I. ABSTRACT

In this talk I will try to describe how the interplay between the system environment coupling and external driving frequency shapes the dynamical properties and steady state behavior in a periodically driven transverse field Ising chain subject to measurement [1]. I will describe fate of the steady state entanglement scaling properties as a result of measurement induced phase transition [2]. I will briefly explain how such steady state entanglement scaling can be exactly computed using asymptotic analysis of the determinant of associated correlation matrix which turned out to be of block Toeplitz form. I will try to point out the differences from the Hermitian systems in understanding the entanglement scaling behaviour in regimes where the asymptotic analysis can be performed using Fisher-Hartwig conjecture. I will end the talk with some open questions in this direction.

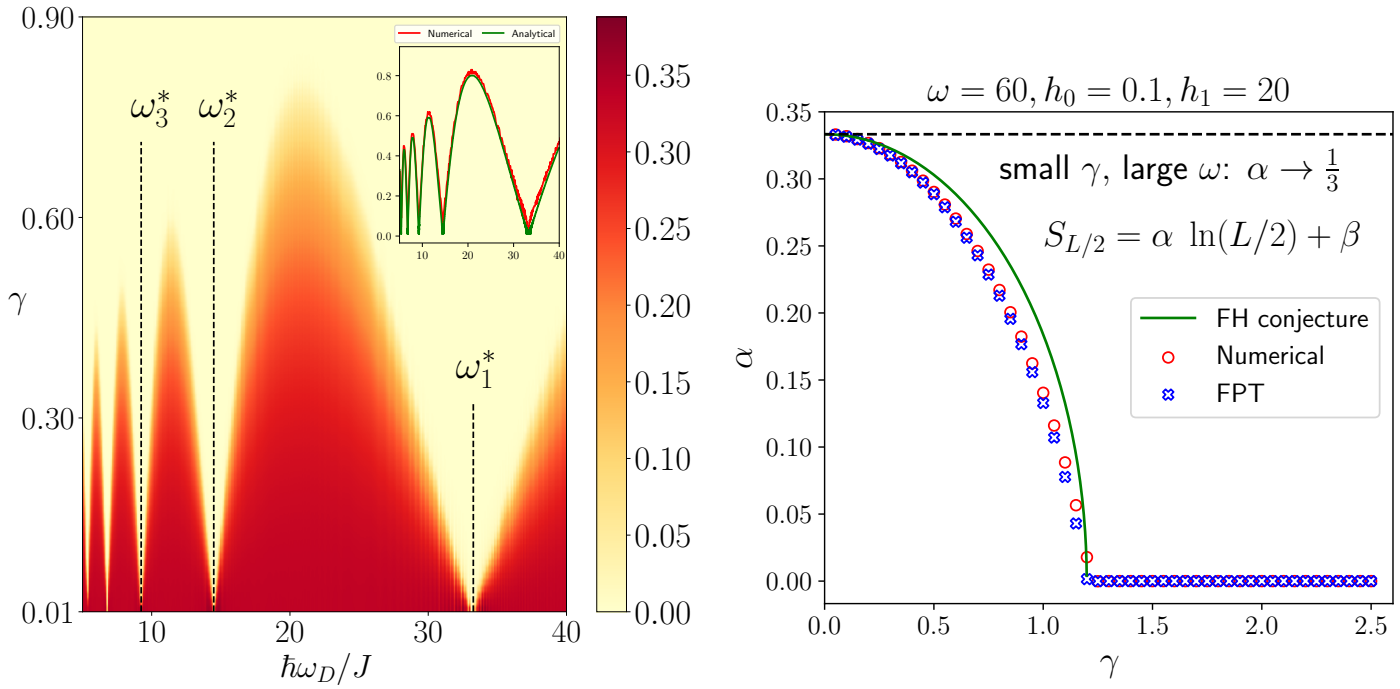

FIG. 1. Left panel: steady state von-Neumann entanglement entropy scaling property shows transition from logarithmic (Red) to area law (Yellow) in the drive frequency (ω_D) and rate of dissipation (γ) plane. Right panel : variation of slope of logarithmic scaling of von-Neumann entanglement entropy as a function of dissipation rate for a fixed driving frequency signifying a transition to area law a critical value (γ_c) of the measurement rate (γ).

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Saturday, 21st December, 2024: [Day1]

List of Posters

Magnetic hard axis ordering in quasi one-dimensional antiferromagnet Ce_3ZrBi_5

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Hypervalent chemical bonds have been identified as one key feature for discovering new topological materials.[1] While an extensive amount of work has been performed on the hypervalent 2D square-net materials, their lower dimensional, electron-rich structural motifs still remain relatively unexplored.[2] Herein, we investigate the electronic structure, transport and magnetic properties of Ce_3ZrBi_5 (CZB) a quasi-one-dimensional (1D) compound in the Ln_3MPn_5 (Ln = lanthanide; M = metal; Pn = pnictide) family that crystallizes in the hexagonal non-symmorphic $P6_3/mcm$ space group. The temperature dependent susceptibility data for CZB single crystals show the presence of two antiferromagnetic (AFM) transitions below T_N = 4.9 K; highlighting a complex and highly anisotropic magnetic landscape. The magnetization shows a peculiar nature where the moments align along the crystal electric field (CEF) hard axis; contrary to the easy axis magnetization in most AFMs. Such observations, although are common for Kondo ferromagnets (FM), are rarely observed in AFMs.[3] The CEF hard axis magnetic moment switching can be attributed to multiple observables: strong competing FM forces in an AFM lattice, presence of competing Kondo and CEF anisotropy energy scales and strong spin-orbit coupling (SOC).[3] The M-H curve shows the presence of first-order metamagnetic transitions demonstrating the presence of strong field induce FM fluctuations in CZB. The temperature and magnetic field variation of the specific heat data shows heavy fermion behavior along with a signature of the Kondo effect.[4] Density functional theory (DFT) calculations reveal the presence of a non-trivial electronic structure, resulting from the half-filled Bi atoms in the 1D chains and $ZrBi_6$ octahedra, that changes significantly in the presence of SOC.[2] A comparative study with a conventional AFM material Ce_3ZrSb_5, in which Bi is replaced by Sb, is performed to investigate the effect of SOC on the electronic and magnetic ground state. Clearly, the quasi-1D structural network in Ce_3ZrBi_5 provides an interesting platform to investigate a host of emergent phenomena giving rise to complex magnetism and electronic structure in a correlated electron system.

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Title : Site-selective polar compensation of Mott electrons in a double perovskite heterointerface

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One of the boundary conditions of the classical electromagnetic theory demands continuous electric potential across any interface, which may not be naturally satisfied in atomically engineered heterostructure and may even lead to an unstable diverging potential profile termed as 'polar catastrophe'. Such instability in oxide heterointerface is avoided through some (electronic/chemical/structural) reconstructions, leading to many emergent phenomena [1-4]. However, most often the compensation mechanisms are viewed from a semiconductor-like band bending perspective when in reality transition metal oxides also host a crucial set of correlated energy scales. In this work [5] , we demonstrate the role of electron correlation in the polarity compensation mechanism by investigating the interface between a prototypical insulating double perovskite Nd_2NiMnO_6 and wide-bandgap insulator $SrTiO_3$, which offers a similar polarity scenario as the famous $LaAlO_3/SrTiO_3$ system [6,7] but with an exception - multiple transition metal (TM) sites with two sets of correlated energy scales. The interface is found to be insulating. By combining several experimental techniques with density functional theory, we establish a site-selective charge compensation process that occurs explicitly at the Mn site of the film, leaving the Ni sites inert. This surprising selectivity, which challenges the well-accepted semiconductor-like scenario for oxide heterostructure, can be attributed to TM cations' relative correlation energy scales. This study establishes the crucial role of Mott physics in polar compensation process and paves the way for designer doping strategies in complex oxides.

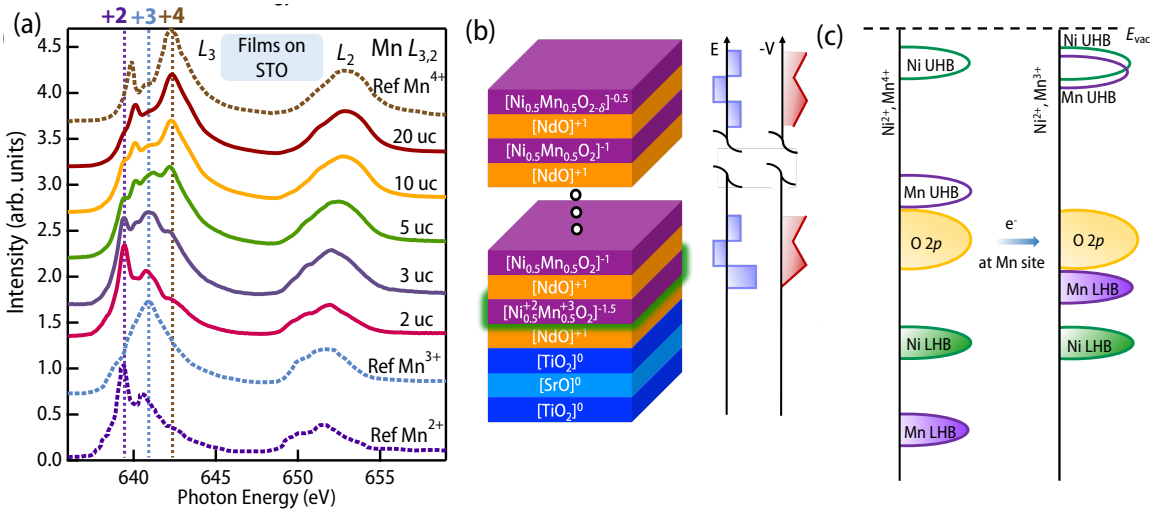

Figure 1: *(a) Mn $L_{3,2}$ X-ray absorption spectra for Nd_2NiMnO_6 films of various thicknesses on $SrTiO_3$ showing electron addition at Mn site . (b) Proposed charge compensation mechanism (c) Visualising site selectivity at Mn using Hubbard band picture.*

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Exotic ferromagnetism in Nd_2TSi_3 (T= Pd, Rh) unlike other members of these rare-earth families

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Compounds belonging to the family R_2TSi_3 (R = rare-earth and T = transition metals), crystallising in AlB_2 derived hexagonal structure, have been known to exhibit exotic magnetic and transport anomalies. Among these families, the rare-earth compounds containing Pd/Rh, are known to order antiferromagnetically. We present the electronic properties of compounds Nd_2PdSi_3 and Nd_2RhSi_3, ordering ferromagnetically around 15.5 K and 16.5 K respectively, with complexities at lower temperatures, making these compounds unique magnetic materials when compared with antiferromagnetism of other rare-earth members in these families. In addition, both these compounds show features attributable to cluster spin dynamics below 16 K, while, in the case of Nd_2RhSi_3 these glassy features are seen at temperatures slightly higher than the Curie temperature, indicating the gradual evolution of cluster magnetism in this compound as the temperature is lowered. Apparently, the 4*f* hybridization of Nd plays a major role in determining magnetism of these compounds, making them exotic.

Critical Scaling Analysis and Magnetic Phase diagram of Mn intercalated TaS_2

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Abstract

Topological chiral magnetic configurations are generally stable, spin protected, and insensitive to defects, making them ideal for developing highly stable, high-efficiency, and low-power spintronic device[1-3]. In this study, we have focused on the investigation of critical phenomenon of a chiral magnetic soliton host compound $MnTa_3S_6$[4], grown through the chemical vapor transport (CVT) method. The compound has magnetic (FM-PM) phase transition at the $T_C \sim 30$ K (See Fig.(a)). The detailed analysis of magnetization isotherms measured in vicinity of T_C with magnetic applied field $H \parallel ab$ plane yields the critical exponents $\beta = 0.377$, $\gamma = 1.345$, and $\delta = 4.677$ (See Fig.(d,e)). Those are very close to the theoretical prediction of three-dimensional Heisenberg model (See Fig.(c)). The Renormalization-group theory analysis suggests the exchange coupling $J(r)$ decays with distance r as $r^{-4.956}$ which is long range type. Based on the scaling equation and the critical exponents, the H-T phase diagram around the phase transition is constructed from where, we have inferred that $MnTa_3S_6$ possess both chiral helimagnetic phase (CHM) and chiral magnetic soliton lattice phase (CSL) (See Fig.(f)). Both these phases are sensitive to applied external field.

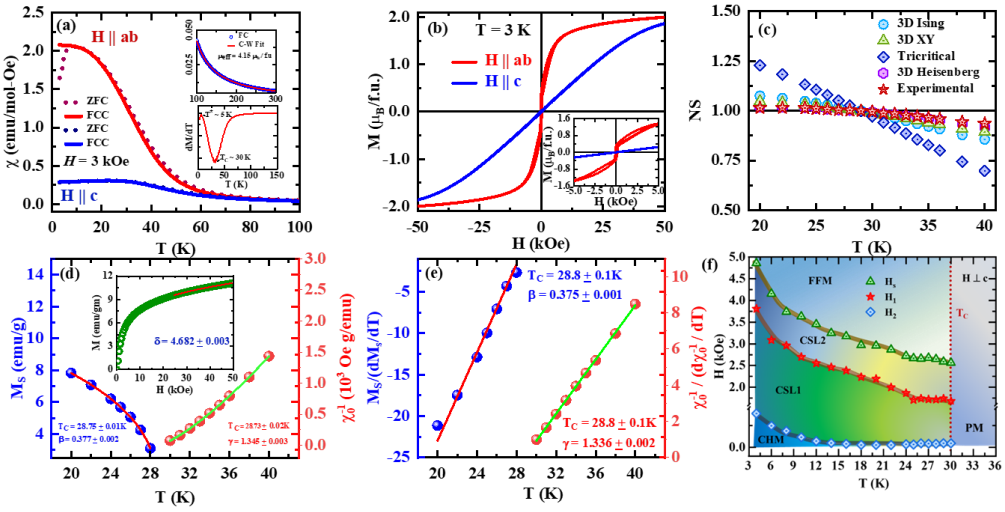

Fig (a) Temperature-dependent magnetization data at H=3kOe along $H||ab$ and $H||c$. Inset shows modified Curie-Weiss Fitting in paramagnetic region. The minima of dM/dT curve at $T \sim 30$K is FM to PM transition. At $T \sim 5$K, there is an additional transition. **(b)** Field dependent magnetization $M(H)$ curves along two different crystal orientations at $T = 3$K. **(c)** Temperature-dependent normalized slopes $(NS) = S(T)/S(T_C)$ for different theoretical models. **(d)** Temperature-dependent spontaneous magnetization M_S and initial inverse susceptibility χ^{-1}_0 with fitting. Inset: M-H curve collected at $T = 29$K and the line (red color) is the fitting. The critical exponent mentioned in graph is obtained from fitting. **(e)** $M_S/(dM_S/dT)^{-1}$ (left) and $\chi^{-1}_0 / (d\chi^{-1}_0/dT)^{-1}$ vs temperature. **(f)** The H-T phase diagram for $MnTa_3S_6$.

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Magnetic Microstate and Configurational Anisotropy Modulated Spin Wave Dynamics in Three-Dimensional Artificial Spin Ice

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Three-dimensional artificial spin ice (3D-ASI), a frustrated magnetic system where the spins (magnetic moments) cannot all simultaneously satisfy their interactions, has emerged as a key area of research due to its fascinating properties [1]. These systems consist of single-domain nanomagnets arranged in specific 3D configurations and coupled by exchange and dipolar interactions. They exhibit a wide variety of interesting phenomena, including emergent magnetic monopoles, vertex-based frustration, chiral dynamics, and phase transitions, among others [2]. 3D-ASI systems arranged in a diamond-bond lattice (DBL) geometry fabricated using two-photon lithography, have emerged as an important candidate due to their fascinating properties. These properties include the observation of coherent spin waves (SWs) [3], magnetic charge propagation [4], and interesting phase characteristics [5].

In this work, we have utilized the Brillouin Light Scattering (BLS) technique to explore the role of the magnetic microstate and configurational anisotropy in tuning the collective SW dynamics of a 3D-ASI array. This array, consisting of crescent-shaped nanowires arranged in a DBL geometry, has been fabricated using two-photon lithography. The observed BLS spectra show the presence of three localized SW modes in the array of 3D-ASI systems with spin ice vertices of type-2. In contrast, four localized SW modes are observed in the system where spin ice vertices of type-2 and type-3 are present in a 1:2 ratio, respectively. This is direct evidence that the magnetic microstate plays a dominant role in affecting the localized SW dynamics. Furthermore, the exploration of the field-dependent SW dynamics along the different sublattices of the DBL array shows a drastic variation in the number of SW modes and their characteristics. This confirms the dominant role of configurational anisotropy in tuning the collective excitation of the SW modes in these complex 3D-ASI systems.

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Prethermalization in the PXP Model under Continuous Quasiperiodic Driving

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Motivated by recent experiments realizing long-lived non-equilibrium states in aperiodically driven quantum many-body systems, we investigate the dynamics of a quasiperiodically driven Rydberg atom chain in the strong Rydberg blockage regime. In this regime, the system is kinetically constrained and the 'PXP' model describes its dynamics. Even without driving, the PXP model exhibits many-body scarring and resultant persistent oscillations for dynamics originating from the Néel-ordered initial state [1–3]. We demonstrate that a rich array of dynamical behaviors emerge when the system is subjected to a continuous drive. In the high-frequency regime, the system exhibits revivals and oscillations for the Néel ordered initial state both for periodic and quasi-periodic drives. We trace the origin of this non-ergodicity to an effective PXP Hamiltonian for both of these driving protocols in this regime. Furthermore, we demonstrate that the behavior of the fidelity and the entanglement entropy is non-monotonic at low frequencies in the high-amplitude regime. This leads to several re-entrant scarring transitions both for both the Néel-ordered and the fully polarized initial state. Our results demonstrate that continuous quasi-periodic drive protocols can provide a promising route to realize prethermal phases of matter in kinetically constrained systems.

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Correlation between Negative Dielectric Permittivity and Magnetism in spinel ferrite nano-structures

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Abstract:

Metamaterials with negative dielectric permittivity have become a research hotspot due to their potential effectiveness in a variety of electromagnetic applications, including filter and antenna design, innovative capacitance and inductor design, electromagnetic absorber, etc. This study opens up a world of possibilities for manipulating the morphology of magnesium ferrite, a naturally occurring compound, to induce metamaterial features like negative dielectric permittivity. In this study, we present the relationship between the structural, dielectric, and magnetic characteristics of the system in the same chemical composition but distinct morphologies, namely, nano solid spheres (NSSs) and nano hollow spheres (NHS). Remarkably, the Lorentz dielectric resonance at a metamagnetic transition causes only NHSs to exhibit negative dielectric permittivity. Subsequent studies reveal that the uncompensated charges store inside NHSs and discharge at specific frequencies and temperatures, resulting in the backscattering of dipoles, which in turn creates the resonance. NHSs have hollow cores and more interfaces than NSSs. Negative dielectric permittivity is not observed in NSSs with concrete morphology and higher anti-ferromagnetic interaction.

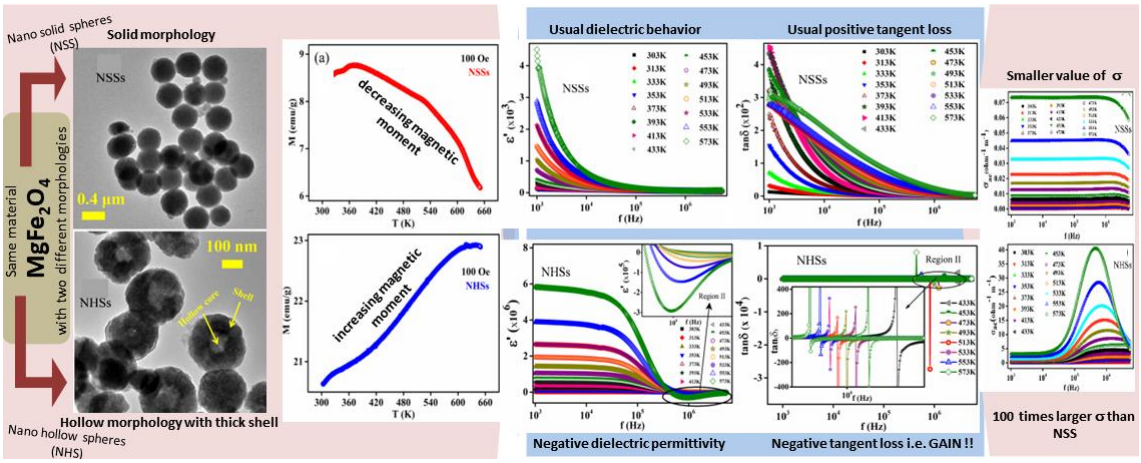

Figure: Correlation between negative dielectric permittivity and magnetism in $MgFe_2O_4$ nano-spheres.

These metamaterials, with their unique physical properties such as negative refractive index, reversed Doppler Effect, etc, can be classified into ordered and random metamaterials. In comparison to the artificially designed ordered metamaterials, random metamaterials have found wide interest due to low cost, ease of fabrication, high availability, and higher control over modification of the negative behaviour. Among the random metamaterials, composites show very high dielectric loss due to high concentration of free electrons, and high temperature instability due to the oxidation of the conductive fillers. In comparison to composites, single phase metamaterials have better temperature stability, favourable homogeneous composition, and feasible methods exist to control their electron concentration. In this backdrop, we propose $MgFe_2O_4$, synthesized in a particular morphology, as one of the very few single-phase random metamaterials. This work attempts to find a credible correlation between the unusual dielectric property and magnetism in the system.

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Low-frequency resistance noise in near magic-angle twisted bilayer graphene

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The low-frequency resistance fluctuations, or noise, in electrical resistance not only set a performance benchmark in devices, but also form a sensitive tool to probe non-trivial electronic phases and band structure in solids. Here we report the measurement of such noise in the electrical resistance in twisted bilayer graphene (tBLG), where the layers are misoriented close to the magic angle ($\theta \sim 1^{\circ}$). At high temperatures ($T \geq 60 - 70$ K), the power spectral density (PSD) of the fluctuations inside the low-energy moiré bands is predominantly $\propto 1/f$, where f is the frequency, being generally lowest close to the magic angle, and can be well-explained within the conventional McWhorter model of the '*1/f* noise' with trap-assisted density-mobility fluctuations [1]. At low T (≤ 10 K) the measured noise exhibits strong two-level random telegraphic signal (RTS), especially close to moiré gap, which exhibits a $\propto 1/f^2$ -like PSD that can be attributed to poorly-screened resonances of the Fermi energy to specific bands of defects in the encapsulating boron nitride (hBN) layers. Remarkably, the low- T noise within the moiré band exhibits series of minima at the integral as well as half-integral fillings, which align with the frequently-observed van Hove singularities in the density-of-states driven by strong Coulomb interaction [2,3,4]. Apart from providing a comprehensive account of the origin and the magnitude of noise in tBLG, our experiment also reveals noise to be significantly more sensitive to the underlying interaction effects in tBLG than the conventional time-averaged transport.

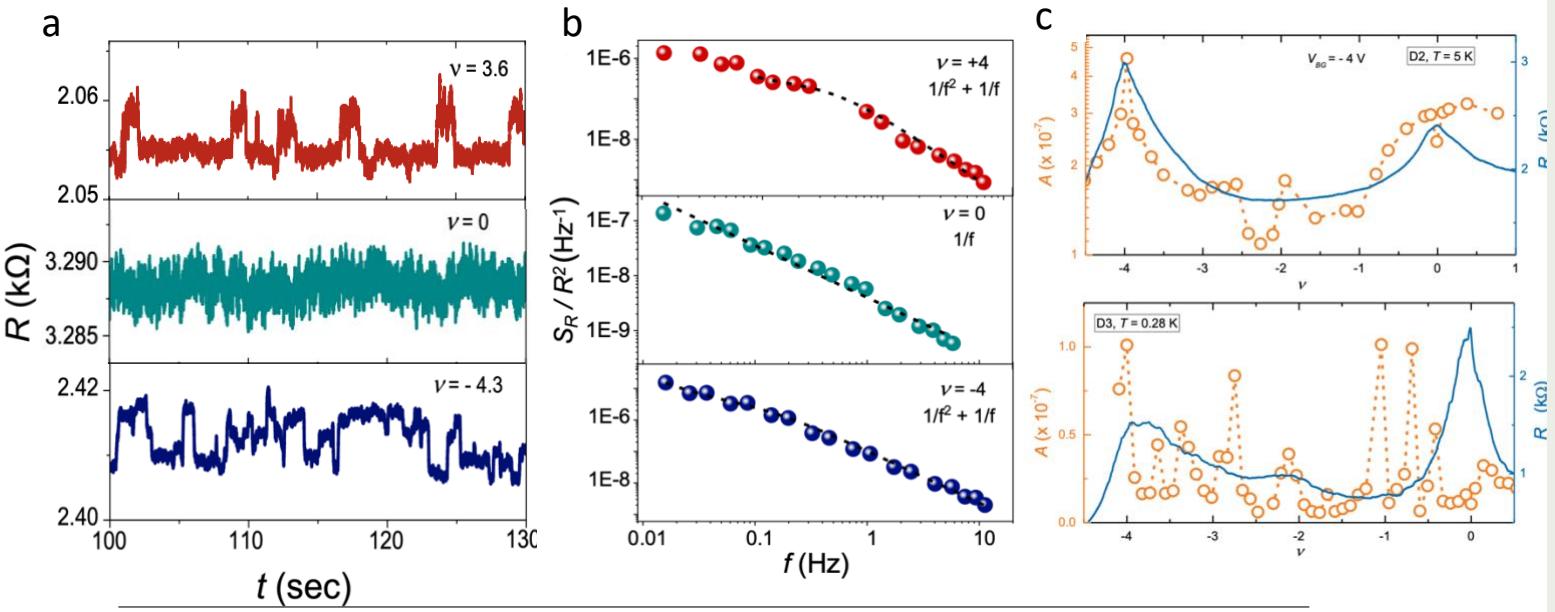

Fig. 1: (a) *R*- fluctuation data in near magic-angle tBLG sample. (b) *f*- dependence of PSD. and, (c) filling factor dependence of noise.

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Frustrated spin-1 triangular lattice antiferromagnet $Ca_3NiNb_2O_9$: A proximate spin liquid

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Abstract

The frustrated model has recently attracted much attention as a probable candidate for the highly entangled quantum spin-liquid (QSL) phase that can host non-Abelian quasiparticle excitations [1-2], and the exotic quasiparticle (QP) excitations known as spinons [3]. The spin-1 triangular lattice Heisenberg antiferromagnet $Ca_3NiNb_2O_9$ and its sister compounds are conjectured to promote the formation of many-body quantum entangled states such as a QSL, an exotic phase which features fractionalized QP excitations and emergent gauges. We probe the single crystal of $Ca_3NiNb_2O_9$ using an in-depth Raman spectroscopic technique [4]. Our measurements provide evidence for the fractionalized excitations, suggesting that the current system is in close proximity to the QSL phase. This is also in line with the proposed higher-order fractional magnetization plateau in this system, as these plateaus have an intricate relationship with the spin entanglement. We observed unconventional underlying scattering as a broad continuum with an intensity that shows fermionic statistics. We observed strong anomalies in the self-energy parameters of the phonons (i.e. frequencies and linewidth) at ~ 50 K (T_{SC} - short-range spin-spin correlation transition temperature) much higher than the long-range magnetic ordering temperature (T_N ~ 4 K), which suggest, these anomalies do not arise from the conventional spin-phonon coupling as the spins are deep inside the thermal paramagnetic regime with $\langle S_i \rangle = 0$. We attribute these anomalies in the phonons to the quantum spin and orbital fluctuations and possible coupling with the Majorana Fermions. We also observed changes in the phonons self-energy parameters in the vicinity of ~ 200 K (T^*). As the temperature reaches T_{SC}, there is a significant redistribution of spectral weight at the demarcating Raman shift $\omega_F \sim 203\ cm^{-1}$ also reflected in the anomalous phonon-mode intensity evolution and show fermionic statistics in their intensity evolution. Additionally, phonon modes show Fano asymmetry, also conjectured as a fingerprint of the spin-liquid phase.

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Band tuning in 2d nanoplatelets due to Geometrical Curvature

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Over the years, the study of bent and curved geometries in nanomaterials [1] has remained of great interest to researchers, as it provides a new platform for investigating fundamental physical properties such as mechanical deformation led generation of pseudo-electric and magnetic fields [2,3] or introducing strain via curvature-induced molecular adsorbates on a graphene sheet [4]. However, the effect of geometrical curvature on the energy levels of nanoscale materials remains an open question. In this project, using scanning tunnelling microscopy (STM) and spectroscopy (STS) measurements, we have demonstrated that in ultrathin CdSe nanoplatelets exhibit a significant variation in the location of conduction and valence band edges and their difference i.e. band gap as a function of curvature from the edge to the centre of the nanoplatelet. Our experimental findings, supported by theoretical calculations, reveal that the higher band gap at the edge, compared to the centre of the nanoplatelet is associated with the larger magnitude of curvature between the edge and the centre. These scientific findings open a new avenue for studying electron transport at the nanoscale influenced by curved geometries.

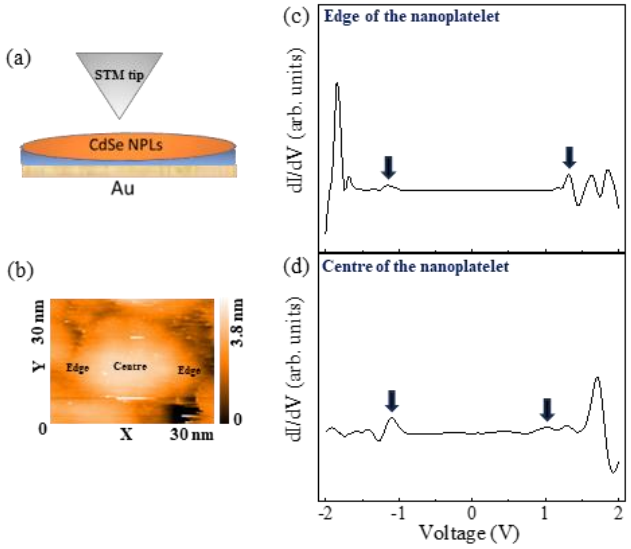

Figure 1 (a) Schematic representation of a scanning tunneling microscopy (STM) tip – CdSe nanoplatelet – Au substrate. (b) Constant current topography image of a CdSe nanoplatelet with the edge and center of the nanoplatelet is marked. Density of states (DOS) at the edge (c) and centre (d) of the nanoplatelet as obtained from scanning tunneling spectroscopy (STS) measurements. The location of peaks as indicated by arrows are the conduction and valence band edges and their difference is the band gap.

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Light Induced Resonant Nonlinear Spin Magnetization

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Spin magnetization is at the forefront of spintronics, which is actively studied to control field-free magnetization dynamics. Here, we formulate a comprehensive theory of light-induced nonlinear spin polarization in centrosymmetric materials. We reveal the quantum geometric origins of various nonlinear spin polarization components applicable to both the metallic and insulating systems. Guided by the symmetry analysis, we predict sizable nonlinear spin polarization in antiferromagnetic CuMnAs and ferromagnetic $MnBi_2Te_4$. Our findings show that the spin-orbit torque resulting from light induced nonlinear spin polarization can be strong enough to switch the magnetization in centrosymmetric ferromagnets and create light-induced THz oscillator in antiferromagnets. Our work motivates the use of photo-induced nonlinear spin polarization as a powerful tool to optically control the magnetization dynamics.

Entanglement signatures of a percolating quantum system

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Entanglement measures have emerged as one of the versatile probes to diagnose quantum phases and their transitions. Universal features in them expand their applicability to a range of systems, including those with quenched disorders. In this work [1], we show that when the underlying lattice has percolation disorder, free fermions at a finite density show interesting entanglement properties due to massively degenerate ground states. We define and calculate appropriate entanglement measures such as typical, annealed, and quenched entanglement entropy in both one and two dimensions, showing they can capture both geometrical aspects and electronic correlations of the percolated quantum system. In particular, while typical and annealed entanglement show volume law character directly dependent on the number of zero modes in the system, quenched entanglement is generally area law albeit showing characteristic signatures of the classical percolation transition. Our work presents an exotic interplay between the geometrical properties of a lattice and quantum entanglement in a many-body quantum system.

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Emergence of tunable exceptional points in altermagnet-ferromagnet junctions

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Abstract:

The existence of exceptional points (EPs) – where both eigenvalues and eigenvectors converge – is a key characteristic of non-Hermitian physics [1-2]. A newly-discovered class of magnets – termed as altermagnets (AMs) – are characterized by a net zero magnetization as well as spin-split bands [3-4]. In this study, we propose the emergence of non-Hermitian physics at AM-ferromagnet (FM) junctions. We discover that such a junction hosts tunable EPs. We demonstrate that the positions of these emergent EPs can be tuned using an external applied magnetic field and show that for a critical value of the applied magnetic field the EPs can annihilate [5]. Notably, the number and position of the EPs crucially depends on the type of AM and its orientation with respect to the FM. Our work puts forth a promising platform of exploration of non-Hermitian physics in an emerging class of magnetic materials.

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Robust Majorana bound state in pseudo-spin domain wall of 2-D topological insulator

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We investigate helical edge states (HES) emerging at the composite domain wall of spin and pseudo-spin degrees of freedom in a 2-D bulk governed by the Bernevig-Hughes-Zhang Hamiltonian which underwent quantum spin Hall to anomalous Hall transition. We numerically study the stability of Majorana bound state (MBS) formed due to proximity induced superconductivity in these helical edge states. We establish exceptional robustness of MBS against moderate chemical potential or magnetic disorder owing to the existence of the simultaneous orthogonality between the right and the left moving modes both in spin and pseudo-spin space. Hence our proposal could pave the way to realizing robust Majorana bound state on 2-D platforms.

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QMAT -2024

Exploring topological phase transitions via Josephson current in *p*-wave superconductors with magnetic-textured barriers

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Topological superconductors hosting Majorana fermions are proposed to be the building blocks for topological quantum computation. However, their experimental reliance heavily depends on spin-orbit coupling and external magnetic fields that can adversely affect superconductivity. To address these challenges, a novel Josephson junction is proposed that employs a magnetic-textured barrier composed of antiferromagnetic or ferromagnetic insulators with periodic domains. This approach eliminates the need for spin-orbit coupling and external Zeeman fields, offering a more viable platform for realizing topological superconductivity.

Our work extends this by incorporating *p*-wave superconductivity, which naturally exhibits non-trivial topological properties by anchoring Majorana edge modes in two dimensions. We investigate the Josephson current signature in two-dimensional *p*-wave superconductor when a textured magnetic tunnel barrier is implanted at the Josephson junction. We expect the topological phase to be influenced by the magnitude of barrier's magnetization and periodicity, with the superconducting phase potentially driving transitions between Majorana edge and end modes and eventually leading to the trivial phase. This transition may be detected as a significant change in the supercurrent across the junction, offering new insights into the behavior of *p*-wave superconductors in presence of magnetic tunnel barriers.

Anomalous Hall effect and thermal transport in the magnetic nodal line semimetals: Mn_3XC (X = Sn, Ga)

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Abstract

Mn-based antiperovskite Mn_3XC (X = Zn, Ga, Sn) materials have gained renewed interest recently due to the observation of topological electronic states [1,2]. Mn_3ZnC shows first order antiferromagnetic (AFM) to ferromagnetic (FM) transition at T_N ~ 233 K and second order FM to paramagnetic (PM) transition at T_c ~ 380 K [1]. Another antiperovskite, Mn_3SnC shows paramagnetic (PM) to concurrent antiferromagnetic (AFM)/ferromagnetic (FM) transition at T_c ~ 286 K [3]. Mn_3GaC shows a FM transition at T_C ~ 310 K and reduction in magnetization indicative of an AFM transition around T_N ~ 150 K. Here, we present magnetotransport and thermoelectric properties of Mn_3SnC and Mn_3GaC. The upturn in the low-temperature electrical resistivity follows Hamann expression with the Kondo temperature T_K = 16 K, whereas low-temperature resistivity of Mn_3SnC exhibits presence of electron-magnon scattering. Mn_3SnC shows anomalous Hall effect (AHE) below T_c ~ 286 K and ordinary Hall above T_C. Whereas, Mn_3GaC exhibits AHE throughout the temperature range. The scaling analysis of the anomalous Hall conductivity (AHC) suggests that the AHE is primarily governed by coexistence of both intrinsic contribution due to Berry curvature and extrinsic contribution due to skew scattering in both Mn_3SnC and Mn_3GaC. The anomalous Hall resistivity (ρ^A_{xy}) shows the signature of the Kondo effect. The value of AHC is found to be 50 $\Omega^{-1}cm^{-1}$ and 0.9 $\Omega^{-1}cm^{-}1$ for Mn_3GaC and Mn_3SnC respectively. Moreover, we also calculate anomalous Hall angle, θ_A (~ 2.3 % and 0.01 %) and anomalous Hall factor, S_H (~ 0.2 V^{-1} and 0.0012 V^{-1}) for Mn_3GaC and Mn_3SnC respectively. The low temperature Seebeck data suggests the presence of significant contribution of electron–magnon scattering, and a large value of Nernst coefficient is consistent with finite Berry curvature effects.

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"Anomalous Hall effect in disordered Co_2TiSi Heusler alloy thin film: An Experimental and DFT study"

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We have reported the anomalous Hall effect in B2-type disordered Co_2TiSi thin film. The experimental value of the anomalous Hall conductivity (AHC) measured at 10 K temperature is 245.26 S/cm with an intrinsic Karplus-Luttinger or Berry phase + side-jump contribution and skew-scattering contribution. From the first principles DFT calculation, we have shown the disorder effect on anomalous Hall conductivity for this material and explained how to analyze the experimentally obtained value with theoretical calculation. Theoretically, we have incorporated a 50 % positional disorder effect into the ordered structure. The disorder effect changes the hybridization between the atomic orbitals of the atoms in the crystal structure. Hence, the density of states of the electronic orbitals' changes. 50 % B2-type disorder effect destroys the half metallicity of the pure ordered $L2_1$ structure as the Fermi level shifts its position relative to the spin-down channel. This results in changing the topology of the Fermi surface, magnonic excitations of the disordered structures compared to pure ordered structure. The residual impurity or defect is generating the disorder impurity scattering potential. The quite large AHC of B2 disordered Co_2TiSi thin film is a promising candidate material for spin Hall effect measurement as spin Hall conductivity is proportional to anomalous Hall conductivity and for future spintronics applications.

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Planar Hall Effect in Quasi-Two-Dimensional Materials

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ABSTRACT

The planar Hall effect (PHE) is the generation of longitudinal and transverse voltages [see Fig. 1(a)] in the plane of the applied electric ($\boldsymbol{E}$) and magnetic fields ($\boldsymbol{B}$). PHE has extensive applications in magnetic sensors and memory devices. In 3D materials, PHE generally originates from the coupling of the Berry curvature ($\boldsymbol{\Omega}$, BC) and orbital magnetic moment ($\boldsymbol{m}$, OMM) to the band velocity and in-plane magnetic field, which generates a longitudinal and transverse planar response [1]. However, the Berry curvature and orbital magnetic moment-induced conventional planar Hall effect are forbidden in 2D systems as the out-of-plane Berry curvature and orbital magnetic moment cannot couple to the band velocity of the electrons moving in the 2D plane and externally applied in-plane magnetic field, respectively. In our paper [2], we demonstrate a unique 2D planar Hall effect (2DPHE) originating from the hidden planar components of the Berry curvature and orbital magnetic moment in quasi-2D multi-layered materials. We identify all planar band geometric contributions to 2DPHE and classify their crystalline symmetry restrictions. Using gated bilayer graphene as an example, we show that in addition to capturing the hidden band geometric effects, 2DPHE is also sensitive to the Lifshitz transitions of the Fermi surface. Our discovery of 2DPHE brings the vast class of layered 2D materials under the purview of planar Hall effect probes, which were limited to 3D materials, and motivates further study on planar band geometric quantity-induced other transport phenomena for innovative applications.

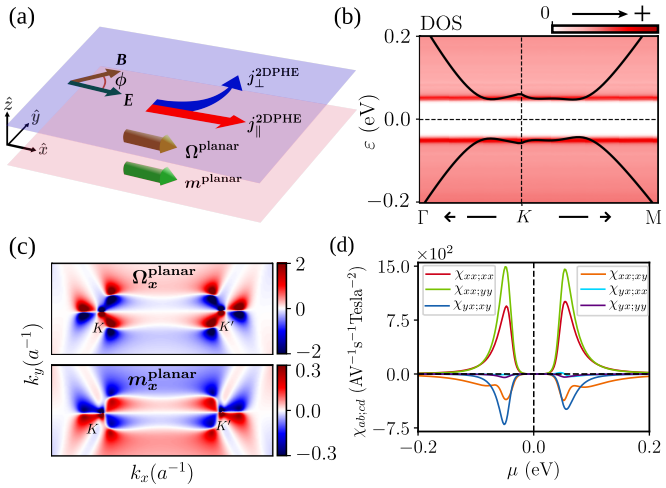

FIG. 1. **Two-dimensional planar Hall effect in strained bilayer graphene.** (a) A transverse and longitudinal current is produced in the presence of in-plane electric and magnetic fields. (b) The low-energy electronic band structure of strained BLG around the K point, with the background color showing the density of states (DOS). The Van Hove singularity in the DOS near the band edges [also seen in (b)] is accompanied by a Lifshitz transition, where the system evolves from hosting three Fermi pockets around the K (or K') point to one Fermi pocket. (c) The upper (lower) panel shows the k-space distribution of the x-component of the planar BC (OMM) for the first conduction band in the unit of a^2 $\left(\frac{e}{\hbar}a^2\mathrm{eV}\right)$, where a is the lattice constant. (d) Different components of 2DPHE response tensors $\chi_{ab;cd}$ defined as $j_a = \chi_{ab;cd}E_bB_cB_d$, as a function of μ evaluated at temperature $T = 50$ K. In Fig (b), (c), and (d), we choose interlayer potential $\Delta = 0.05$ eV.

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Electronic and thermal transport properties of superconducting topological 3D Dirac Semimetal PdTe

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Topological semimetals are materials with special electronic properties, featuring topologically nontrivial bulk band crossings and robust surface states [1]. Recent discoveries of materials that show both topological semimetal behavior and superconductivity have further advanced this research. PdTe is a 3D Dirac semimetal, exhibiting type- II superconducting behavior with a transition temperature (T_C) ~ 4.5 K [2,3]. Recent Angle-Resolved Photo-emission Spectroscopy (ARPES) experiments have revealed the coexistence of bulk-nodal and surface-nodeless Cooper pairings in PdTe [4]. However, the low-temperature thermal-conductivity measurements on PdTe single crystals suggest that PdTe has multiple nodeless superconducting gaps, which contradicts the bulk-nodal gap claim [5]. We carried out electronic and thermal transport experiments on PdTe single crystals. Our field-dependent specific heat data down to temperatures ~ 58 mK shows a power-law field dependence, which differs from the usual linear behavior expected for an isotropic fully gapped s-wave superconductor [6]. Additionally, our zero-field specific heat data reveals a clear ~ T^3 temperature dependence at low temperatures ($T < T_C/3$), suggesting the presence of bulk point nodes in the superconducting order parameter of PdTe. A weak-coupling BCS-type order parameter with *p*-wave symmetry and point nodes fits the zero-field data well. These bulk specific heat measurements indicate that PdTe is likely an odd-parity *p*-wave superconductor [7]. In thermal transport measurements, the superconducting transition is observed in Seebeck coefficient, which suppresses with applied magnetic field. We observed $S(T) \propto T$ (electron diffusion dominant) behavior in the range of 200 – 300 K, giving Fermi temperature $T_F = 1.5\times10^4$ K, and $S(T) \propto T^3$ (phonon drag dominant) behavior was observed near 50 K. Moreover, future experiments on doped PdTe samples are expected to show unusual transport properties near superconducting transitions. These findings make PdTe an intriguing candidate for studying the underlying physics in the topological superconducting state.

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Transmigration of Edge States with Interaction in Su-Schrieffer-Heeger Chain

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Abstract

The effect of Hubbard and Kondo interactions on the edge states in the half-filled Su-Schrieffer- Heeger chain of electrons is investigated by studying the behaviour of charge quasiparticles using Kumar representation and density matrix renormalization group method. For any finite dimerization of hopping, by increasing the Hubbard interaction, the edge states are found to transmigrate from the physical charge gap to a high energy gap through an intermediate phase without the edge states. The extent of this phase with no edge states shrinks smoothly upon increasing the dimerization. The transmigration of edge states from the charge gap to the high energy gap is also found to occur with Kondo interaction, but through an intermediate phase which itself changes from having no edge states for weak dimerization to having the edge states in the physical as well as the high energy gaps coexisting from moderate to strong dimerization.

Reference :: J.Bisht, S.Jalal, B.Kumar,arXiv:2404.02259

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Exactly Solvable Kitaev Spin-Orbital Bilayer Model

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(Manuscript under preparation)

In condensed matter physics, spin liquids represent a unique and puzzling state of matter characterized by their lack of conventional magnetic order. Understanding these phases has long been a fascinating challenge and exact solvable models offer a powerful tool to explore their intricate properties. In this talk, we propose an exactly solvable spin-orbital bilayer model on a honeycomb lattice. This model can be reduced to two species of free Majorana fermions coupled to the background Z2 gauge field, in a similar spirit of the original Kitaev model. Through a variational analysis, we obtain a rich ground state phase diagram. Lastly, we demonstrate that an essence of Lieb's theorem still holds true, even when we step beyond the planar regime.

Other Publications:

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Evolution of BCS Superconductors following a Sudden Quench

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In this study, we investigate the dynamics of S-wave superconductors following a quench in the interaction parameter within the framework of the attractive Hubbard model. Starting from an initial state at $t \leq 0$ characterized by a given interaction parameter and average density, we examine the evolution of the system for times $t > 0$, under a sudden change (quench) in the interaction parameter. Our focus is on understanding the time-dependent behavior of onsite densities, the evolution of order parameters both spatially and in phase, the corresponding density of states etc. We also examine the potential rise of off-diagonal order parameters and the possibility of charge density wave formation within the system. The analysis is performed across both weak and strong coupling regimes, as well as for weak and strong quench scenarios. The time-dependent equations of motion are solved using the 4th order Runge-Kutta method, providing detailed insights into the dynamics of the superconducting state under different quench conditions.

Resonant bulk photogalvanic effect in centrosymmetric metals

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We investigate dominant photogalvanic effects in centrosymmetric systems where the usual second-order photogalvanic response vanishes. We specifically focus on the Fermi surface effects and elaborate on the band geometric quantities. We predict several new contributions: nonresonant Berry curvature quadrupole contribution, resonant Fermi surface injection, and shift contributions where the position of the Fermi surface determines the response peaks. We study the physical mechanisms behind these new contributions and associate them with the Riemannian geometry of the Bloch bands. Our study provides a new perspective on the photogalvanic responses in centrosymmetric semimetallic systems where the second-order photogalvanic effects are identically zero and a finite Fermi surface is present.

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Observation of Magnetic Skyrmions and Unusual Transport Phenomena in Tetragonal Ferrimagnet Mn_2Sb

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Magnetic skyrmions are swirling kinds of spin textures with a topological protection against continuous deformation. Their topological magnetic states allow them to be moved, created, and annihilated efficiently, thereby making them one of the most promising candidates in future information storage and computing applications. The stabilization of skyrmions depends on the nature of magnetic interactions which originate from the crystal symmetry of the respective materials. In non-centrosymmetric magnetic materials Dzyaloshinskii– Moriya interaction (DMI) plays a vital role in stabilizing skyrmions/antiskyrmions. In contrast, in centrosymmetric magnets, the stabilization of skyrmions is governed by competing dipolar interaction and easy axis magnetic anisotropy, frustrated magnetic exchange, and higher-order magnetic interactions. The absence of DMI in the centrosymmetric magnets leads to the observation of energetically degenerate skyrmions with both clockwise and counter-clockwise helicities. Recently, ferrimagnetic skyrmion host materials have attracted a lot of attention for their potential room-temperature applications since most of these materials exhibit very high ordering temperatures and comparatively smaller magnetic moments. One fascinating case is the tetragonal centrosymmetric ferrimagnet Mn_2Sb which shows an ordering temperature of 550 K and a spin reorientation transition at 240 K. We have done a comprehensive investigation on the real space observation of different types of magnetic spin textures using Lorentz transmission electron microscopy (LTEM) and electrical transport properties. The LTEM study shows the stabilization of magnetic skyrmions and bubbles at room temperature. Also, we observe a directional dependence of the Hall resistivity in the system from the Hall Effect measurements. These findings significantly advance the broader exploration of Mn_2Sb, highlighting its potential applications in skyrmion-based magnetic technologies and providing valuable insights into novel magnetic phenomena.

Adsorption of H_2 Molecules over Hexagonal Boron Nitride Monolayer: A Combined DFT and Kinetic Monte-Carlo Study

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Abstract: One of the main challenges faced during the use of hydrogen (H_2) 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 H_2 molecules over a hexagonal boron nitride (h-BN) monolayer [1]. The adsorption and diffusion energy over the surface of an h-BN monolayer have been predicted using the revPBE-vdW functional in vdW-DFT framework. The adsorption energy lies between -60 to -70 meV over different sites of an h-BN ring indicating a weak physisorption process. In addition, Bader charge analysis and density of states (DOS) calculations have been utilized to describe the adsorption mechanism. The lateral repulsion present between the H_2 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 H_2 molecules over the h-BN substrate. A quantity, surface coverage can be defined as the fraction between the total number of occupied sites and the total number of adsorption sites. The kMC calculations indicate that the H_2 adsorption is favorable at a low temperature and high pressure. Other than pristine, defective h-BN monolayers have also been considered for the adsorption of H_2 molecules [2]. While the adsorption energy increases above a boron vacancy, it is reduced for a nitrogen vacancy. Moreover, different carbon point defects and carbon clusters over the h-BN substrate have been also considered for our study. The H_2 adsorption energy lies between -65 to -85 meV over different carbon clusters. Thus, boron vacancy and carbon cluster formation can be an effective way to increase the overall storage capacity of the h-BN monolayer.

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Tunable interaction between phonons and the continuum in $Cr_2Ge_2Te_6$: a possible 2D magnetic material for quantum sensing

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$Cr_2Ge_2Te_6$ is a 2D Heisenberg layered van der Waals ferromagnetic semiconductor and this is potential candidate for the next-generation spintronic devices, nanoelectronics, and useful as a substrate in ferromagnetic insulator-topological insulator heterostructures. Here, we comprehensive inelastic light (Raman) scattering measurements on single crystal of $Cr_2Ge_2Te_6$ as a function of temperature and polarization, from 6 to 330 K. Our measurements reveal the long and short-range ordering of the spins below T_c (~60 K) and T^* (~180 K), respectively; setting the stage for broken rotational and time reversal symmetry, gauged via the distinct renormalization of the phonon self-energy parameters. Our comprehensive measurements also uncovered an intriguing dependence of the interaction strength between discrete state (phonon) and the underlying continuum, quantified using the Fano asymmetry parameter, as a function of the polarization at different temperatures. Our results suggest the possibility of tuning the interaction strength using controlled scattered light and symmetry in this 2D magnet. This advancement may pave the way for controlling the interaction strength based on light polarization, and thus open the possibility of potential quantum sensors capable of quantifying interaction strength as a function of the photon polarization. Our investigation of 2D ferromagnetic semiconductor $Cr_2Ge_2Te_6$ using temperature and polarization dependent Raman spectroscopic measurements revealed the prospect to control the quantum pathways of inelastically (Raman) scattered light, offering future platform for application in quantum technology and sensing.

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Origin of peculiar exchange bias phenomena in a hole doped rare-earth double perovskite series

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(Manuscript under preparation)

Developing and understanding the materials that show significant Exchange Bias (EB) are at the forefront of current magnetism research and are of immense scientific and technological importance. Nevertheless, it is crucial to interpret the results with caution, as the presence of non-saturated minor loop like phenomena can obscure the true physics of the EB materials. In pursuit of this objective, we have successfully synthesised a rare-earth double perovskite system $RE_{2-x}Sr_xCoMnO_{6-\delta}$ ($0 \leq x \leq 1$) and investigated their diverse magnetic characteristics, with particular emphasis on EB. At $x = 0.75$, we observed the highest EB field of ~ 4.1 kOe at 8 K temperature when subjected to a cooling field of 6 T and sweep field of 7 T. However, upon subtracting the contribution of minor loop phenomena, we observed the presence of inverse EB (IEB) masquerading as normal EB (NEB) at $x = 0.75$ and two other nearest compositions. The IEB for $x = 0.75$ is found to be robust even at a high cooling field of 6 T, while for the other two nearest compositions, we see conversion of IEB to NEB with increasing cooling field. These peculiar phenomena can be attributed to the competition between ferro-antiferro (causing NEB) and ferro-glass (causing IEB) type interfaces. Furthermore, the entire series demonstrates complex physics, showcasing intriguing phenomena such as re-entrant double glassy states and behaviour resembling non-Griffiths-like phases.

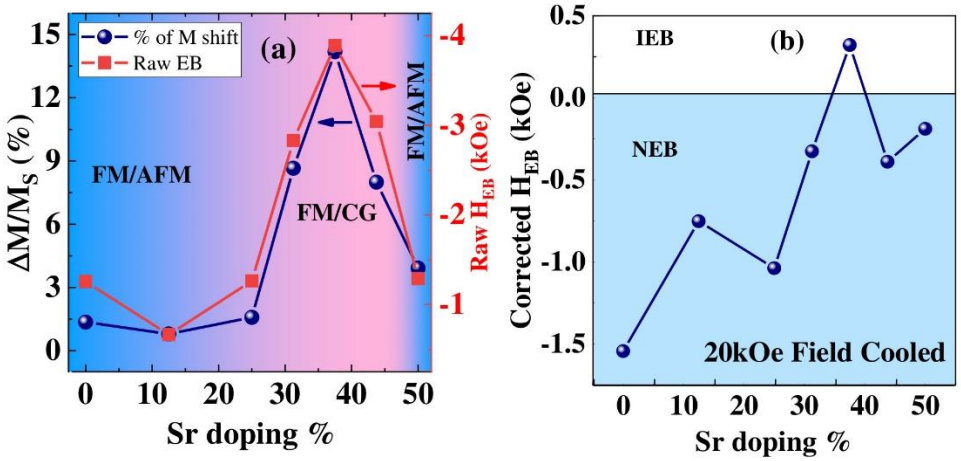

Fig. 1. (a) Variation of EB (2T field cooled) and vertical magnetization shift with hole doping as seen from the raw M(H) data at 8 K. Blue (Red) shade indicates FM/AFM (FM/Cluster-Glass) type interfaces; (b) Variation of *minor loop corrected* EB (2T field cooled) with hole doping at 8 K. 37.5% ($x = 0.75$) shows inverse EB.

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Investigating Low-Frequency Noise and Defect-Induced Impurity Bands in Topological Insulators

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Low-frequency noise in topological insulators (TIs) serves as a crucial indicator of the dynamic processes occurring within these materials. TIs, characterized by their unique electronic properties, are highly sensitive to disruptions, with defects like antisite defects and vacancies playing a significant role. These imperfections can introduce impurity bands, which alter the material's noise characteristics, potentially affecting the performance and stability of TIs in practical applications.

To gain insights into the magnitude and behavior of noise within our TI sample, we've established a low-frequency spectroscopy setup. This advanced system allows us to meticulously measure and analyze the noise, providing valuable data on how it correlates with the inherent properties and defects within the TI.

Moreover, our investigation extends to examining the impact of substituting indium in the TI. By replacing a portion of the material with indium, we aim to observe any changes in the noise behavior, shedding light on how such modifications influence the TI's electronic dynamics. This study is essential for optimizing TIs for future technological applications, where understanding and controlling noise is critical.

Topological and antiferromagnetic ordering in two-dimensional van der Waals crystals of $(Ni_xFe_{1-x})_2P_2S_6$ probed by Raman spectroscopy

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Abstract

Mermin-Wagner theorem states that isotropic spins can't have long-range order in one/two-dimensions at finite temperature by breaking the continuous global symmetry. However, it does not apply to all types of phase transitions in low dimensions such as topologically ordered phase rigorously shown by Berezinskii-Kosterlitz-Thouless (BKT) and experimentally realized in very limited systems such as superfluids, superconducting thin films. Quasi two-dimensional van der Waals magnets provide an ideal platform to investigate the fundamentals of low-dimensional magnetism. We explored the quasi two-dimensional (2D) honeycomb antiferromagnetic single crystals of $(Ni_xFe_{1-x})_2P_2S_6$ (x = 1, 0.7, 0.5, 0.3 & 0) with varying spins using in depth temperature dependent Raman measurements. As a function of chemical substitution, a tunable transition from paramagnetic to antiferromagnetic ordering is shown via phonons reflected in the strong renormalization of the self-energy parameters of the Raman active phonon modes. Interestingly, our observation of a broad magnetic continuum and its anomalous broad linewidth and coupling with the nearby phonon mode hints for a strong magnetostrictive coupling. Quite surprisingly, we also observed renormalization of the phonon modes much below the long-range magnetic ordered temperature attributed to the topological ordered state, namely the BKT phase, varying as a function of substitution and opens the possibility of identifying the topological ordering of spins using Raman scattering as a probe in quasi 2D magnetic systems. The extracted critical exponent of the order-parameter [spin-spin correlation length] evince the signature of topologically active state driven by vortex-antivortex excitations.

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Beyond being free: glassy dynamics of $SrTiO_3$-based two-dimensional electron gas

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Electron glasses offer a convenient laboratory platform to study glassy dynamics. Traditionally, the interplay between long-range Coulomb interactions and disorder is deemed instrumental in stabilizing the electron glass phase [1]. Existing experimental studies on electron glass have focused on doped semiconductors, strongly correlated systems, granular systems, etc., all of which are far from the well-delocalized limit. In this work we expand the study of electron glasses to a well-known quantum paraelectric $SrTiO_3$ (STO) and unveil a new scenario: how naturally occurring ferroelastic twin walls of STO [2,3] could result in glassy electrons, even in a metallic state. We show that the emergent two-dimensional electron gas at the γ-Al_2O_3/STO interface exhibits long-lasting temporal relaxations in resistance and memory effects at low temperatures, which are hallmarks of glassiness [4,5]. We also demonstrate that the glass-like relaxations could be further tuned by application of an electric field. This implies that the observed glassy dynamics is connected with the development of polarity near the structural twin walls of STO and the complex interactions among them, arising from the coupling between ferroelastic and ferroelectric orders. The observation of this glassy metal phase not only extends the concept of electron glasses to metallic systems with multiple order parameters but also contributes to the growing understanding of the fascinating and diverse physical phenomena that emerge near the quantum critical point.

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Subjugating extensive magnetostructural temperature window and giant magnetocaloric effect in B-doped MnNiSi hexagonal system

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Abstract

Coupled first-order magnetic transformations (FOMTs) with narrow widths governed by low external stimuli play a crucial role in magnetic refrigeration for ferromagnetic hexagonal systems. In this work, we report a family of magnetocaloric materials named interstitial boron (B) doped-$(MnNiSi)_{0.67}(Fe_2Ge)_{0.33}$ compounds that are devoid of rare-earth elements. Our results show that varying B concentrations up to 5 at % can tailor the robust FOMTs between the low-temperature ferromagnetic orthorhombic phase and the high-temperature paramagnetic hexagonal phase in a wider temperature regime. A dramatic change in hysteresis (ΔT_{hys}) from ~ 25 K for x = 0 to ~ 8 (9) K as well as increases in the saturation magnetization for specific 2 (3) at % of B dopants is pronounced. Henceforth, the origin of the reducing hysteresis is illustrated based on the geometrical compatibility conditions ($\lambda_2 \sim 1$) between the austenite and martensite phases using temperature-dependent powder XRD analysis. Moreover, we found the samples performed good functional stability from the thermal cycling run. The branch of these B doping materials exhibits robust features of a large magnetocaloric effect (MCE) and temperature-averaged magnetic entropy change (TEC) over an extensive temperature range (~71 K) at a lower magnetic field change of 2T. These several tangible benefits, such as reduced ΔT_{hys}, geometrical compatibility, and robust MCE properties are first reported in the studied hexagonal system. Therefore, our results offer a viable approach to improve the cascading of these materials towards the application of cooling technology.

Quantum kinetic theory of the nonlinear thermal currents

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&

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We present a comprehensive study of second-order nonlinear thermal transport in electronic and bosonic systems using a quantum kinetic theory framework. Our investigation reveals the presence of intrinsic scattering time-independent nonlinear thermal currents, in addition to the known extrinsic nonlinear Drude and Berry curvature dipole contributions. These intrinsic currents have a quantum mechanical origin and are generally governed by the quantum metric tensor a band geometric quantity. The quantum metric represents the distance between two neighboring Bloch wavefunctions in Hilbert space or eigenstate-space. Intrinsic currents become nonzero only in systems where both space inversion and time-reversal symmetries are broken.

In electronic systems, we specifically analyze the nonlinear thermal responses in tilted massive Dirac systems, demonstrating the dominance of the intrinsic contribution over Drude and anomalous Hall contributions. Additionally, apart from the scattering time dependency, we show distinct temperature dependencies of various current contributions in the low-temperature limit. In bosonic systems, we uncover an intrinsic nonlinear thermal Hall current arising from the quantum metric and demonstrate its dominance in topological magnons in a two-dimensional ferromagnetic honeycomb lattice without Dzyaloshinskii-Moriya interaction.

Our findings underscore the critical role of band geometry in nonlinear thermal transport and pave the way for future theoretical and experimental studies on intrinsic thermal responses, with significant implications for quantum material research and applications in quantum magnonics and power-efficient thermal devices.

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Strong spin-lattice coupling in two-dimensional $CrTe_2$

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Keywords : $CrTe_2$, two-dimensional magnetism, room-temperature ferromagnetism, spin-lattice coupling

ABSTRACT:

Recent experimental studies on ultrathin films of $CrTe_2$ have shown potential for achieving room-temperature ferromagnetism. However, the results in single-layer $CrTe_2$ are widely debated in the literature, with conflicting findings ranging from intrinsic ferromagnetism to a ground state characterized by zigzag antiferromagnetism. We correlate these contrasting results to a very strong spin-lattice coupling, which is atypical for two-dimensional van der Waals materials. We examine the underlying phase diagram to understand these phenomena better and explore exchange interactions and magnetic anisotropies. Moreover, we employ long-range anisotropic Heisenberg Monte Carlo simulations to calculate ordering temperatures and investigate methods for manipulating the magnetic properties, focusing on compatibility with potential device applications.

QMAT - ABSTRACT

The interplay between the quantum effects from low-dimensionality and the spin-orbit coupling leads to exotic ground states with unusual excitations. Among the diverse 2D spin systems, the S = ½ 2D square lattice has piqued the curiosity of researchers due to its connection with the High-Temperature Superconductivity (HTSC). Studying the Crystal electric field (CEF) and spin-orbit coupling (SOC) effects in a J_{eff} = ½ 2D square lattice magnets is one of the recent fundamental interests in condensed matter physics. While a few transition metal-based square lattice materials exist, the experimental exploration of rare-earth magnetic materials with a perfect 2D square lattice structure is very limited. Herein, we report the structural, magnetic, heat capacity, and electronic structure studies of Bi_2REO_4Cl (RE = Yb, Er), which constitutes a structurally perfect 2D square lattice with rare-earth magnetic ions. The magnetization and heat capacity data analysis confirms that both the Yb^{3+} and Er^{3+} ion hosts the spin-orbit driven J_{eff} = ½ state at low temperatures. The Curie-Weiss temperature for the low temperature region in the case of Bi_2YbO_4Cl and Bi_2ErO_4Cl come out to be -1 K and -2.1 K, implying the presence of antiferromagnetic (AFM) coupling between the magnetic moments. The heat capacity measurements for Bi_2YbO_4Cl reveal a broad peak at 0.3 K, with no distinct magnetic anomaly detected down to 0.09 K, suggesting the development of short-range correlations. In contrast, Bi_2ErO_4Cl exhibits magnetic long-range order at 0.47 K. Our first-principles calculations based on density functional theory provide further insight into crucial role of spin-orbit coupling and magnetic anisotropy of the spins.

Topological Magnetism and Superconductivity in Magnet-Superconductor Hybrid Systems

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This study presents a practical and adaptable strategy for crafting two-dimensional (2D) topological superconductors (TSCs) within magnet/superconductor hybrid materials featuring Majorana flat edge modes (MFEM). Utilizing a noncollinear magnetic texture in proximity to the common s-wave superconductor, we explore an alternative to unconventional p-wave superconductors, providing a promising route to realize the 2D Kitaev model experimentally.

The study first presents a continuum model illustrating a technique for inducing a gapless TSC phase featuring MFEMs by manipulating noncollinear spin-spiral states in the presence of an s-wave pairing. Furthermore, the constructed minimal Hamiltonian applicable to magnet/superconductor heterostructures, with its numerically solved magnetic ground state, demonstrates resilient MFEM within the gap of Shiba bands. These modes are spatially confined to the edges of a 2D magnetic domain characterized by a spin-spiral arrangement. Employing Mn (Cr) monolayers on a strained s-wave superconducting substrate, specifically Nb(110) under strain (Nb(001)), validates the occurrence of a non-collinear magnetic ground state. This study highlights the intricate interplay between such a magnetic state and s-wave superconductivity, showcasing the appearance of MFEM at distinct domain edges. This innovative approach extends the scope of TSCs into the 2D domain, demonstrating the potential for applications in antiferromagnetic-superconductor spintronics and topological quantum computation. The method provides a unique approach to uncover topological superconducting phases in prototype transition-metal/superconductor materials—akin to the 2D Kitaev model.

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- Topological superconductivity by engineering noncollinear magnetism in magnet/superconductor heterostructures: A realistic prescription for the two-dimensional Kitaev model.
  Pritam Chatterjee, Sayan Banik*, Sandip Bera, Arnob Kumar Ghosh, Saurabh Pradhan, Arijit Saha, and Ashis K. Nandy*; Phys Rev B (Letter) **109** 121301.
  (*These authors contributed equally to this work)

Title - Realizing non-trivial doublon formation using a quantum computer

Authors name - Biswajit Paul, Tapan Mishra

Abstract - Dynamical formation of doublons or onsite repulsively bound pairs of particles on a lattice is a highly non-trivial phenomenon. In this work, we show the signatures of doublon formation in a quantum computer by simulating the continuous time quantum walk in the framework of the one dimensional extended Fermi-Hubbard model. By considering two up-component and one down-component particles initially created at the three neighbouring sites at the middle of the lattice and allowing intra- (inter-) component nearest neighbour (onsite) interactions we show the formation a stable onsite doublon in the quantum walk. The probability of such doublon formation is more (less) if the hopping strength of the down particle is weaker (stronger) compared to the up particle. On the contrary, for an initial doublon along with a free up particle, the stability of the doublon is more prominent than the doublon dissociation in the dynamics irrespective of the hopping asymmetry between the two components. We first numerically obtain the signatures of the stable doublon formation in the dynamics and then observe them using Noisy Intermediate-Scale Quantum (NISQ) devices.

Impact of Band-ordering Reversal and Scattering Mechanisms on Carrier Mobility in Scandium Nitride

Sourav Rudra, Dheemahi Rao, Samuel Poncé, and Bivas Saha

Low hole mobility in nitride semiconductors poses a significant challenge for achieving high-efficiency device applications. Scandium nitride (ScN), a promising rocksalt group III(B)-nitride semiconductor that has recently attracted for potential applications in thermoelectricity, low-loss and high figure-of-merit infrared plasmon- and phonon-polaritons and optoelectronic artificial synaptic functionalities with memory and learning abilities. Despite such functionalities, ScN suffers from low hole mobility due to ionized impurity scattering, as demonstrated through *ab initio* Boltzmann transport formalism including spin-orbit coupling. A potential solution to enhance hole mobility in ScN thin films is strain engineering, which can reverse band-ordering. Biaxial tensile strain lifts the split-off hole band above the heavy hole and light hole bands, resulting in a lower hole-effective mass and increased mobility. Alongside impurity scattering, Fröhlich interaction plays a crucial role in the carrier scattering mechanism due to the polar nature of ScN. Improving hole mobility in ScN could boost thermoelectric, plasmonics, and neuromorphic computing device efficiencies.

Similarly, the electron mobility in ScN is hindered by electron-phonon interactions, defects, grain boundary, and dislocation scatterings. The electron mobility varies based on growth conditions, and understanding these scattering mechanisms is critical for device applications. *Ab initio* Boltzmann transport formalism and experimental measurements reveal that while Fröhlich interaction sets an intrinsic upper bound for ScN's electron mobility at ~521 $cm^2/V.s$ at room temperature, ionized-impurity and grain-boundary scatterings significantly lower this mobility. Experimental data on temperature dependence and room-temperature doping dependency aligns with the Caughey-Thomas model, emphasizing the importance of mitigating ionized-impurity scattering. Modulation doping and polar-discontinuity doping are proposed as strategies to achieve high-mobility ScN, enhancing its potential for various device applications.

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Exploring anisotropic superconductivity in a ternary boride superconductor through Migdal-Eliashberg theory

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(Dated: August 13, 2024)

In the field of condensed matter physics and material science, the discovery of novel superconducting materials remains a formidable challenge. Although superconductivity in binary borides has been verified through numerous experiments and computations, superconductivity in ternary borides is still relatively unexplored. In this work, We have explored the anisotropic superconductivity of a ternary boride superconductor utilising the Migdal-Eliashberg theory implemented in Electron Phonon Wannier (EPW) code. Our substance comprises Mo atoms that are confined within a specific plane. This results in a significant coupling between the σ-bonding states of Mo d-orbitals and the in-plane vibration of Mo atoms, namely the E_{2g} phonon mode situated in the acoustic branch of the phonon dispersion, which is influenced by Mo atoms. As a result, it leads to anisotropic superconductivity with a critical temperature of 19.30 K. Due to the relatively large distance between Mo atoms, π-bonding states are unable to form an additional gap as seen in MgB_2, resulting in our system being a single-gap superconductor. We also conducted a high-pressure study on the anisotropic superconductivity of our system. Up to 77 GPa, the system does not undergo any structural phase transition, but it becomes thermodynamically unstable beyond this point. We observed a decreasing trend in electron-phonon coupling strength and superconductivity with increasing pressure, which can be attributed to the reduction in the density of states of Mo atoms at the Fermi level and the stiffening of phonon in the phonon dispersion.

ABSTRACT

Rare coexistence of Griffith's phase and spin glass state with intrinsic dominant anomalous Hall in inverse Heusler alloy Mn_2PdIn

Heusler alloys are a family of compounds with promising characteristics for exploring and controlling topological phases. In this work, we have synthesized a bulk polycrystalline inverse Heusler alloy, Mn_2PdIn, due to its predicted nontrivial band topology. The compound violates the Slater–Pauling rule and exhibits ferrimagnetic ordering around 280 K. D.C. magnetization measurements reveal spin glass nature and an exchange bias effect at low temperatures, below 100 K, along with Griffiths phase behavior above the transition temperature. Two different types of spin glassy phases were detected in our A.C. susceptibility measurements. The spin fluctuation-dominant scattering of conduction electrons at low temperatures (below 100 K) in our resistivity measurements also aligns with the spin glassy phase of the compound. Additionally, a substantial intrinsic anomalous Hall conductivity of 52 S cm^{-1} suggests the nontrivial band topology of this compound. The two different magnetic sublattices of Mn play a dominant role in geometric frustration and symmetry-breaking interactions, which are responsible for the spin glassy states and intrinsic anomalous Hall conductivity.

Title:- Interaction driven topological phase transitions of hardcore bosons on a two-leg ladder

Abstract:- We investigate the topological properties of hardcore bosons possessing nearest-neighbor repulsive interactions on a two-leg ladder. We show that by allowing nearest neighbour dimerized interactions instead of hopping dimerization, the system exhibits topological phases and phase transitions under proper conditions. First, by assuming uniform hopping throughout the ladder, we show that when interaction along the legs are dimerized and the dimerization pattern is different in the legs, a trivial rung-Mott insulator to a topological bond order phase transition occurs as a function of the dimerization strength. However, for a fixed dimerization strength, the system exhibits a topological to trivial phase transition with increase in the rung hopping. A completely different scenario appears when the rung interaction is turned on. We obtain that for a ladder with uniform hopping, the repulsive interaction either turns the topological phase into a trivial rung-Mott insulator or a charge density wave phase. Such topological features are absent when the dimerization pattern in the nearest neighbour interaction is considered to be identical in both the legs of the ladder. We numerically obtain the ground state properties and also show the signatures of topological phase transitions through Thouless charge pumping.

Enhanced Dielectric Performance of ZIF-8 through Nanoparticle Integration

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Abstract:

Metal-organic frameworks (MOFs) have recently emerged as innovative materials with considerable interest from the scientific and technological fields. Among the various 3D MOFs, zinc imidazole framework 8 (ZIF-8) stands out due to its unique structural and electrical properties. While ZIF-8 typically exhibits low dielectric values, making it suitable for low-dielectric applications, incorporating nanoparticles can enhance its dielectric constant. This study aims to improve ZIF-8's dielectric properties by integrating nanoparticles, specifically ZnO nanoparticles were chosen due to their high electron mobility, wide band gap, and exciton binding energy[1]. When introduced as fillers in ZIF-8, ZnO nanoparticles influence the framework's morphology, porosity, pore size distribution, and interconnectivity, thereby affecting the material's polarization and dielectric characteristics. ZnO's inherent ionic polarization helps reduce dielectric loss while increasing the dielectric constant, a critical attribute for dielectric materials. Following the doping of ZIF-8 with 5wt% ZnO, the dielectric constant increased by 1.5 times at ambient temperature and nearly five times at 150°C. Concurrently, the dielectric loss decreased compared to pure ZIF-8[2]. The changes in dielectric properties are attributed to variations in porosity, pore size, defects, and oxygen vacancies. These findings validate the interaction between ZnO and ZIF-8 and offer insights into the intrinsic and extrinsic electrical properties of ZIF-8 composites. This work aims to leverage MOF's potential for low-loss, high-k dielectrics through the straightforward integration of nanoparticles.

Key Words: MOF, nanoparticles, defects, dielectric, loss

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Multifunctional Graphene-Based metal oxide Nanocomposites towards Dielectric, Magnetic and Photocatalytic Activity

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ABSTRACT

The growing population needs innovative solutions in health, environment, energy storage, and drinking water to ensure sustainability and enhance quality of life. Graphene-based materials have the potential to revolutionize energy (dielectric), water (waste-water treatment), and data storage (magnetic), addressing the primary concerns of modern society through their unique and dynamic properties. This has been accomplished by adding ZnO and Fe-doped ZnO (ZnO@Fe) to graphene oxide (GO) and controlling its structural and optical properties. GO has an initial dielectric (ε_r) of 350, according to the research. This increases significantly when the loss decreases with the addition of ZnO (470) and ZnO@Fe (2240) to the GO [2]. The composites exhibit increased thermal stability as indicated by the temperature-dependent ε_r, which may be attributed to the synergistic action of Fe and ZnO ions with GO. This has promise and may find application in a range of high-temperature apparatuses. Additionally, photocatalytic applications employ these graphene-based nanocomposites, showing that at 1 hour, the catalytic activity of GO (32%) is increased to 99% for 5% Fe-doped GO@ZnO composites [3]. This might be because of adding ZnO and Fe changed the rate at which electrons recombined, which affected the photodegradation process. Applying the sample in real-time to Mahanadi river water, demonstrated a 96% degradation efficiency, suggesting that it might be a promising candidate for an adaptive photocatalyst that effectively removes organic dyes from water. The technique has also been expanded to include spintronics applications. ZnO and GO behave in a diamagnetic manner. However, after adding 10% Fe-doped ZnO to GO, a room-temperature ferromagnetic feature was obtained. We obtain the effective anisotropy value up to the order of 10^6 erg/cc and enhancement of Tc from 46 K (GO-ZnO) to 377 K (GO-ZnO@Fe10) which is more than RT. In this approach, we may control and apply the same created sample cost-effectively for multi-purpose applications.

Keywords: - GO, Nanofillers, Percolation, Dielectric, magnetic, Photocatalytic degradation

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Fabrication of trench array of different depths and their application in the enhancement of the Raman & Photoluminescence intensity of monolayer MoS_2

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The two-dimensional (2D) materials' optoelectronics are influenced by their surrounding dielectric environment. By altering the underlying substrate material, thickness, or trench depth for suspended samples, optical signals can be either enhanced or suppressed. Different thicknesses and depths of substrates and trenches are commonly utilized as dielectric platforms for 2D materials. However, finding the optimal substrate thickness or trench depth requires multiple samples, which can result in variations between samples. To address this issue, we propose an optimized electron beam dose-modulated scheme for fabricating trenches with varying depths and thicknesses in the same SiO_2/Si substrate, followed by reactive ion etching [1]. We then transfer a single 2D flake (monolayer MoS_2) to cover all the steps or trenches on the same SiO_2/Si substrate. Our results show that the relative ratio of the air gap and SiO_2 thickness can be adjusted to significantly tune the photoluminescence (PL) and Raman intensities of the monolayer MoS_2 compared to MoS_2 on the SiO_2 substrate alone (Figs. (b) and (c), respectively). The experimental data (Raman and PL intensities) are consistent with the simulated data using a multi-reflection model [2]. We also observe a clear Raman peak shift with SiO_2 thickness or trench depth, which is attributed to the thickness and depth-dependent power absorption in the monolayer MoS_2. Therefore, we demonstrate a novel approach to enhancing the outcoupled light emitted by the monolayer MoS_2 by combining the air gap and SiO_2. This fabrication technique has potential applications in photonic band gap crystals and micro/nano-electromechanical systems (M/NEMS).

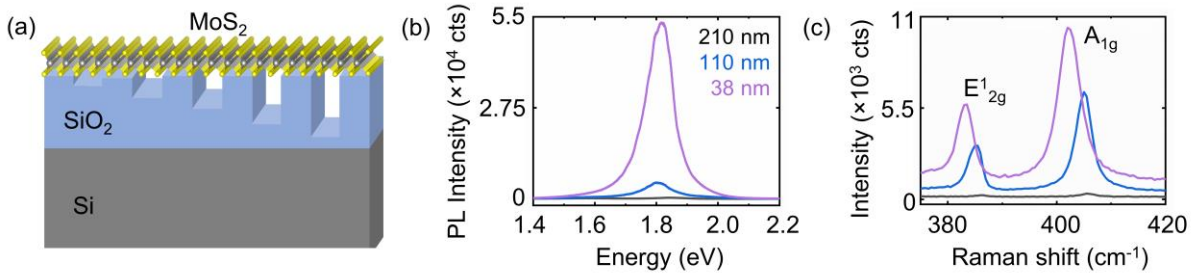

Figure: (a) Schematic of the suspended MoS_2 monolayer over square holes of different depths in SiO_2. (b) & (c) Room temperature PL & Raman spectra at the centre of the holes with remaining SiO_2 thickness of 38 nm, 110 nm, and 210 nm. The maximum thickness of SiO_2 is 210 nm.

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Crossed Andreev reflection in altermagnets

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Crossed Andreev reflection (CAR) is a scattering phenomenon occurring in a superconductor (SC) connected to two metallic leads, where an incident electron on one side of the SC emerges on the opposite side as a hole. Despite its significance, CAR detection is often impeded by the prevalent electron tunneling (ET), wherein the incident electron exits on the opposing side as an electron. One approach to augment CAR over ET involves employing two antiparallel ferromagnets across the SC. However, this method is constrained by the low polarization in ferromagnets and necessitates the application of a magnetic field. Altermagnets (AMs) present a promising avenue for detecting and enhancing CAR due to their distinct Fermi surfaces for the two spins. Here, we propose a configuration utilizing two AMs rotated by 90° with respect to each other on either side of an SC to enhance CAR. We calculate local and nonlocal conductivities across the AM-SC-AM junction using the Landauer-Büttiker scattering approach. Our findings reveal that in the strong phase of AMs, CAR overwhelmingly dominates nonlocal transport. In the weak phase, CAR can exhibit significant enhancement for larger values of the altermagnetic parameter compared to the scenario where AMs are in the normal metallic phase. As a function of the length of the SC, the conductivities exhibit oscillations reminiscent of Fabry-Pérot interference.

Keywords: Altermagnet, Crossed Andreev reflection, Nonlocal conductivity, Fabry-Pérot oscillations
Crossed Andreev reflection in altermagnets
Sachchidanand Das and Abhiram Soori, PHYS. REV. B 109, 245424 (2024)

Persistent currents in mesoscopic spin-orbit coupled rings due to an applied Zeeman field

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Persistent currents (PCs) in mesoscopic rings have been a subject of intense investigation since their proposal by Buttiker, Landauer, and Imry in 1983. In this work, we investigate the behavior of PC in spin-orbit coupled rings under the influence of a Zeeman field, which contrasts with traditional PC observed in rings threaded by magnetic flux. We find that the emergence of PC requires the nonzero values of spin-orbit coupling and the Zeeman field. Through theoretical analysis and numerical calculations, we unveil some intriguing phenomena. Mainly, in ballistic rings, we observe that PC varies inversely with system size, along with PC being zero at half-filling for even number of sites. Moreover, the introduction of on-site disorder results in a suppression of PC, with exponential decay observed for large disorder strengths and quadratic decay for smaller disorder strengths. Notably, disorder can enhance PC in individual samples, albeit with a configuration-averaged PC of zero. Furthermore, we find that the standard deviation of PC increases with disorder strength, reaching a maximum before decreasing to zero at high disorder strengths. Furthermore, we find that the standard deviation of PC increases with disorder strength, reaching a maximum before decreasing to zero at high disorder strengths. We also study persistent spin current which shows behavior similar to that of PC except that at half-filling, it is not zero. Our findings shed light on the intricate interplay between spin-orbit coupling, Zeeman fields, and disorder in mesoscopic quantum systems, offering new avenues for theoretical exploration and experimental verification.

Keywords: Persistent current, spin-orbit coupling, Persistent spin current, mesoscopic ring.

- Bijay Kumar Sahoo, Subroto Mukerjee and Abhiram Soori arXiv:2406.07405

von Neumann entropy and quantum version of thermodynamic entropy

Smitarani Mishra, Shaon Sahoo

Abstract

There has been an unsettled debate on what the quantum analog of the thermodynamic (TH) entropy is. More specifically, it is deliberated if the von Neumann (VN) entropy can be considered as the quantum counterpart of the TH entropy. In our work, we investigate if the VN entropy corresponds to the TH entropy in the large-system limit. We find that, for a large non-integrable quantum system, the VN entropy and the TH entropy are equivalent. This result is shown to be valid for both isolated systems and subsystems of a larger system. Our results help us establish a correspondence principle for the entropy. For supporting numerical results, we analyze here a one-dimensional spin-1/2 chain with next-nearest neighbor interactions.

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

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

Single and multi-frequency driving protocols in a Rashba nanowire proximitized to a *s*-wave superconductor

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Abstract

We perform systematic analyses of single and multi-frequency driving protocols on a Rashba nanowire with superconducting correlations induced by proximity effects. The results for the single-mode drive reveal interesting frequency dependencies of the Majorana modes, in the sense that the parameters corresponding to the trivial and the topological limits of the undriven (static) case host Majorana zero modes, respectively at low and high frequencies. Further, emergence of long-range interactions are noted that give rise to multiple gap-closing scenarios, where the latter implies occurrence of multiple Majorana modes. On the other hand, the multi-frequency driving protocol, sub-grouped into commensurate and incommensurate ratios of the frequencies, demonstrates intriguing consequences. The commensurate case yields dynamical control over the stability of the edge modes. Moreover, complex driving protocols such as those with larger ratio of frequencies harm the Majoranas by pushing them into the bulk. Finally, the incommensurate case yields independent Majorana modes occurring at low-symmetry points in the Brillouin zone. While the single and the commensurate multi-frequency driving protocols admit the usage of symmetric time frames for the computation of the topological invariants, the incommensurate case relies on the framework of many-mode Floquet theory, where the topological properties are ascertained via calculating the Berry phase. We present band structure and phase diagrams to substantiate all our results. The robustness and concurrent existence of these unique Majorana modes, even amidst a very dense energy spectrum along with a lack of global time-periodicity, hold promise for future applications in the field of quantum computation.

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Study of Magnon Band Topology in Antiferromagnets

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August 14, 2024

Abstract

In this work, we study topological properties of magnons via creating spin excitations in presence of an external magnetic field on a two-dimensional antiferromagnetic square lattice. It is known that Dzyaloshinskii-Moriya interaction (DMI) plays an important role in coupling between different particle (spin excitation) sectors, here we consider an anisotropic DMI and ascertain the role of the anisotropy parameter in inducing topological phase transitions. While the scenario, for dealing with ferromagnets, albeit with isotropic DMI is established in literature, we have developed the formalism for studying magnon band topology for the antiferromagnetic case. Owing to the presence of a two-sublattice structure of an antiferromagnet, a large number of magnon bands participate in deciding upon the topological properties. The nature of the phases and the phase transitions therein are characterized by the band structure, presence (or absence) of the chiral edge modes observed in a semi-infinite nano-ribbon geometry, computation of the thermal Hall effect, etc. Moreover, the strength of the magnetic field is found to play a decisive role in controlling the critical point that demarcates various topological phases.

Magnetic systems with transition metals show rich phases in electronic and magnetic properties. The co-existence of antiferromagnetism and metalicity is found in a Hubbard model. Faster spin dynamics (THz) in antiferromagnets (AFM) than in ferromagnets (FM) (GHz) make them attractive for faster memory read-write operation. The net-zero magnetization in AFM leads to a higher density of magnetic memory chunks overcoming the shortcomings of FM. The highly mobile electrons in a metal can carry the read-write instructions faster. That makes the AFM metal an advanced alternative to the current FM based MRAM devices. However, the AFM metals are rare. Here I will discuss a topologically protected antiferromagnetic Dirac metal. The ab initio calculations for a long range of Hubbard interactions show the AFM metal state. The phase diagram, based on The semi-classical Monte Carlo method, also shows the large region of AFM metalicity. And, the symmetry protection of the Dirac nodal points makes the system a topological metal with non-trivial spin-polarized surface states.

Antiferromagnets have emerged as promising materials for spintronic devices due to their strong resistance to external perturbations and their rapid operational speeds. Within this category, non-collinear antiferromagnets are gaining prominence as a new class of spintronic materials because of their unique magnetic and transport properties [1]-[4]. These materials, similar to their collinear counterparts, exhibit ultrafast spin dynamics and effectively avoid stray field effects. Among them, the kagome magnet Mn_3Sn stands out because of its various magnetic ordered states, including a triangular antiferromagnetic (AFM) configuration. Despite having negligible net magnetization, Mn_3Sn shows a substantial anomalous Hall effect, attributed to its cluster octupole magnetic order, which breaks time-reversal symmetry. In Mn_3Sn, replacing Mn with Fe results in the dominance of higher-order exchange interactions, which is reflected in the non-coplanar magnetic ground state and exhibits a pronounced anomalous Hall effect [5]. Instead of using a d-element for electron doping, the same can be achieved by introducing a p-element like antimony. Antimony is particularly effective for this purpose because it has an additional electron compared to the Sn atom. Sb doping causes a transition from the inverse triangular AFM ground state to a helical AFM phase. Also, the temperature range over which the helical phase remains stable with increasing Sb doping. We would present the role of the Kagome lattice in generating berry curvature and its contribution to the AHE in the Sb-doped Mn_3Sn. Furthermore, the tunability of the material properties through external parameters such as temperature, magnetic field and pressure will be presented.

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Halogen Modification of M–N_6 Single-Atom Catalysts for Enhanced Electrocatalytic Hydrogen Evolution Reaction

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The utilization of renewable energy sources for the electrochemical reduction of carbon dioxide (CO_2RR) into valuable fuels and chemicals is a promising approach to address energy security and environmental concerns. Single-metal atom catalysts have emerged as attractive alternatives due to their superior efficiency in overcoming limitations associated with conventional metal nanocatalysts. Our comprehensive first principle study,we focuses on fine-tuning chlorinated single-atom-based active sites on a graphitic carbon nitride (g-C_3N_4) monolayer to achieve absolute selectivity for HCOOH. Our research demonstrates that halogenation significantly inhibits the hydrogen evolution reaction (HER), which competes with the CO_2RR, by enhancing electronic stability. To achieve selectivity for a single product among all reduced products, we fine-tuned the chemical environment of the catalyst to neutral conditions. Our findings reveal that the catalyst exhibited enhanced selectivity for HCOOH, with a notably low onset potential and a broad potential range where HCOOH selectivity was sustained at the FeCl site at pH 7 compared to the acidic region.These results underscore the FeCl active site of FeCl-decorated g-C_3N_4 as a highly efficient and selective electrocatalyst for the CO_2RR. The insights gleaned from our study provide valuable guidance for the design of new CO_2RR catalysts with enhanced selectivity and efficiency.

Publication:

1. Renna Shakir, Hannu-Pekka Komsa, Karan Kumar Paswan, A. S. K. Sinha, and J. Karthikeyan, *The Journal of Physical Chemistry C* 2024, 128, 13, 5505–5514.

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QMAT -2024

Realizing Fulde-Ferrell-Larkin-Ovchinnikov pairing assisted topological Majorana zero modes and superconducting diode effect in helical Shiba chain

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We propose a theoretical perspective for the realization of Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) pairing in a helical Shiba chain subjected to an out-of-plane Zeeman field, analyzed through a self-consistent Bogoliubov-de-Gennes (BDG) mean-field formalism approach. An *s*-wave superconductor in proximity to a chain of magnetic adatoms with helical spin texture has emerged as a pivotal platform for realizing topological Majorana zero modes (MZMs). Our study reveals the crucial role of finite momentum pairing of Cooper pairs in the emergence of FFLO-pairing assisted topological MZMs. Notably, we demonstrate that FFLO pairing facilitates non-reciprocal charge transport, giving rise to a superconducting diode effect in systems where time-reversal and inversion symmetries are broken. This diode effect stems directly from the asymmetric FFLO state. Our comprehensive analysis highlights the intricate interplay between the helical Shiba chain, the out-of-plane Zeeman field, and FFLO pairing in the emergence of MZMs and driving the diode effect. These findings offer valuable insights into the design and realization of topological superconducting devices with diode-like properties, potentially advancing technological applications in quantum computing and superconducting electronics.

Generic construction of volume-law entangled eigenstates in spin Hamiltonians

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One of the fundamental challenges in understanding thermalization in isolated quantum many-body systems lies in the inherent difficulty in finding exact solutions for excited states of generic non-integrable models. Here, we propose a method to analytically construct a specific set of athermal volume-law-entangled exact excited eigenstates in a large class of spin Hamiltonians in any dimension. We illustrate the power of our method by identifying and providing exact analytic expressions for excited eigenstates for several physically relevant integrable and non-integrable spin Hamiltonians. Our construction also encompasses the recently obtained examples of volume-law entangled eigenstates, including those in the PXP models, and sheds light on their general structure.

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Quasi-Majorana Zero Modes in Kitaev Chains: The Role of Next-Nearest-Neighbor Couplings on Square Lattices

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Abstract:
We study the topological features of a Kitaev chain with nearest-neighbor hopping and pairing interaction on a square lattice model, which exhibits a topological gapless phase that hosts edge modes. These edge modes are not present at exactly zero energy but can be differentiated from the bulk, called pseudo- or quasi Majorana Zero Modes (qMZMs)[1]. These lower energy modes are robust against disorder and, under certain circumstances, also mimic the characteristics of Majorana Zero Modes (MZMs), like the non-Abelian statistics. We begin our analysis by investigating the bulk spectrum and the Berry connection vector, which show the presence of singularities and flux-carrying vortices in the Brillouin Zone. Further, we analyze the Hamiltonian under cylinder geometry to reveal the edge properties of the model. To differentiate between the presence of multiple MZMs and qMZMs, we explore the system under open boundary conditions. Our results include the study of normalized site-dependent Linear Density of States (LDOS), which locates the presence of edge states[2]. Also, we present numerical results that confirm the robustness of the obtained edge modes against disorder perturbations.

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Orbital Hall Conductivity in a Graphene/Haldane and Haldane/Haldane Bilayers

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We investigate the orbital Hall conductivity in bilayer graphene (G/G) by modifying one or both the layers as Haldane type (G/\tilde{G} : Graphene/Haldane and \tilde{G}/ \tilde{G} : Haldane/Haldane) with the inclusion of next nearest neighbour (NNN) hopping strength (t_2) and flux (φ). It is observed that the low energy bands of G/\tilde{G} and \tilde{G}/ \tilde{G} are isolated with a gap at charge neutrality with the next nearest neighbour (NNN) hopping term $t_2e^{\pm i\varphi}$. The time reversal (TR) symmetry breaking with $t_2e^{\pm i\varphi}$ induces a large orbital magnetic moment ($m_n(k)$) for the nth band in G/\tilde{G} and \tilde{G}/ \tilde{G} bilayers. This TR symmetry breaking, modulated by the t2 strength, leads to the emergence of Orbital Ferromagnetism and Valley Orbital Magnetism within the BZ for the Haldane single layer as well for both G/\tilde{G} and \tilde{G}/ \tilde{G}. We show that for the applied longitudinal electric fields, the intrinsic angular momentum (L^z) gives the orbital current ($J^{z,orb}$) along a transverse direction and generates the orbital Hall conductivity (OHC). We further show that the orbital magnetic polarity leads the Haldane single layer to Orbital Chern Insulator with the quantized OHC in the gap over the occupied bands. Moreover, the accumulation of orbital magnetic moment of the bands in Haldane graphene bilayer shows Quantum Orbital Hall Insulator and Orbital Chern Insulators.

Keywords: Bilayer Graphene, Orbital magnetization, Obital Hall conductivity.

Reference: Orbital Hall Conductivity in Bilayer Graphene, Ghosh, Sovan and Chittari, Bheema Lingam, Nov 2023. arXiv:2311.06447v1

Driven-dissipative fermionized topological phases of strongly interacting composite bosons

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We theoretically investigate the optical response of polaritons in a one-dimensional driven-dissipative Bose-Hubbard model with topological couplings. Strong correlations, accompanied by particle gain and loss can create non-trivial fermionised' non-equilibrium steady states(NESS). We observe clear signatures of Bose-Fermi mapping in the NESS and further investigate how changing experimentally controllable drive parameters can allow selective excitation of either the bulk, the edge or both, establishing non-trivial topological properties in the responses and correlations.

Quench dynamics of two-component quantum gases in optical lattice

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We explore the dynamics of a two-component Bose-Hubbard model in square optical lattice[1]. By systematically varying interspecies interactions, we obtain additional quantum phases: immiscible and miscible phases[2]. Miscible phase is a homogeneous mixture of the two components and in immiscible phase the two components separate spatially. We investigate the dynamics of the system with a focus on the distinct properties of immiscible and miscible phases using the time-dependent Gutzwiller mean field theory[3]. We quench the tunneling amplitude of the system keeping the onsite interaction fixed and study the non-equilibrium dynamics as the system evolves from Mott insulator (MI) to superfluid (SF) phase. We analyze the dynamics of the SF order parameter and study the formation of vortices. We also calculate the critical exponents to examine the physics of Kibble-Zurek mechanism[4,5]. Then we investigate how the introduction of nearest neighbor interactions affects the non-equilibrium dynamics.

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Ultracold bosons in 2D optical lattices with long-range interactions and synthetic gauge potential

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We study the effects of synthetic gauge potential on the quantum phases of an extended Bose-Hubbard model (eBHM) that describes ultracold atoms in optical lattices with long-range interactions[1,3] (nearest neighbor and next nearest neighbor). We determine the effects of gauge potential on various quantum phases using single-site mean-field theory[2]. In the model we consider inter-atomic repulsive interactions as attractive interactions makes the system unstable and leads to collapse. As the potential depth of the lattice is increased, a phase transition from superfluid to supersolid (SF-SS), supersolid to density-wave (SS-DW) and superfluid to mott insulator (SF-MI) is observed[2,3]. The introduction of artificial gauge potential enhances the quantum phases but the enhancement is not monotonic with the strength of the synthetic field. In lower values of synthetic strength there are vortices and super current in supersolid phase and superfluid phase[4].

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Abstract for QMAT 2024

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August 15, 2024

Abstract

We introduce a novel approach for detecting the rotation of persistent current in an annularly trapped Bose-Einstein condensate. Our method integrates the concepts of cavity optomechanics with atomic superfluid rotation, allowing for an in situ, in real-time, and minimally destructive detection of the condensate rotation. This is in contrast to currently used methods that completely destroy the condensate. Cavity optomechanics involves the coupling of mechanical motion to electromagnetic fields confined in resonators. By utilizing dispersive light-matter interaction, our approach facilitates minimally destructive measurements of persistent currents. Specifically, we consider a ring-trapped BEC interacting with an optical cavity mode that carries orbital angular momentum. The optical cavity induces Bragg scattering among the atoms in the condensate, leading to BEC density modulation due to the interference among different rotational states. The transmitted light from the cavity picks up these modulations, and the resulting cavity output spectrum reveals the winding number of the persistent current. We employ a mean-field stochastic Gross-Pitaevskii simulation technique to model the persistent current for weakly repulsive interatomic interactions. We also provide the first analysis of optomechanical detection of matter-wave bright soliton motion for weakly attractive atomic interactions. The cavity transmission spectra, which contain signatures of condensate rotation, are obtained. We also analyze the sensitivity of rotation measurement as a function of the system's response frequency that demonstrates the effectiveness of this optomechanical configuration as a rotation sensor, revealing that the best sensitivity of our method to the BEC rotation is three orders of magnitude better than other available proposals. Our method can have significant implications for characterizing rotating matter waves across various fields, including atomtronics, superfluid hydrodynamics, matter-wave soliton interferometry, and optomechanical sensing.

"Electric field driven conformational modifications in metal-molecule-metal junction"

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Abstract Poster Presentation

Development of next-generation organic electronic devices depends on understanding of charge transport at single molecular level. Single-molecule junctions, consisting of individual molecules sandwiched between two electrodes, are commonly used in charge transport studies. During the past few decades, rapid technical and theoretical advances have improved our understanding of charge transport phenomena and different physical properties at the atomistic limit. Importantly, in recent times, there has been a great interest in combining single-molecule junctions with different control systems to study and optimize the important physical phenomena, including planarization, folding, trans-to-cis isomerization, and so forth. Our work focuses on how electric fields affect the conformation of the molecule and consequently its impact on the charge transfer to or from the molecule.

Here we show that conformation of the benzidine molecular junction can be greatly tuned by modifying bias voltage, and this junction can have two distinct conductance states with conductance values either high or low. While high conductance states become more dominant with the rise of bias voltage. The effect is opposite for the low-conducting state. Further experiment with benzene-1,4-diamine and 4,4'-(ethyne-1,2-diyl)dianiline molecular junctions reveals no such effect. Thus, our findings demonstrate that applied bias voltage is a key factor in realizing the desirable configuration of the benzidine molecular junction. Increase in bias voltage leads to change in the dihedral angle between two phenyl rings of benzidine molecule, which might be reflected in bias-sensitive molecular conformation. Theoretical MD simulation and transport calculation also support our observation. Overall, important role of the electric field in nano electromechanics is identified through our study, which enriches our knowledge for future generation nano-electronics applications.

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Effect of spin-orbit and Rabi coupling on the modulational instability of spin-1 Bose-Einstein condensates

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August 15, 2024

In this work, we present the analytical and numerical results of the effect of spin-orbit and Rabi coupling on the collective excitation spectrum of the spin-1 Bose-Einstein condensates. We use the Bogoliubov-de-Gennes theory to obtain the collective excitation spectrum and characterize the dynamical instability regime using the modulational instability gain factor. We exhibit the eigenspectrum for ferromagnetic and antiferromagnetic interactions, showing stable, unstable, avoided crossing among the branches. The eigenvectors show the transition from density-like (in-phase) to spin-like (out-of-phase) mode and reveal spin-density mixed mode in the case of multi-band instability. Spin-flip occurs in the eigenvector component at the point of stable avoided crossing. Based on the eigenspectrum, we report modulational instability analysis in two regimes: (i) $k_L^2 < \Omega$ and (ii) $k_L^2 > \Omega$, for a specific range of interaction strengths, also for a specific range of SO and Rabi coupling strengths. The spin-orbit (SO) coupling increases the instability gain. The positive strength of Rabi coupling decreases the instability gain, while negative Rai coupling increases the instability gain. In the (i) regimes, we obtain modulation instability only if the sum of interaction strengths is attractive. To complement our analytical results, we also provide the results of the numerical simulations to study the condensate dynamics, which we achieve by quenching the weak trap strength.

Keywords: Bose-Einstein condensate, spin-orbit coupling, stable/unstable avoided crossing, modulation instability, etc.

Enhancement of localization in 2D-disordered optical lattice due to long-range interactions

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In this work, we explore the localization phenomena of ultracold quantum gases in disordered optical lattices under the influence of long-range interactions. Recent advances in experimental techniques have enabled the precise manipulation of ultracold atoms in optical lattices, where disorder and interaction play a crucial role [1]. The interplay of disorder, hopping and interactions leads to the emergence of localization [2]. We employ time-dependent Gutzwiller Mean Field Theory to study the dynamics of the system [3]. We show that an enhancement of localization occurs in the domain where the average filling factor is less than unity. However, delocalization occurs in the domain where the average filling factor is larger than unity.

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Abstract

The intricate nature of quantum correlations and entanglement in quantum many-body systems plays a pivotal role in understanding quantum phase transitions, quantum computation, and quantum communication protocols. Numerous measures have been proposed to quantify local and non-local quantum correlations, with entanglement being thoroughly studied in many quantum spin-chain models. The critical properties of $1-D$ spin-chain models have been extensively investigated in the ground state using pairwise correlations such as concurrence, quantum discord, and quantum mutual information, as well as multipartite correlations, for instance, global entanglement. In this work, we conduct an in-depth analysis of quantum correlations in exactly solvable $1-D$ three-spin cluster-like interaction models, specifically the cluster $X-Y$ model in a transverse magnetic field, known for its highly entangled cluster state in the ground state, both in the absence of a magnetic field and for various interaction strengths. We investigate bipartite and multipartite correlations in nearest neighbors and next-nearest neighbors using the measures defined above. We find that, unlike the commonly studied spin chains such as the transverse $X-Y$ model, the nearest neighbors do not exhibit any quantum correlations for any parameter values due to the non-existence of off-diagonal correlations in the Hamiltonian. However, the next-nearest pair concurrence is non-zero and shows maxima close to quantum critical points. The derivative of the pair concurrence with respect to the magnetic field h and cluster coupling strength J_y exhibits singular behavior at critical points, indicating a topological quantum phase transition. Similar behavior is observed in quantum discord and quantum mutual information. However, the multipartite measure of global entanglement does not exhibit any singular behavior at the critical points. Additionally, three-spin correlations are investigated, showing maximal correlations for the cluster state.

Frustrated spin-1/2 model on kagome strip chain: An analogy to Kugel Khomskii model

The discovery of quantum spin liquids (QSL) in frustrated magnetic materials has sparked significant interest in the realm of quantum magnetism. Among the promising candidates for QSL, the Kagome strip chain (KSC) stands out. These system exhibits different exotic phases such as magnetization plateaus [1], quantum spin liquid [2]. In this study, we delve into the ground state quantum phases of a frustrated antiferromagnetic Heisenberg spin-1/2 model Hamiltonian on a KSC (Fig. 1), which is a one-dimensional counterpart of the Kagome lattice. We map out the quantum phase diagram within the two-dimensional exchange parameter space of this system.

The KSC's isolated unit cell, comprising five spin-1/2 particles, gives rise to three unique magnetic states: a spin-3/2 state, a spin-1/2 state with an orbital degree of freedom, and a spin-1/2 state with dimerized base spins. These states emerge based on the exchange ratio within the unit cell. To explore the ground state properties, we employ exact diagonalization and density matrix renormalization group methods, revealing five distinct quantum phases.

Among these, two types of dimerized ground states are particularly intriguing due to their inversion symmetry-breaking, resulting in doubly degenerate ground states. Phase III showcases gapless spin excitations, while Phase IV features a small but finite spin gap arising from translation symmetry breaking. The other phases are characterized by gapless spectra and antiferromagnetic quasi-long-range order in the central spins. Specifically, Phase I displays a spin-3/2 state, and in Phase II, neighboring unit cell base spins form singlet dimers. In Phase V, the base spins create strong singlet dimers, with the central spin-1/2 forming an isotropic effective spin-1/2 chain.

Furthermore, we develop an effective model incorporating both spin-1/2 and orbital degrees of freedom, reminiscent of the Kugel-Khomskii model [3], but with highly anisotropic orbital interactions. This comprehensive investigation advances our understanding of quantum magnetism and the potential realization of QSL in Kagome strip chains.

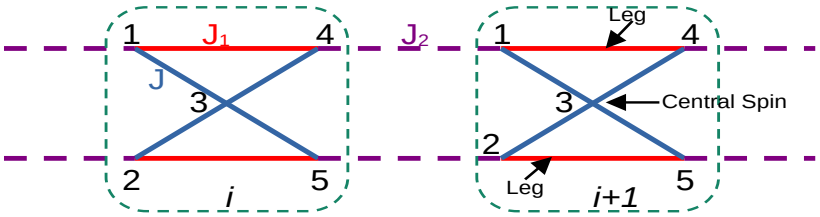

Fig 1 : Structure of KSC with their interactions

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Magneto-elastic coupling effect in Co_2FeAl Heusler alloy deposited on flexible polyimide.

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Spintronics has garnered significant attention since its inception, prompting numerous research groups to focus on developing spin-related electronic devices. Recently, there has been a high demand for flexible and wearable devices due to their exceptional potential in practical applications [1,2]. However, in order to develop flexible spintronic devices, materials with high spin polarization are highly desirable. Heusler alloys have become prominent in spintronics due to their high spin polarization and elevated Curie temperature and low magnetic damping. Among half-metallic materials, Co-based Heusler alloys, such as Co_2FeAl (CFA), typically exhibit high Curie temperatures compared to oxide half-metals, making them promising candidates for spintronics applications at room temperature [3]. The magnetoelastic properties of Heusler alloys are not well understood, despite their potential to undergo high strains when used in flexible devices. For a magnetic material grown on flexible substrates, the substrate deformation induces a tensile or compressive strain to the magnetic layer, which may change its magnetic anisotropy. In this work we studied the magneto mechanical coupling effect under various compressive and tensile strains generated by inward and outward bending of the films. The coercivities were adjusted by applying strains along the easy or hard axes of the Co_2FeAl films. The results indicate that the easy axis can be converted to the hard axis and vice versa for application of compressive strain. This work demonstrates that it is possible to rotate the magnetic anisotropy by 90 degrees simply by changing the direction of curvature, thereby switching the film from uniaxial tension to uniaxial compression and vice versa.

Keywords: Flexible spintronics, Magneto-elastic Coupling, Heusler alloy, Anisotropy

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Phase diagram of disordered extended Bose-Hubbard model

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Abstract

Dipolar atoms, molecules, and Rydberg atoms have long-range interactions and are suitable to study the effects of long-range interactions in optical lattices [1,2]. In these systems disorder can be introduced using speckle lasers [3] to simulate condensed matter systems with impurities. Dipolar atoms loaded in disordered optical lattices can be described using disordered extended Bose-Hubbard model [4,5]. This model exhibits six quantum phases: Mott insulator, Bose glass, supersolid, superfluid, disordered solid and checkerboard density wave. We use the single-site Gutzwiller mean-field theory [6] to study the phase diagram of the model for different disorder strengths. We also study the phase diagram by introducing nearest neighbour and next-nearest neighbour long-range interactions [1,2]. The quantum phases can be distinguished from each other using different order parameters [4].

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Understanding the Dynamics and Correlations of Intralayer Moiré Excitons in WSe_2/WS_2 Heterostructure

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Vertical stacking of two-dimensional layered material having slight lattice mismatch and small relative twist angle provides a large periodic moiré superlattice. The spatially modulated moiré potential can influence the behaviour of electrons and holes in the supercell and modulate the bandgap of the system. Recent studies on moiré superlattices of transition metal dichalcogenides (TMDCs) reveal their potential role for studying exotic quantum phases like tunable Mott insulating states, Wigner crystal, moiré polarons and offer new avenues to explore correlated excitonic physics.

In a WSe_2/WS_2 heterostructure, due to type II band alignment of stacked layers, ultrafast charge transfer occurs between the layers and results in intralayer and interlayer exciton states. Recent observations show multiple intralayer moiré excitons near resonance of WSe_2 A exciton in nearly aligned WSe_2/WS_2 heterostructure [1], with different moiré states exhibiting distinct characters such as Wannier-type exciton and charge-transfer exciton [2]. However, the fundamental microscopic understanding of the dynamical behaviour and correlation amongst these moiré intralayer excitons remains elusive. In this work, we study the dynamics of intralayer moiré exciton states (and exciton-exciton correlations) in a nearly aligned WSe_2/WS_2 heterostructure using broad-band white-light absorption spectroscopy and time-resolved two-colour pump-probe measurements. We find modified dynamics for different exciton states and find signatures of coupling. Our study experimentally confirms the distinct nature of site-dependent moiré intralayer states and provides the understanding of unexplored non-equilibrium correlation among these moiré excitonic species.

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Layered Growth of 2D Magnetic Material

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Two-dimensional (2D) magnetic materials have emerged as an exciting frontier for fundamental research and in a wide range of applications, including spintronics and magnetic storage devices. They exhibit intriguing properties, including layer-dependent magnetic behaviour; for example, $CrCl_3$, in the monolayer limit, behaves as a ferromagnet (FM), while, in the bilayer limit, it is an antiferromagnet (AFM)[1]. Additionally, they have a tunable magnetic anisotropy aided by the application of strain or dopant intercalation[2]. These fascinating properties, among others of 2D magnetic materials, have enabled the demonstration of isolated high-performance devices. However, to incorporate these 2D magnetic materials in application-relevant devices, the development of large-scale growth processes for them is critical.

We perform the Physical Vapour Transport Deposition (PVTD) growth of atomically thin $CrCl_3$, which provides unique advantages of thickness control and scalability over the conventional method, i.e., exfoliation of the bulk crystal[3]. PVTD can also allow the in-situ doping of the grown flakes by the introduction of dopants during the growth process, as well as the tunability of the strain by varying substrates and/or quenching speeds. We report the large-scale synthesis of 2D $CrCl_3$ flakes over different substrates, i.e., amorphous SiO_2/Si, crystalline Sapphire, and crystalline fluorophlogopite mica (F-Mica) substrates. Large-scale growth with the signature of directional epitaxy and growth down to atomic thickness are observed on the crystalline F-Mica substrate. In addition, thin faceted growths have also been demonstrated on amorphous SiO_2/Si and crystalline Sapphire (Al_2O_3) substrates. Additionally, the deposition temperature has been identified as the control knob for the thickness of the as-grown flakes. Raman and Photoluminescence spectroscopy confirms the $CrCl_3$ growth. Scanning Electron Microscopy – EDS (Energy Dispersive X-ray spectroscopy) additionally confirms the stoichiometric chemical composition. Magnetic Force Microscopy (MFM) is done to study the magnetic properties of the as-grown flakes. In conclusion, we demonstrate, for the first time, a systematic method to grow large-scale 2D magnetic materials, which could pave the way for their potential incorporation into technologies and for creating highly tunable materials.

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Competing topological phases in a non-Hermitian time-reversal symmetry-broken Bernevig-Hughes-Zhang model

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The Bernevig-Hughes-Zhang (BHZ) model is one of the most celebrated examples of a quantum spin Hall (QSH) insulator exhibiting helical edge states characterized by a Z_2 invariant. The Z_2 topology is primarily protected by the presence of time reversal symmetry (TRS) in the system which is responsible for the robustness of the helical states. In the presence of an in-plane magnetic field, which breaks TRS, these first-order helical states gap out to be replaced by second-order corner states under suitable open-boundary conditions. Here, we show that the inclusion of a spin-dependent non-Hermitian balanced gain/loss potential, in addition to the in-plane magnetic field, induces a competition between the first and second-order topological phases. We observe that the first-order helical edge states that were gapped out in a nanoribbon geometry, resurface as the non-Hermitian effect intensifies, effectively neutralizing the role played by the magnetic field. By employing the projected spin spectra and the spin Chern number, we conclusively explain the resurgence of the first-order topological properties in the time-reversal symmetry-broken BHZ model in presence of non-Hermiticity. Finally, the biorthogonal spin-resolved Berry phase, exhibiting a non-trivial winding, definitively establishes the topological nature of these revived edge states, emphasizing the triumph of non-Hermiticity over the magnetic field.

Room-temperature topological phase transition with Pierl's instability in a quasi-one-dimensional Bi_4I_4

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Higher-order topological insulators emerged as an extension to the traditionally existing domain of topological insulators with symmetry-protected states in edges or corners. Pristine Bi_4I_4 is a unique quasi-1-dimensional candidate with the simultaneous existence of edge/hinge modes [1]. We report resistance fluctuation dynamics at the very vicinity of room temperature topological phase transition from α-Bi4I4 (hinge modes) to β-Bi4I4 (surface states) mediated by the thermodynamically first-order structural transition inferred from differential Scanning Calorimetry. Inter-band transition is identified from the temperature-dependent Seebeck study. It is also established from the crystal structure that there is Pierl's instability in the α-phase along the c*(2b-a)-axis direction. On the other hand, in β -phase there is no such distortion. The phase transition is accompanied by enhanced fluctuations in resistance fluctuations with spectral weight shifting to lower frequencies. Additionally, we identify a coexisting meta-stable phase from time-series resistance fluctuations and their inherent bi-modal distributions. This has been identified as Random Telegraphic Noise (RTN) [2,3]. This nature in the time domain resistance fluctuation is observed at around 306.8K, a bit prior to the phase transition that suggests a metastable phase persisting in the hysteretic domain of the resistivity curve. At the very vicinity of the phase transition (~309.3K) where the system transitions from α to β, we have observed a distinct nucleation like resistance does remain in a stable value rather it keeps falling to the lower resistive state in the same time duration of measurement suggesting an unstable equilibrium state. A shift in mean value of the probability distribution function also indicates the abruptness of the phase transition.

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Progress in Next-Generation Biomedical Implants through Pulsed Laser Deposition Surface Coatings

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Biomaterials are generally designed to integrate seamlessly with biological systems, causing minimal adverse tissue reactions. The development of bioactive coatings for orthopedic implants is essential for improving osseointegration and ensuring the longevity of implants. Recent advancements in biomedical science advocate incorporating electrically active coatings into implants, promising improved in-vivo performance. This interest arises from the noted benefits of pulsed electromagnetic stimulation in accelerating fracture healing. In this research, pulsed laser deposition (PLD) has been utilized for the deposition and analysis of composite coatings composed of 80 At.% potassium sodium niobate (KNN) and 20 At.% hydroxyapatite (HAP) onto titanium (Ti) substrates. The basic aim of choosing the ceramic composite is because of enhanced electrical and biological properties. Titanium (Ti) implants are widely used in biomedical applications due to their excellent mechanical properties and biocompatibility. However, they face significant limitations, including poor wear resistance, potential for corrosion, and suboptimal osseointegration, which can lead to implant failure. To overcome these challenges, bioceramic composite coatings have emerged as a promising solution, offering superior surface properties that enhance biological interactions.

This study investigates the multifunctional properties of bioceramic coatings designed to improve cell adhesion, biocompatibility, surface potential, roughness, and wettability behaviour which are critical for successful implant integration. The coatings were characterized using a combination of techniques, including band gap analysis, photoluminescence spectroscopy, X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS), to evaluate their structural and optical properties. Surface potential measurements were conducted to understand the influence of surface charge on cell interactions. The study uncovered a significant relationship between the films' dielectric properties and protein adsorption behaviour, as assessed with bovine serum albumin (BSA), highlighting the critical role of film surface roughness in tuning protein interactions.

In vitro biocompatibility tests, including cell adhesion studies, demonstrated that the surface modifications significantly enhanced cell proliferation and attachment, highlighting the potential of these coatings for tissue engineering applications. Additionally, wettability studies revealed a strong correlation between surface hydrophilicity and cell adhesion, with coatings exhibiting enhanced wettability showing superior cell compatibility. The results suggest that tailoring the surface properties of bioceramic coatings can lead to optimized performance in biomedical implants, offering a promising approach to improving the integration and longevity of these materials in biological environments.

Higher order gaps in the renormalized band structure of doubly aligned hBN/bilayer graphene moiré superlattice.

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Abstract

Heterostructures of graphene encapsulated between two thin, rotationally misaligned hBN flakes form a stimulating platform for probing topological phases of matter [1]. The difference in the lattice constants of hBN and graphene and the angular misalignment between the layers generate two distinct long-wavelength moiré superlattices at the top and bottom interfaces of graphene with hBN [2]. In this work, we present our findings on the recursive band gap engineering of chiral fermions in bilayer graphene doubly aligned with hBN [3]. By utilizing two interfering moire potentials, we generate a super moiré pattern that renormalizes the electronic bands of the pristine bilayer graphene, resulting in higher-order fractal gaps even at very low energies. These Bragg gaps can be mapped using a unique linear combination of periodic areas within the system. To validate our findings, we used electronic transport measurements to identify the position of these gaps as functions of the carrier density and establish their agreement with the predicted carrier densities and corresponding quantum numbers obtained using the continuum model, as shown in Fig.1. Our work provides direct experimental evidence of the quantization of the area of quasi-Brillouin zones in super moiré systems [4]. It fills essential gaps in understanding the band structure engineering of Dirac fermions by a recursive doubly periodic superlattice potential.

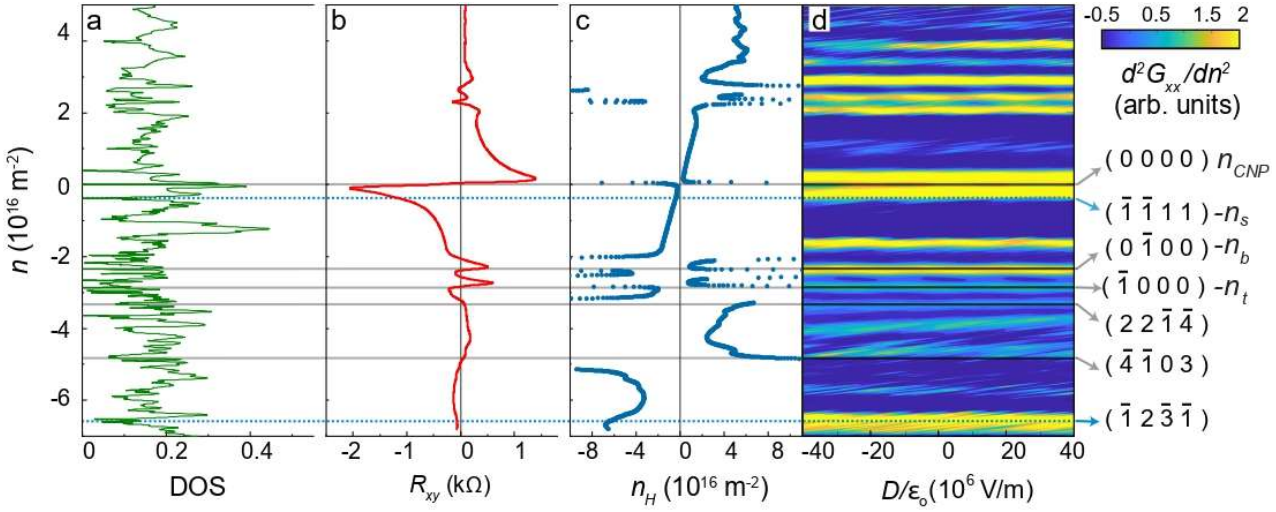

Figure 1. Experimentally obtained and theoretically calculated Bragg gaps. (a) Plot of the calculated density of states (DOS) for $\theta_b = 0.026°$ and $\theta_t = 0.44°$. Horizontal lines represent prominent dips in the DOS. (b) Plot of transverse resistance R_{xy} versus n measured at B = 0.7 T and T = 2 K. (c) Plot of hall carrier density n_H versus n. (d) Map of the normalized d^2G_{xx} (B = 0)/dn^2 in the n − D plane; the data have been plotted on a logarithmic scale. The quantum numbers of the Bragg gaps are marked on the right.

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Nonlinear electrical transport unveils Fermi surface malleability in a moiré heterostructure

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Graphene moiré superlattices host van Hove singularities appear at low energies, which are malleable with progressive band filling, leading to a sequence of Lifshitz transitions and resets observable in Hall measurements. However, at zero magnetic fields, transport measurements in the linear response regime have limited sensitivity to the band's topology. Here, we probe these unique features in twisted bilayer graphene at zero magnetic field using second-order transport measurements. We demonstrate that the nonlinear responses, induced by the Berry curvature dipole and extrinsic scattering processes, intricately map the Fermi surface reconstructions at various partial fillings of the band. Importantly, our study confirms that the applied magnetic field does not induce or stabilize the probed transitions, highlighting these features as intrinsic to the moiré bands. Additionally, we show the tunability of the Berry curvature dipole and extrinsic scattering process with an out-of-plane electric field near the conduction band edge. Beyond corroborating the insights from linear Hall measurements, our findings establish nonlinear transport as a pivotal tool for probing band topology and correlated phenomena.

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Low temperature Electrical and Thermal transport studies of 4H-$NbSe_2$ crystals

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Abstract

Transition metal dichalcogenides (TMDCs) have the formula MX_2, where M is a transition metal like V, Nb, or Ta, and X is a chalcogenide such as S, Se, or Te.These materials are known for their layered structures and interesting properties, including charge density waves (CDW) and superconductivity [1,2]. This study focuses on 4H-$NbSe_2$ which is a polymorph of well known 2H-$NbSe_2$ [1,3]. We have synthesized both polycrystalline and single-crystal forms of 4H $NbSe_2$. The polycrystalline material was obtained using a solid-state chemical reaction [1,2], while the single crystals were grown using the chemical vapor transport method with iodine as a transport agent. Structural characterization through powder X-ray diffraction (XRD) confirmed the phase purity and hexagonal nature of the samples. We performed temperature-dependent measurements of electrical resistivity and the Seebeck coefficient at low temperature. Our findings revealed a superconducting transition at T ~ 6.4 K. Evidence from Seebeck coefficient measurement suggests the possibility of CDW transition at ~ 43 K. We'll present detailed electrical and thermal transport properties of the 4H- NbSe2. These studies have the potential to advance our understanding of its potential applications in quantum technologies and thermoelectrics.

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Efficient and Affordable Fabrication of Low Entropy Oxide: Exploiting Dual Band Gap Characteristics for Future Optoelectronic Devices

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Abstract: Considering the extraordinary physicochemical properties of the high entropy oxides and their tremendous potential in various applications, in this study, we present a novel Low Entropy Oxide (LEO) material exhibiting uniquely both direct and indirect band gaps within a single material. This report demonstrates and explains the successful formation of single-phase chemically homogeneous $(NiMn)_3O_4$ LEO with spinel ($Fd\bar{3}m$) structure and configurational entropy less than 1 R. The X-ray photoelectron spectroscopy (XPS) study of $(NiMn)_3O_4$ reveals the charge compensation mechanism that underlies the structural change. These LEOs can be suitable candidates for future applications in advanced optoelectronic devices and energy systems.

1. INTRODUCTION

Entropy-stabilized oxides (ESOs) have become increasingly recognized in materials science and condensed matter physics for their complex structures and tunable functional properties. The discovery of the (CuCoMgNiMn)O HEO by Rost et al. [1] was a turning point in the investigation of High Entropy Oxides (HEOs), and it significantly sped up interest in these materials. Most research on Entropy-Stabilized Oxides (ESOs) has focused on systems with five or more cations in a single lattice, leaving a significant gap between mono-cation and penta-cation oxides. Hence, there exists a valuable opportunity to explore the novel properties of ESOs by varying the number and types of cations used. On the other hand, the coexistence of both direct and indirect band gaps within a very useful range in a material is a unique and valuable property. The direct band gap allows for efficient light absorption and emission, which is ideal for LEDs and lasers, while the indirect band gap enhances carrier mobility, benefiting electronic devices. This dual nature offers substantial potential for optoelectronic applications [2], such as photocatalysis, solar cells, thermoelectric devices, and photodetectors.

2. EXPERIMENTAL DETAILS

The equimolar proportion of high-quality NiO and MnO were milled for 30 hrs in an argon atmosphere with a ball-to-powder ratio of 10:1. Then, the as-milled powder was annealed at 800 ºC for 12 hrs in an air atmosphere followed by slow cooling. The structural analysis was carried out using an X-ray diffractometer. Morphological analysis was done by using FESEM. XPS was employed to evaluate the electronic states of elements in the films. Optical properties were characterized using Uv-Vis Spectroscopy.

3. RESULTS AND DISCUSSIONS

Room temperature XRD pattern (as shown in Fig. 1a) reveals that the final LEO sample matched with spinel structure [M(=Ni, Mn)$_3$O$_4$ type structure, space group $Fd\bar{3}m$, group number 227, where M is a metal]. The same phase appears when the milled sample is annealed at 900 ºC. Further, the LEO exhibits an interesting particle morphology (see Fig 1(b)). Though the parent oxides have only a 2^+ cationic state, the existence of both 2^+ and 3^+ states in 2*p* XPS spectra of Ni and Mn justifies the formation of Fe_3O_4 like spinel structure with both 2^+ and 3^+ cationic states. After extrapolating the Kubelka-Munk function obtained from the reflectivity measurements (Figs. 1e and 1f), it was determined that the LEO has a direct band gap of 1.60 eV in addition to an indirect band gap of 0.64 eV.

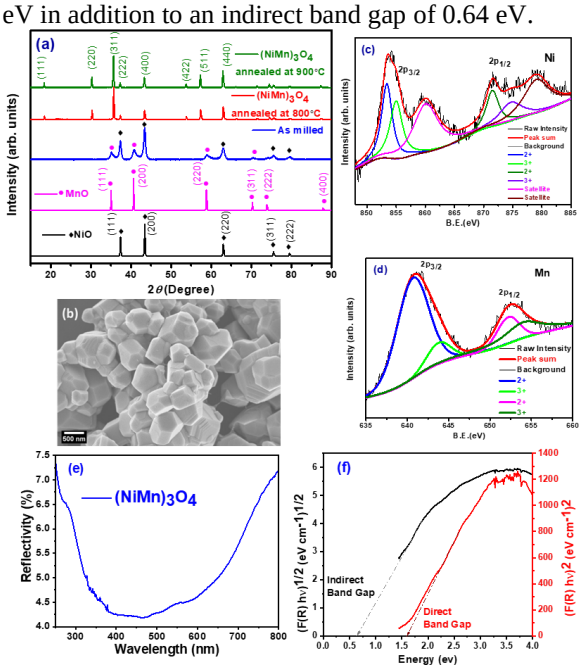

Fig.1(a) Room temperature XRD patterns of parent oxides, milled NiO-MnO sample, and the LEO. (b) FESEM image of $(NiMn)_3O_4$ LEO. (c) and (d) XPS Ni 2*p* and Mn 2*p* spectra of LEO. (e) Reflectivity vs Wavelength plot. (f) Kubelka-Munk plot (Direct and indirect band gap) of $(NiMn)_3O_4$.

4. CONCLUSIONS

The easy, affordable synthesis and dual-band gap characteristics of this LEO position it as a strong candidate for future exploration in diverse applications in advanced optoelectronic devices and energy systems.

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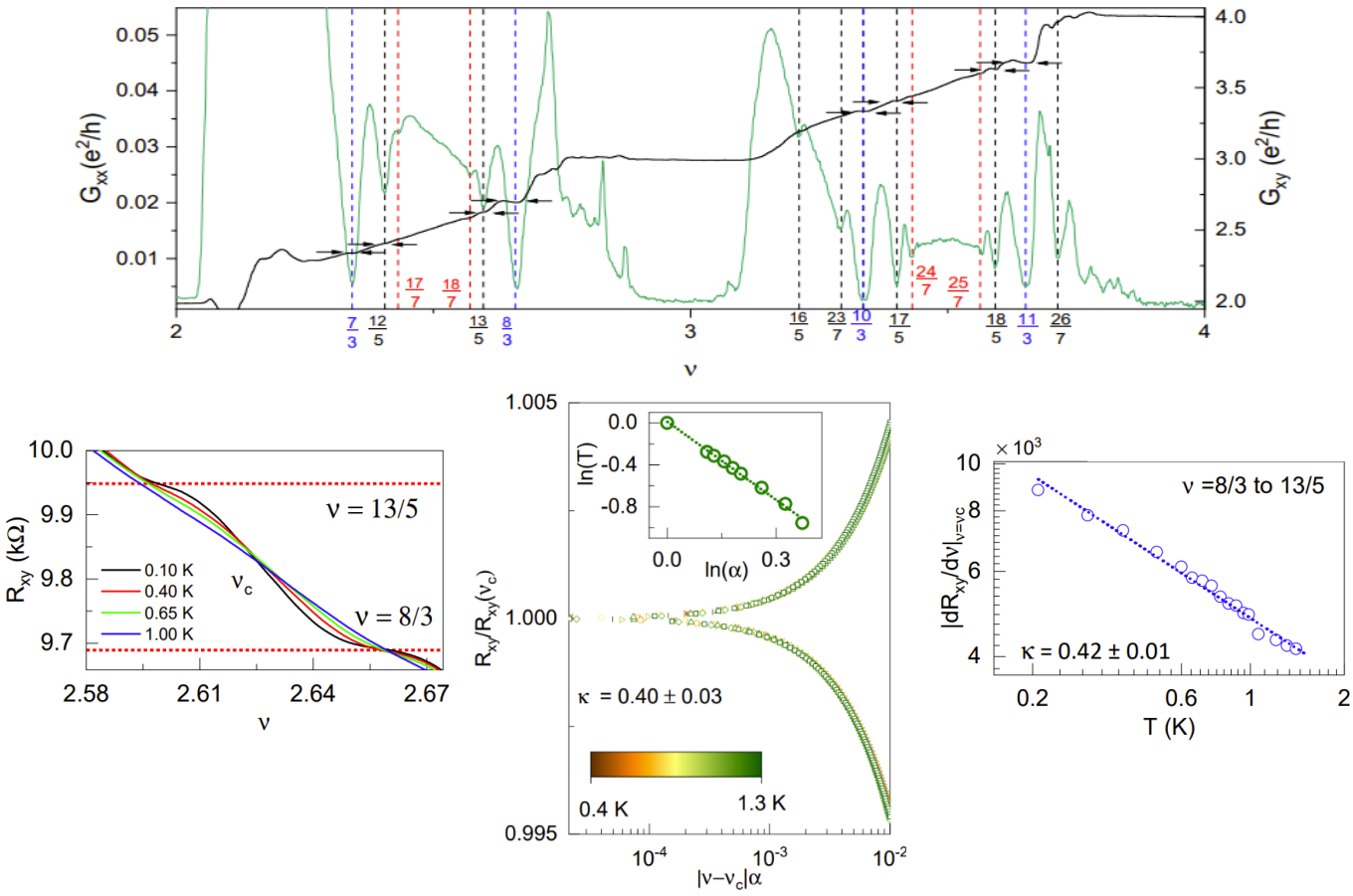
Universality of Quantum Phase Transitions in the Integer and Fractional Quantum Hall Regimes

Quantum Hall Regimes Fractional quantum Hall (FQH) phases emerge due to strong electronic interactions and are characterized by anyonic quasiparticles, each distinguished by unique topological parameters, fractional charge, and statistics. In contrast, the integer quantum Hall (IQH) effects can be understood from the band topology of non-interacting electrons. We report a surprising super-universality of the critical behavior across all FQH and IQH transitions. Contrary to the anticipated state-dependent critical exponents, our findings reveal the same critical scaling exponent κ = 0.41 ± 0.02 and localization length exponent γ = 2.4 ± 0.2 for fractional and integer quantum Hall transitions. From these, we extract the value of the dynamical exponent z ≈ 1. We have achieved this in ultra-high mobility trilayer graphene devices with a metallic screening layer close to the conduction channels. The observation of these global critical exponents across various quantum Hall phase transitions was masked in previous studies by significant sample-to-sample variation in the measured values of κ in conventional semiconductor heterostructures, where long-range correlated disorder dominates. We show that the robust scaling exponents are valid in the limit of short-range disorder correlations



Coupled electron-phonon dynamics in polar semiconductors: A first-principles Boltzmann transport approach

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The energy transport properties of materials such as the thermal conductivity, the electronic mobility and the Seebeck coefficient are strongly dependent on the interactions among elementary energy carriers - electrons and phonons. The physics of coupled electron-phonon transport is of primary interest to study various phenomena such as superconductivity, thermoelectricity, phonon drag and hydrodynamic transport [1]. Here, we present an efficient computational tool to obtain a full numerical solution of the coupled electron-phonon linearized Boltzmann transport equation (BTE) to predict the energy transport properties in polar semiconductors such as GaAs, GaN and BAs. We focus on low temperatures, where the momentum-conserving collisions among phonons and electrons - the Normal processes - dominate over the momentum-dissipating collisions - the Umklapp processes, thus necessitating the development of an iterative scheme to fully solve the coupled BTE beyond the commonly used relaxation time approximation (RTA). In our approach, we allow the phonon and the electron system to go out of equilibrium, unlike many of the previous approaches that assume that the phonons remain in equilibrium while calculating the transport coefficients [2]. We address the computational complexity involved in these calculations by constructing two different discretizations of the Brillouin zone for electrons and phonons respectively, that enabling us to selectively refine the regions of the electronic and the phononic Brillouin zones of interest, depending on the temperature and the number density of electrons under consideration. From our calculations, we find that the effect of phonon drag on the phonon thermal conductivity is relatively weak in GaAs, GaN and BAs at all temperatures. However, there is a giant enhancement in the absolute value of the Seebeck coefficient at low temperatures, driven by the phonon drag effect, in all of these materials. Our approach enables a rapid, yet accurate evaluation of thermal, electrical and thermoelectric transport coefficients in doped semiconductors at a fraction of the computational cost, compared to the approaches available in the literature [3,4].

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First principles prediction of anharmonic phonon lineshapes and free energies in alkali halides beyond the quasiharmonic approximation

Ashita K. Baburaj and Navaneetha K. Ravichandran

Abstract

The quasiharmonic model provides insights into energy transport mechanisms and accurately predicts the thermodynamic and thermal properties of semiconductors and insulators at low temperatures. However, it overlooks phonon-phonon interactions, which become increasingly significant as temperature rises [1]. Here we show that the incorporation of anharmonic (cubic and quartic) terms into the crystal potential energy from first principles enables us to accurately capture the vibrational thermodynamics of phonons at elevated temperatures. This fourth-order anharmonic theory offers improved predictions of the thermal and thermodynamic properties of materials, while its effects at lower temperatures remain consistent with the quasiharmonic theory.

We demonstrate the predictive power of this fourth-order anharmonic first principles theory by applying it on alkali halides such as NaCl, which are ionic crystals with strong anharmonicity owing to their weak bonding. We find that the inclusion of higher-order terms in crystal potential energy at higher temperatures is necessary for accurately predicting the phonon free-energy and, consequently, the thermodynamic properties. In these calculations, we account for anharmonic effects through perturbation theory as well as employ phonon renormalization techniques developed recently [2]. We calculate phonon frequencies, line shapes observed in inelastic neutron scattering experiments and the anharmonic free energy for various phonons modes within the Brillouin zone to quantify the effect of the higher-order anharmonic terms of the crystal potential on individual phonon modes. Using these phonon-specific properties, we quantify the large effect of the crystal anharmonicity on several important thermodynamic quantities such as the Grüneisen parameter, the coefficient of thermal expansion, and the heat capacity. In particular, we analyze the temperature-dependent changes in the Grüneisen parameter, derived from mean fractional energy shifts [3], to elucidate the impact of anharmonicities on thermal properties—an effect inadequately described by the quasiharmonic model alone. Our predictions from this new fourth-order anharmonic thermodynamics framework compare favourably with the experimental data on phonon lineshapes and heat capacity available in the literature over a broad temperature range, thus confirming the need for going beyond the commonly used quasiharmonic approximation.

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Enhancement of superconductivity in Zr_2S_2C arising from phonon softening on transition from bulk to monolayer

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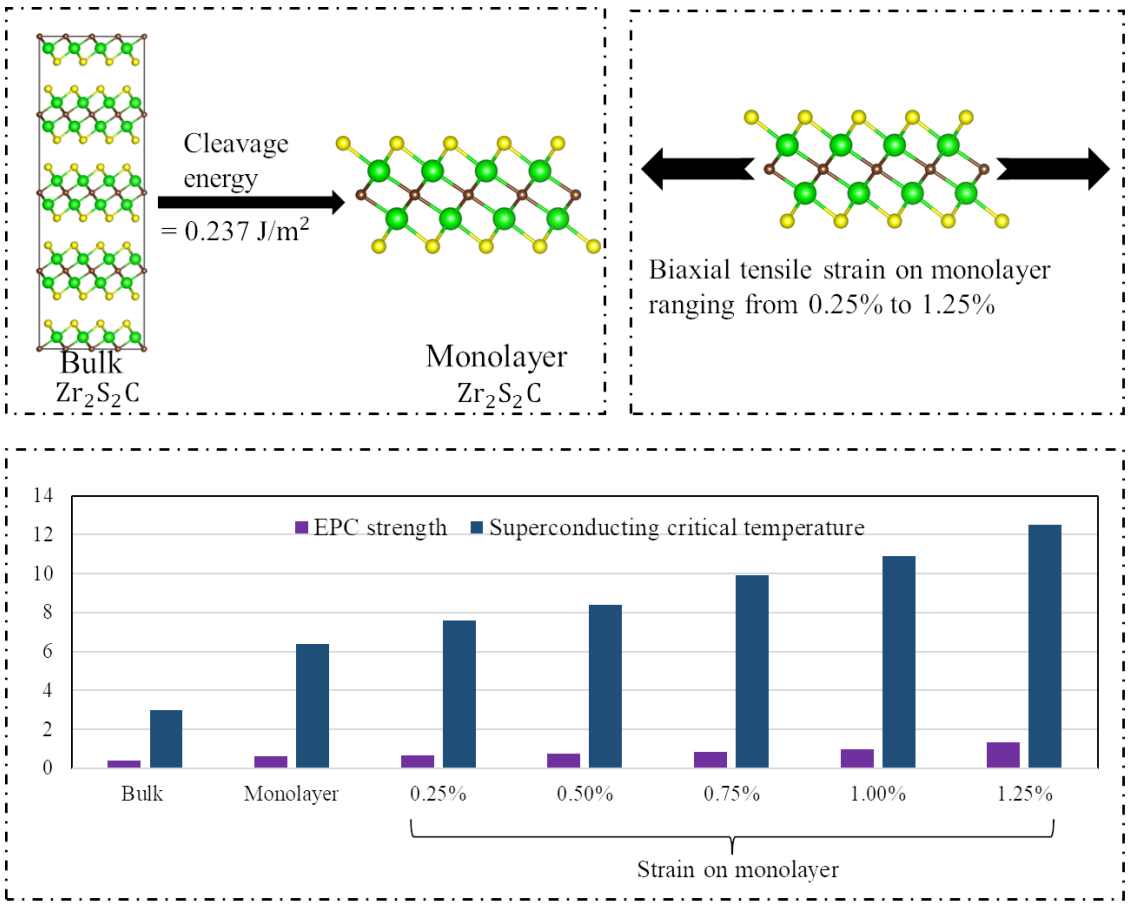
We report a new compound, Zr_2S_2C, belonging to the transition metal carbo-chalcogenide (TMCC) family. Through first-principles calculations, our analysis of phonon dispersion spectra indicates that the compound is dynamically stable in both bulk and monolayer forms. We systematically investigated the electronic structure, phonon dispersion, and electron–phonon coupling (EPC) driven superconducting properties in bulk and monolayer Zr_2S_2C. The results demonstrate the metallic character of bulk Zr_2S_2C, with a weak EPC strength (λ) of 0.41 and superconducting critical temperature (T_c) of ~3 K. The monolayer Zr_2S_2C has an enhanced λ of 0.62 and T_c of ~6.4 K. The increased λ value in the monolayer results from the softening of the acoustic phonon mode. We found that when biaxial strain is applied, the low energy acoustic phonon mode in monolayer becomes even softer. This softening leads to a transformation of the Zr_2S_2C monolayer from its initial weak coupling state (λ = 0.62) to a strongly coupled state, resulting in an increased λ value of 1.33. Consequently, the superconducting critical temperature experiences a twofold increase. These findings provide a theoretical framework for further exploration of the layered two-dimensional TMCC family, in addition to offering valuable insights.



Investigating Magnetocaloric Properties and Magnetic Anisotropy 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 generalised 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.

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Effect of W doping on Structural, Dielectric and Magnetic properties of Co-Zn Spinel Ferrites

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Abstract

Due to its high coercivity, large magneto-crystalline anisotropy, low eddy current loss, high electrical resistivity, moderate saturation magnetization, and high dielectric constant, Co-Zn spinel ferrites have huge application in modern technology like high frequency device, magnetic switches, biosensors, satellite communication, read-write head of high speed digital tapes, etc. Apart from this, doping different rare earth ion and transition metal ion induces them to exhibit considerably more interesting behavior. In this work, we have doped different percentage of tungsten (W) on Fe site of Co-Zn spinel ferrites ($Co_{0.65}Zn_{0.35}Fe_{2-x}W_xO_4$; x = 0.0, 0.1, 0.2). All the polycrystalline samples have been prepared using conventional solid-state reaction method. The structural analysis, performed using high resolution X-ray diffraction and Rietveld refinement, confirmed the formation of a single-phase cubic inverse spinel structure with space group Fd3m with slight lattice parameter expansion upon W doping. This reduction is attributed to the larger ionic radius of W^{6+} ions substituting the Fe^{3+} ions in the lattice. Based on the FESEM analysis of the samples, we can say that the grain size is getting bigger as the W doping concentration goes up. Dielectric measurements are carried out over a wide range of frequencies (100 Hz to 10 MHz) and temperatures. The dielectric constant (ε') showed a decrease with increasing W content, which can be explained by the Maxwell-Wagner model of interfacial polarization. The loss tangent (tan δ) exhibited a similar decreasing trend, indicating reduced energy losses in the W-doped samples. The magnetic properties, analyzed using a vibrating sample magnetometer (VSM), revealed that saturation magnetization (Ms) decreased with increasing W content but Curie temperature (T_C) increased with doping W. This decrease is due to the non-magnetic nature of W^{6+} ions replacing magnetic Fe^{3+} ions, leading to a dilution of the magnetic sublattices. In conclusion, W doping in Co-Zn spinel ferrites significantly influences their structural, dielectric, and magnetic properties.

Efficient Ultrathin Solar Cells Based on TiS_3-NbS_3 Van der Waals Hetero-surface

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Abstract:

The pursuit of the ideal solar cell design is a cornerstone of progress in the photovoltaic industry. A promising approach lies in the development of ultrathin two-dimensional (2D) materials, arranged in Van der Waals (vdW) heterostructures, which offer exceptional interfaces for the efficient separation and transfer of photoinduced charge carriers—crucial for the generation of photocurrent.This study delves into the potential of hetero-interfaces formed from monolayers of **TiS_3** and **NbS_3**. We systematically analyze three distinct stacking configurations (AA, AB, AB') through comprehensive electronic structure calculations using Density Functional Theory (DFT). Our hybrid functional computations, carried out with the **GPAW** code, a real-space grid-based electronic structure program—reveal that **TiS_3** monolayers exhibit direct bandgap semiconducting behavior with an approximate bandgap of ~1.2 eV. In stark contrast, **NbS_3** emerges as a metallic compound, highlighting its potential to serve as a pivotal component in Schottky Barrier Solar Cells (SBSC).The pronounced optical absorption of **TiS_3** in the visible light spectrum, combined with its high carrier mobility, positions it as a strong contender for next-generation photovoltaic technologies. These attributes suggest that **TiS_3** could achieve remarkable power conversion efficiency (PCE), thereby opening new avenues for advanced solar energy devices. Moreover, our theoretical framework provides critical insights into key photovoltaic parameters—such as open-circuit voltage, short-circuit current, Schottky barrier height, and work function, ensuring a thorough evaluation of these materials for their performance in solar cell applications.

Keywords: Schottkybarrier solar cell, van der Waals, DFT, optical absorption.

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Flexible Near-Infrared Plasmon-Polaritons and Electronic Transport in Scandium Nitride

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As device technologies continue to miniaturize, it is crucial to understand and engineer the electronic properties of semiconductors at the nanoscale. Scandium nitride (ScN), an emerging rocksalt indirect bandgap semiconductor, has garnered significant interest due to its promising applications in thermoelectrics, plasmonics, neuromorphic computing, and Schottky barrier devices. However, a comprehensive understanding of electronic transport, carrier scattering mechanisms, and optical properties in ultrathin ScN films remains lacking. Our findings shed light on the impact of surface scattering in these ultrathin ScN films, which could lead to more efficient miniaturized devices. Additionally, the flexibility and near-infrared plasmonic properties of ScN expand its potential applications in photonics and bio-photonics, including antifogging, smart windows, and bioimaging. van der Waals heteroepitaxy, a technique for growing strain- and misfit-dislocation-free flexible epitaxial films on layered substrates, has enabled the deposition of polaritonic ScN heterostructures on fluorophlogopite-mica (F-mica) substrates using molecular beam epitaxy. These heterostructures are the first semiconducting nitrides to exhibit plasmon resonance within the biological transmission window of 1200-1300 nm. Remarkably, the optical properties of these ScN structures remain stable even after being bent over 100 times or heated to 500°C. Developing low-cost, high-quality, flexible yet refractory plasmonic ScN heterostructures for the near-infrared spectral range could revolutionize flexible optics and bio-photonic devices. The unique properties of ultrathin, flexible, and CMOS-compatible ScN make it highly efficient for modern device applications.

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Optical control of multiple resistance levels in graphene for memristic applications

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Neuromorphic computing has highlighted components such as memristors, neural processing units, and threshold switches, which mimic the behavior of biological synapses and neurons. A memristor is a fundamental electronic component whose resistance depends on the charge that has flown through it; it is a resistor with a memory. Hexagonal boron nitride (h-BN)/Graphene heterostructures can be optically doped using visible light and electrostatic gating. h-BN has a wide band gap (6eV) and many intermediate defect states in the visible range. Violet light excites electrons in the valence nitrogen state of h-BN, which can subsequently be transferred to graphene via electrostatic gating. We used this technique to achieve high electron doping densities in graphene, where doping levels can be controlled by the illumination time or the back gate voltage, thereby creating memristors with multiple resistance levels.

Tuning the Properties of MnAl Alloy for Rare Earth Free Magnet Applications

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Abstract: The ever-growing automobile industry with green transportation and green energy harvesting demand magnets of large quantity at the industrial scale. However, most of the magnets are made of rare-earth-based materials. In this regard, there is a quest for making rare-earth-free magnets. In this study, we report the tuning of properties of MnAl alloys. The high-temperature ε-phase of the MnAl alloy is formed by heat-treating $Mn_{51}Al_{49}$ powder followed by rapid quenching. The hard magnetic τ-phase is then obtained through milling and subsequent vacuum annealing. The prepared sample exhibits a ferromagnetic nature with magnetization ranging from 37.35 emu/g to 24.52 emu/g at 16 kOe applied field and a large coercivity of 3.95 kOe is obtained in 4 h milled powder followed by annealing at 500 ℃. The second-order ferromagnetic to paramagnetic transition (Curie temperature) was observed at 611 K. These results make MnAl alloy a potential candidate for permanent magnet application.

1. INTRODUCTION

The increasing demand for permanent magnets in this technology-driven world and the scarcity of rare-earth (RE) resources demand alternatives to conventional RE-based permanent magnets. In this regard, MnAl alloy is a potential candidate to fill the gap between high-performance RE-magnets and inferior ferrites because of their excellent theoretical magnetic properties, including saturation magnetization (M_s) over 140 emu/g, anisotropy constant (K_1) of 1.67 MJ/m^3 and maximum energy product (BH_{max}) of 12.64 MGOe [1,2].

2. EXPERIMENTAL SECTION

A high purity of Manganese (99.5%) and Aluminium (99.9%) powders were taken in a composition $Mn_{51}Al_{49}$ and heated in an air furnace at 1000 ℃ for 10 h and then quenched in ice water, followed by planetary ball milling for 4 h and annealing in the temperature ranges of 400 - 600 ℃. The structural analysis was done by X-ray diffractometer (XRD) and morphological study was performed using FESEM techniques. The magnetic properties were characterized by vibrating sample magnetometer (VSM).

3. RESULTS AND DISCUSSION

Fig. 1(a) depicts the room temperature XRD pattern of initial heat-treated $Mn_{51}Al_{49}$ powder at 1000 ℃ for 10 hours (sample A). The formation of high-temperature ε-phase (Space group 194, *P63/mmc*) is evident, which decomposes into hard magnetic τ-phase (space group 123, *P4/mmm*) and other stable phases after milled for 4 h. The as-milled powder was heated at low temperatures ranging 400 - 600 ℃ for a short duration to enhance the τ-phase.

The FESEM micrograph of the 4 h milled powder displays the uniform particle morphology (see Fig. 1 (b)). Fig. 1 (c) shows the *M-H* loop of the as-milled and heat-treated powders, revealing the existence of hard magnetic properties. As the annealing temperature increases, the coercivity of the sample decreases to 2.71 kOe after heating at 600 ℃ because of the crystallization of the phases. On the other hand, the decrease in magnetization can be attributed to the formation of a non-magnetic stable phase as the annealing temperature is increased. Temperature dependence of the magnetization (*M–T*) recorded at high temperature under an applied field of 500 Oe and shown in Fig. 1(e) clearly shows the magnetic phase transition from ferromagnetic to paramagnetic state around 611 K.

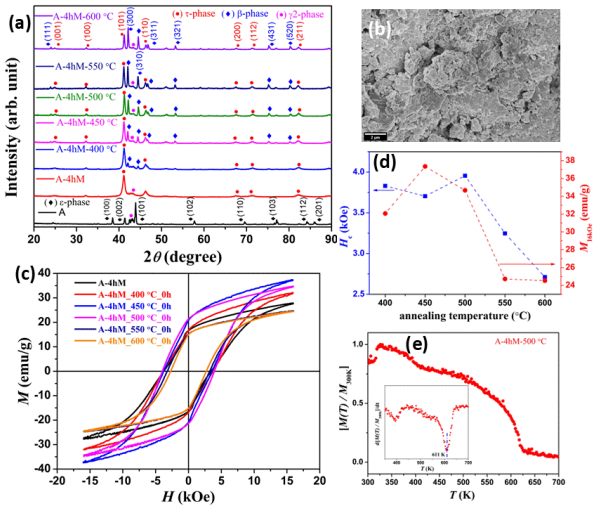

Fig.1 (a) Room temperature XRD patterns of $Mn_{51}Al_{49}$ heated at 1000 ℃ for 10 h (A), then milled for 4 h and heated at different temperatures, (b) FESEM image of 4 h milled powder, (c) *M-H* loop of as-milled and heat-treated powders, (d) Variation of coercivity and magnetization at 16 kOe, and (e) *M-T* curve of 4 h milled and annealed at 500 ℃ sample with inset depicting the thermal derivative of magnetization.

4. CONCLUSIONS

A careful optimization of sample preparation techniques in MnAl alloy helps to form the ε-phase, which decomposes into hard magnetic τ-phase and other stable phases. As a result, a large coercivity of 3.95 kOe and magnetization 37.35 emu/g at 16 kOe is achieved in milled and annealed powders. The detailed investigations to achieve such a rare-earther free magnet will be presented.

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Josephson Junctions with ferromagnet-Heavy metal barrier

Superconductivity and ferromagnetism are well-known physical properties of solid states that have been widely studied and they have antagonistic phenomena because superconductivity favors electrons of opposite spins in form of singlet Cooperpairs, while magnetism tries to align electron spins. So superconductivity and ferromagnetism do not exist simultaneously, but still, the combination of both superconductor and ferromagnet leads to a very rich and interesting physics. One particular example, the phase oscillations of the superconducting order parameter inside the ferromagnet. This is known as proximity effect at S/f interface. Ferromagnetic exchange field breaks the Cooper Pair which exponentially reduces the proximity length, ζF to a few nanometer, whereas in normal metal this length is a few hundred nanometer. The singlet cooperpair can transform into long-range triplet cooper-pair while passing supercurrent through ferromagnet having magnetic inhomogeneity in Josephson junction geometry. To eliminate challenges in fabricating magnetic inhomogeneity in multi-layered magnetic heterostructures Bergeret & et.al[1] and Jacobsen & et.al[2] demonstrated that spin-orbit coupling offers an alternative approach to generate such triplet Cooper pairs, having a single magnetic layer. Here the relative angle between this spin density and the magnetization of an adjacent ferromagnetic layer is proposed to act as a facilitator for the spin rotation of s_z=0 triplet Cooper pairs, effectively transforming them into long-range triplet pairs.

Here we have fabricated a Josephson junction in a transverse geometry as Nb(80nm)/Pt(3nm)/Nb(80nm)/[Pt(5nm)/Ni(10nm,20nm,40nm)/Pt(5nm)]/ Nb(80nm)/Pt(3nm)/Nb(80nm). Pt is used as a spin-orbit coupling material and 3nm Pt in between Nb layers is used as a marker layer to ease the fabrication process. The Josephson coupling beyond the singlet proximity length of ferromagnet Ni[3] 8nm, signifies the existence of long-range triplet supercurrent in the system.

In the device fabrication process, Si/SiO_2(250nm) substrate is patterned using standard UV lithography technique. All the metal heterostructures are then deposited using DC magnetron sputtering at a base pressure 6*10E-8mbar. The desired pattern is achieved by the lift-off process in acetone. Further Focused Ion Beam is used to fabricate Josephson junctions on these chips. The low-temperature transport measurements are performed in a cryogen-free cryostat system.

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Theoretical Prediction of novel 2D Rashba Systems based on Inverse Design Approach

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Rashba systems are emerging as one of the most promising families in the field of optoelectronic and spintronic application. The two-dimensional structures tend to have the inherent non-centrosymmetric configuration in most of the cases. The prediction of new Rashba materials, containing heavy element as constituent, could be pertinent as a pivotal aspiration in advancing device applications, where precise control over spin textures is crucial. We have leveraged the Inverse Design Approach based on the invertible neural network and Monte-Carlo techniques to predict newly possible two-dimensional structures, which could be perceived as Rashba systems. This research explores the integration of machine learning algorithms into the design process, enabling the discovery and optimization of materials with unique Rashba effects, particularly in low dimensional structures. Furthermore, we highlight the potential of hybrid approaches, combining Monte-Carlo with machine learning, to accelerate the exploration of chemical spaces and enhance the quality of material design outcomes.

Probing topological phase transitions in Aubry-Andre-Harper model via high-harmonic generation

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We study the High-order harmonic generation (HHG) using the AAH model with off-diagonal hopping [1] while preserving chiral symmetry. We use the modulating phase of the AAH model as a control parameter. The harmonic yield in a particular energy range exhibits a strong dependence on the control parameter with a clear separation of the region of the system's topologically trivial and nontrivial phases. The threshold for the harmonic yield is found to serve as an all-optical tool for detecting topological phases. The harmonic yield is suppressed due to interference of inter- and intra-band currents when the control parameter is around the topological phase transitions. We extended our study with broken chiral symmetry by including the onsite potential [2]. The introduction of the onsite potential lifts the degeneracy in the edge states, which affects the harmonic enhancement.

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Energy spectra and fluxes of two dimensional turbulent quantum droplets

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In this work, we numerically examine the scalings of the energy spectra of the turbulent state of the two-dimensional quantum droplet. The turbulent state is generated using a time-dependent paddling potential. We have systematically analyzed the effect of the frequency and strength of the paddling potential and the number of atoms on the distribution of the vortex and antivortices that is generated. Using the second order correlation function, we have identified the presence of three regions of different vortex configuration: (I) dominated by randomly distributed vortex and anti-vortex, (II) dominated by clustered vortex or anti vortices and (III) dominated by the paired vortex and antivortices. The incompressible energy spectrum exhibits Kolmogorov-like scaling ($E(k) \sim k^{-5/3}$) for region II and Vinen-like scaling ($E(k) \sim k^{-1}$) for region III. The flux shows the forward kinetic energy cascade in all the regimes. Finally we compute the energy spectra of the turbulent state of the non-uniform structure of the droplet that shows Kolmogorov-like scaling for all the parameters range. We also provide a phase diagram to show the presence of the different turbulence regime in the $N - T_{osc}$ phase space.

Correlation between chalcogen defects and electronic transport in Mo foil Grown monolayer MoS_2 devices

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Abstract: Atomic vacancies, such as chalcogen vacancies in 2D TMDs, are important in changing the host material's electronic structure and transport properties. We present a straightforward one-step method for growing monolayer MoS_2 utilizing oxidized Molybdenum (Mo) foil using CVD and delve into the transport properties of as-grown samples. Devices fabricated from these MoS_2 sheets exhibit excellent electrical responses, with the standout device achieving mobility exceeding 100 $cm^2V^{-1}s^{-1}$. Structural analysis and optical signatures unveiled the presence of chalcogen defects within these samples. To decipher the influence of inherent defects on the electronic transport properties, we measured low-temperature transport on two distinct sets of devices exhibiting relatively high or low mobilities. Combining the thermally activated transport model with quantum capacitance calculations, we have shown the existence of shallow states near the conduction band, likely attributed to sulfur vacancies within MoS_2. These vacancies are responsible for the hopping conduction of electrons in the device channel. Furthermore, our claims were substantiated through low-temperature scanning tunnelling microscopy measurements, which revealed an abundance of isolated and lateral double sulfur vacancies in Mo foil-grown samples. We found that these vacancies increase the density of states near the conduction band, inducing intrinsic n-type doping in the MoS_2 channel. By first-principles density functional theory-based (DFT) calculations, we have further established that it is the presence of S-divacancy that enhances the conductivity of the injected charge carriers through the formation of relatively delocalized shallow states close to the bottom of the conduction band. Consequently, this elevated conductivity enhances the field-effect mobility of MoS2 transistors. Our study offers insights into chalcogen vacancies in CVD-grown monolayer MoS2 and highlights their beneficial impact on electronic transport properties. [1]

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Ultrafast Transient Phonon Dynamics in Complex Crystals Predicted Using Deep Learning-accelerated First Principles Computations

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In crystalline semiconductors and insulators, strong momentum-conserving coupling among phonons leads to quite uncommon, yet important thermal transport phenomena such as hydrodynamic and Poiseuille phonon flow, particularly at low temperatures. These unusual phenomena have attracted significant attention from the research community recently [1,2], due to their potential applicability in the thermal cloaking and shielding of semiconductor devices and in the development of detectors with low thermal noise. To study such ultrafast transient phenomena, solving the complete linearized Peierls Boltzmann equation (LPBE), which depict the phonon dynamics including advection and equilibriation, is crucial. However, accurate solution of the full LPBE demands huge computational overhead requiring ultrafine discretization of the phonon Brillouin zone, accurate description of anharmonic three-phonon and four-phonon interactions with proper distinction of momentum-conserving (Normal) and momentum-dissipating (Umklapp) scattering processes and ultrafine temporal resolution over long physical timescales. Thus, such complete transient solutions of the LPBE have been typically limited to crystals with 1-4 atoms per unit cell and to crystals with high symmetry in the literature [3].

Here we present complete transient solutions of the LPBE in ultrahigh thermal conductivity materials with complex crystal structures, achieved by acceleration of the solution by a neural network (NN) framework [4]. By leveraging the universal approximation theorems of NNs, we adjust the number of neurons and layers to derive approximations of the solution of the LPBE to high accuracy at a fraction of the computational cost, compared to the conventional approaches to solve the LPBE [3]. We demonstrate the capability of this computationally efficient data-driven solution framework for the LPBE by calculating the ultrafast transient response of a spatially localized impulsive heat source in graphite and in the BCN compounds, which are ultrahard materials with complex crystal structures, that have been predicted to possess ultrahigh thermal conductivity recently [5]. Our NN framework is able to accurately predict the diffusive and non-diffusive temporal spreading of the spatially localized heat input in these materials in reasonable computational timeframe. Our solution method opens up new possibilities for predictive simulations of ultrafast thermal transport processes with complex crystal geometries.

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Sunday, 22nd December, 2024

List of Abstracts – Talks

[Day2 Parallel Session -1]

Fractional, Entangled and Quasi Orbitals

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

Unprotected Emergent Conservation Laws in Interacting Quantum Matter

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Abstract

Dynamical freezing refers to the phenomenon of perpetual but approximate freezing or conservation of certain local operators close to their initial values in a generic, disorder-free, quantum chaotic many-body system, under a strong periodic drive. These conservation laws are "emergent", as they are not respected in the undriven system. This is a way to evade Thermalization at late times in the absence of disorder even in the thermodynamic system. We will conjecture a recipe for constructing the conservation laws and show that they are not necessarily protected by high energy costs that can be posed by the strong drive field. This provides a new route to stabilizing and engineering interacting quantum matter far from equilibrium and also helps quantum state preservation. It also raises new questions regarding mechanisms of stabilizing the quantum of matter out of equilibrium and formulating Statistical Mechanics with approximate but perpetual constraints.

Superlattice induced electron percolation within a single Landau level

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In this talk, I will present our recent theoretical work on the quantum Hall effect in a single Landau level in the presence of a square superlattice of δ-function potentials. The interplay between the superlattice spacing (a_s) and the magnetic length (l_B) in clean system leads to three interesting characteristic regimes corresponding to $a_s < l_B$, $a_s \gg l_B$ and the intermediate one where $a_s \sim l_B$. In the intermediate regime, the continuous magnetic translation symmetry breaks down to discrete lattice symmetry. In contrast, we show that in the other two regimes, the same is hardly broken in the topological band despite the presence of the superlattice. In the presence of weak disorder (white-noise), interestingly, we obtain a large fraction of extended states throughout the intermediate regime which maximizes at the special point $a_s = \sqrt{2\pi} l_B$. We argue the superlattice induced percolation phenomenon requires both the breaking of the time reversal symmetry and the continuous magnetic translational symmetry. It could have a direct implication on the integer plateau transitions in both continuous quantum Hall systems and the lattice based anomalous quantum Hall effect which will be explained. In addition, I will also briefly discuss our recent results on the superlattice-induced phenomena in the fractional quantum Hall effect.

Reference: arXiv:2403.17137 (2024) .

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Percolation Transition in a Topological Phase

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Abstract: We study the signatures of the percolation transition in the topological phases of the short-ranged and long-ranged Su-Schrieffer-Heeger (SSH) chains. Under bond-percolation in both the chains, when the end-to-end connectivity is lost, the topological response (polarization) immediately becomes zero. However, the bond-diluted chain can host an extensive number of zero-modes even in the absence of the topological responses, indicating the breakdown of the bulk-edge correspondence. We label this region as a "fractured topological region" (FTR). We find that the presence of topological response of the chain is governed by the geometrical connectivity while the existence of zero-modes is determined by the critical lines of an effective 'mean-field' model. Thus, the interplay of topology and percolation gives rise to two different crossover boundaries in the phase diagram of the bond-diluted chain.

Reference: Saikat Mondal, Subrata Pachhal, Adhip Agarwala, "Percolation transition in a topological phase", Phys. Rev. B (Letter) 108, L220201 (2023)

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Distinguishing between topological Majorana and trivial zero modes via transport and shot noise study in an altermagnet

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We theoretically investigate the transport and shot noise properties of a one-dimensional semiconducting nanowire with Rashba spin-orbit coupling (SOC) placed in closed proximity to a bulk s-wave superconductor and an altermagnet with d-wave symmetry. Such heterostructure with vanishing net magnetization manifests itself as an alternative route to anchor Majorana zero modes (MZMs) characterized by appropriate topological index (winding number W). Interestingly, this system also hosts accidental zero modes (AZMs) emerged with vanishing topological index indicating their non- topological nature. Furthermore, by incorporating three terminal setup, we explore the transport and shot noise signatures of these zero modes. At zero temperature, we obtain zero bias peak (ZBP) in differential conductance to be quantized with value |W| Ã— 2e2/h for MZMs. On the other hand, AZMs exhibit non-quantized value at zero bias. Moreover, zero temperature shot noise manifests negative (positive) value for MZMs (AZMs) within the bulk gap. At finite temperature, shot noise exhibits negative value (negative to positive transition) concerning MZMs (AZMs). Thus, the ob- tained signatures clearly distinguish between the MZMs and non-topological AZMs. We extend our analysis by switching on the next to nearest neighbour hopping amplitude and SOC. Our conclusion remains unaffected for this case as well. Hence, our work paves the way to differentiate between emergent MZMs and AZMs in a semiconductor/ superconductor/ altermagnet heterostructure.

We will discuss the effect of strong sample-to-sample fluctuations in a generic one-dimensional disordered interacting chain at relatively weak disorder potential. It leads to creep dynamics in several observables, which implies a lack of a generic time scale. We propose entanglement as a measure of time to reparametrize the ensemble average dynamics. This approach evidences a remarkably uniform parametrization of the dynamical many-body evolution within the otherwise highly heterogeneous ergodic regime.

Inverse Melting in A Pinned Vortex Liquid

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Random pinning caused by structural defects inherent in materials often disrupts the order in a periodic vortex solid. Additionally, thermal and quantum fluctuations can melt the solid into a vortex liquid (VL). As a result, except in very clean superconductors, the periodic vortex lattice is typically observed well below the upper critical field, H_{C2}, and the critical temperature, T_c. When the magnetic field or temperature increases, the periodic order eventually breaks down, leading to a completely disordered state. However, in some rare cases, increasing the temperature can lead to a transition to a more ordered state, a process known as "inverse melting." Experimental instances of this phenomenon are uncommon. In this study, we observe such a process in the two-dimensional vortex liquid of a moderately pinned amorphous Re_6Zr (a-ReZr) thin film, using a scanning tunneling microscope to directly image the vortex lattice. At low temperatures and magnetic fields, the vortices form a "pinned liquid," characterized by low vortex mobility and spatially inhomogeneous vortex density. As the temperature or magnetic field increases, the vortices eventually form a nearly perfectly ordered state. Beyond this temperature or magnetic field, the ordered vortex lattice melts back into a vortex liquid. This re-entrant transformation from a liquid to a solid-like state, and then back to a liquid, also produces distinct signatures in the superconductor's magneto transport properties.

Revival of the Hofstadter butterfly in the Presence of various disorders and Correlation Strength

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We investigate the revival of the Hofstadter butterfly spectrum influenced by the interplay of four distinct types of disorder and electronic interactions in a two-dimensional square and honeycomb lattice. Employing a mean-field approximation of the unrestricted Hartree Fock method at zero temperature, we explore the deterministic disorders in the systems. Our study reveals that these varied disorders initially obscure the characteristic butterfly nature of the spectrum, while electronic interactions induce a gap at half-filling. Introducing disorder with interactions effectively closes this gap, partially restoring the butterfly spectrum's distinct features.

Furthermore, we analyze the impact of disorders and interactions on entanglement entropy and the entanglement spectrum within the system. We compute the DC conductivity and Chern number using the Kubo formalism to assess the system's topological properties.

This research provides new insights into how different types of disorder and electronic interactions dynamically influence the Hofstadter butterfly spectrum, highlighting their crucial roles in modifying the system's topological characteristics and entanglement properties.

Non-coplanar magnetic structure driven Large Anomalous Hall Effect in electron doped Mn3Sn

Charanpreet Singh, Sk Jamaluddin, Subhadip Pradhan, Ashis K. Nandy, Masashi Tokunaga, Maxim Avdeev , Ajaya K. Nayak

The discovery of a large anomalous Hall effect (AHE) in non-collinear antiferromagnet Mn_3Sn begins a new era of antiferromagnetic (AFM) spintronics. The hexagonal Mn3Sn exhibits an in-plane triangular 120 degree AFM ordering owing to the geometrical frustration in the kagome lattice. In this work, we present a combined theoretical and experimental investigation to show how suitable electron doping in the Mn_3Sn can drastically change the in-plane AFM structure to a tunable non-coplanar magnetic state. We demonstrate that the higher-order exchange interaction in the magnetic Hamiltonian drives the planar magnetic state to the non-coplanar one. We also find a large scalar spin chirality (SSC)-induced topological AHE, whose size is closely correlated with the system's degree of noncoplanarity. Additionally, a unique simultaneous manipulation of the dual order in the system is demonstrated, where the Hall signal due to in-plane AFM order can be switched independently without perturbing the SSC-induced signal. The current work provides a new avenue for investigating unique quantum phenomena in triangular AFM materials where higher order magnetic interactions play a vital role.

Strain-driven magnetic reorientation in transition metal oxides

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The electronic structure can be altered by structural modification because of the close relationship between structure and electronic characteristics. As a result, strain-induced structural change emerges as an effective tool for tuning the electrical properties of perovskites. Under tensile strain, transition metal oxides such as $BiFeO_3$ undergo a magnetic phase change from G-type to C-type antiferromagnet. First, we performed density functional theory-based first-principles calculations to show that combined in- and out-of-plane epitaxial strain produces a magnetic phase change from G-type to C-type antiferromagnet in $BiFeO_3$. We then investigated the effects of strain using the half-filled one-band Hubbard model by using the semiclassical Monte-Carlo approach for U~bandwidth regime. Strain was incorporated by including next nearest neighbor hopping (t') in our model Hamiltonian. Our results show that, in the presence of strain, the long-range staggered antiferromagnetic ordering temperature (T_N) decreases as t' increases. Around $t'=0.5*t_z$ (for $t_z < t_x = t_y$) we observed a magnetic phase transition from G-type to C-type antiferromagnet. Interestingly, for $t_z > t_x = t_y$, our calculations reveal a strain-induced magnetic phase transition from G-type to A-type antiferromagnet. Overall, our theoretical results show the subtle competition between magnetic phases under epitaxial strain.

Unusual magnetic properties of $TbRu_2Ge_2$ compound

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In order to study the magnetic structure of antiferromagnetic $TbRu_2Ge_2$ compound, we have observed multistep metamagnetic transitions below its Neel temperature (T_N =) 38 K. As presented in the inset of Fig. 1(a), the broad maximum observed around 30K is probably not associated with a phase transition, and may be attributed to the crystal field effects. Below a typical temperature, T_t ~ 4 K, a sharp decrease in the magnetization has been observed, which can be associated to the antiphase character of the magnetic structure, associated with a long period commensurate propagation vector. In this region, magnetization also exhibits multiple step like behavior as a function of magnetic field, and get saturated above ~60 kOe magnetic field, as represented in Fig. 1(b). Additionally, the neutron diffraction experiments already revealed that the magnetic structure of $TbRu_2Ge_2$ is sine modulated below T_N and at 4.2K, it becomes square modulated, with a magnetic moment of 9.06μB. For a better understanding of the magnetic behavior below T_t, we have performed magneto-transport and heat capacity measurements with magnetic field variation.

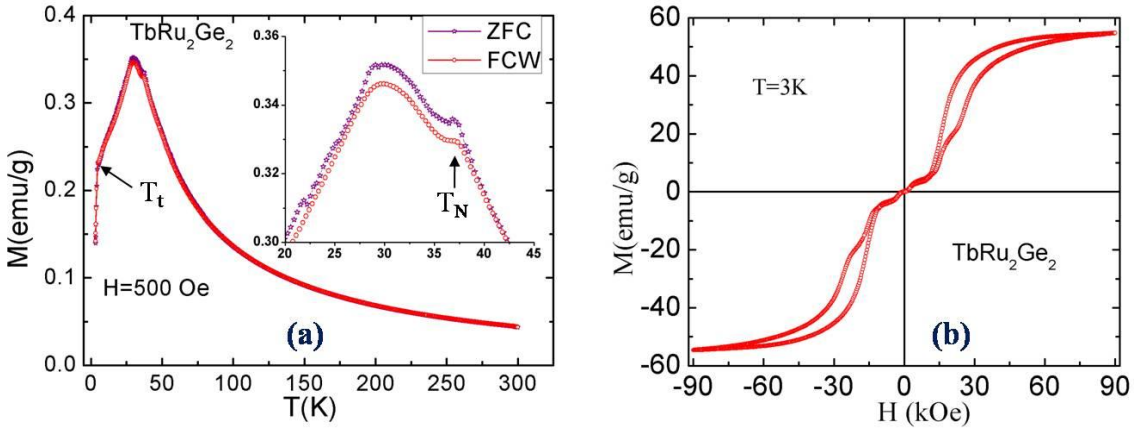

Fig.1. (a) Temperature dependent of magnetization of $TbRu_2Ge_2$ obtained in zero field colled warming (ZFCW) and field cooled warming (FCW) protocol, under measuring field of 500 Oe. (b) Isothermal magnetization curve as a function of magnetic field at 3 K.

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2D broadband FMR data acquisition with Vector Network Analyzer and Determination of Asymptotic Lande g-Factor

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Abstract. The development of spintronic devices requires low microwave losses for energy-efficient devices. Cavity-based ferromagnetic measurements are insufficient for studying the broad frequency response of the material. The VNA-based FMR spectroscopy generates a large data set as it can sweep both frequencies and magnetic fields. We used electronic calibration instead of manual calibration, which was used in many reports, enabling us to acquire better spectra with an excellent signal-to-noise ratio. Additionally, the derivative divide method was implemented to enhance the signal-to-noise ratio, and the spectral analysis in the frequency domain was carried out. 2D mapping of VNA-FMR data enables us to visualize the FMR and additional modes and its response over a broad frequency and magnetic field range. In laboratory conditions, the magnetic field is limited to few Tesla and this low field data acquisition leads to errors in the determination of gyromagnetic ratio and spin and orbit moment quantification. In this work, an asymptotic analysis is carried out to find the correct Lande g factor for spin and orbital moment quantification.

High temperature Josephson diode

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Abstract Body

Many superconducting systems with broken time-reversal and inversion symmetry show a superconducting diode effect, a non-reciprocal phenomenon analogous to semiconducting *p–n*-junction diodes. While the superconducting diode effect lays the foundation for realizing ultralow dissipative circuits, Josephson-phenomena-based diode effect (JDE) can enable the realization of protected qubits. The superconducting diode effect and JDE reported thus far are at low temperatures (~4 K), limiting their applications. Here we demonstrate JDE persisting up to 77 K using an artificial Josephson junction of twisted layers of $Bi_2Sr_2CaCu_2O_{8+\delta}$. JDE manifests as an asymmetry in the magnitude and distributions of switching currents, attaining the maximum at 45° twist. The asymmetry is induced by and tunable with a very small magnetic field applied perpendicular to the junction and arises due to interaction between Josephson and Abrikosov vortices. We report a large asymmetry of 60% at 20 K. Our results provide a path towards realizing superconducting Josephson circuits at liquid-nitrogen temperature.

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Acknowledgment

We acknowledge the Department of Science and Technology (DST), Nanomission grant SR/NM/NS-45/2016, CORE grant CRG/2020/003836 and Department of Atomic Energy (DAE) of the Government of India (12-R&D-TFR-5.10-0100) for support.

Keywords: Superconducting diode, Josephson diode, high Tc superconductor, BSCCO

Signature of point nodal superconductivity in the Dirac semimetal PdTe

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Recent angle-resolved photoemission spectroscopy (ARPES) experiments on PdTe, a 3D-Dirac semimetal and a superconductor with the transition temperature $T_c \sim 4.3$ K, have revealed compelling evidence of the presence of bulk nodes in the superconducting order parameter [1]. To investigate the validity of this proposition, here we present a detailed investigation of the magnetic field dependence of the specific heat of PdTe down to temperatures ~58 mK. We observed that the low-temperature specific heat of PdTe with an externally applied magnetic field exhibits a power-law field dependence, a characteristic of unconventional superconductivity. Furthermore, the zero-field low-temperature electronic specific heat follows a cubic temperature dependence, which is a signature of the presence of bulk point nodes in PdTe [2]. These intriguing observations suggest that PdTe is a rare and fascinating topological material that exhibits both Dirac semimetallic properties and superconductivity with point nodal gap symmetry.

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Diode effect in quantum dot-based Josephson junction

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

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Linear and Non-Linear response in the mixed state of superconducting NbN and a-MoGe thin films using a low-frequency two-coil mutual inductance technique

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We investigate the low-frequency electrodynamics in the vortex state of two type-II superconducting films, namely, a moderate-to-strongly pinned Niobium Nitride (NbN) and a very weakly pinned amorphous Molybdenum Germanium (*a*-MoGe). We employ a two-coil mutual inductance technique to extract the complex penetration depth, $\tilde{\lambda}$.

The linear response is studied through the temperature variation of $\tilde{\lambda}$ in the mixed state, where we employ a model developed by Coffey and Clem (CC model) to extract the different vortex lattice (VL) parameters such as the restoring pinning force constant (Labusch parameter), VL drag coefficient and pinning potential barrier. We observe that a consistent description of the inductive and dissipative part of the response is only possible when we take the viscous drag on the vortices to be several orders of magnitudes larger than viscous drag estimated from the Bardeen-Stephen model.

The nonlinear response is observed by the dependence of screening and dissipative response on the magnitude of AC current in the drive coil at a fixed temperature and magnetic field. With increasing in magnitude of AC current we can drive the system from the superconducting to the normal state.

We develop a computation scheme to analyse the nonlinear response by invoking the local radial variation of $\tilde{\lambda}$ of the superconducting thin film, with a circular geometry.

We use this scheme to extract the local radial variation of different vortex lattice parameters like the pinning force constant, the viscous drag on the vortices and the activation barrier of the superconducting thin film and identify the appropriate the vortex creep model with which we can describe the low frequency response over a range of the driving current.

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Basistha S, Mandal S, Jesudasan J, Bagwe V and Raychaudhuri P **2024** Low frequency electrodynamics in the mixed state of superconducting NbN and a -MoGe films using two-coil mutual inductance technique *Supercond. Sci. Technol.* **DOI** 10.1088/1361-6668/ad5a45

Spin-orbit driven emergent phases in quantum materials.

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Abstract

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 either due to its orbital motion around the positively charged nucleus or due to a gradient of electrostatic potential in non-centrosymmetric systems. As an example of the first case we shall consider strongly correlated Mott insulators with a d4 electronic configuration where the interplay between spin-orbit coupling (SOC) and superexchange interactions can give rise to magnetism, defying the expected formation of atomic J = 0 nonmagnetic singlets leading to unconventional magnetic ground states promoted by anisotropic orbital interactions.[1],[2],[3] In addition, we shall show the emergence of Rashba and Dresselhaus spin–orbit interactions in non-centrosymmetric systems that exhibit characteristic spin textures, in particular persistent spin-textures important for spintronics research. [4],[5],[6]

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In search of spin orbit driven ferroelectric Rashba swtitches in Perovskite oxides

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Abstract

Ferroelectric perovskite oxides are known for their excellent technological applications such as in spintronics research i.e. as spin control devices. One such manifestation of spin control can be seen in Rashba-Dresselhaus effect in non-magnetic insulators with broken inversion symmetry. This phenomenon of spin splitting in the momentum space if it occurs in the band edges can help in realising the spin field effect transistor devices. To achieve the spin control via switching of gate voltage, existence of ferroelectric polarisation in the material is necessary. This has led to a lot of research on ferroelectric Rashba semiconductors (FERSC) and formulation of design principles necessary to search for such materials. Using first principles density functional theory based methods, we analyse the Iodate perovskites viz. AIO_3, A=K, Rb, Cs, and Tl in non-centrosymmetric rhombohedral phases (R3m). More specifically, we study the effect of A cation in the Rashba spin splitting by taking into the account of atomic as well as geometric relaxation, spin polarization, and spin orbit coupling. Our study reveals that the Rashba splitting is inversely proportional while the band gap is directly proportional to the ionic radii of the A cation [1].

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Influence of band convergence on the thermoelectric transport properties of CoBi-based half-Heusler alloys

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Abstract

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) guides experimental efforts to provide insights into the solid solution compounds' electronic structure, band convergence, and phonon properties. By leveraging the unique band structures of both materials, we explore the possibility of designing solid solutions with improved power factor and reduced lattice thermal conductivity (due to mass fluctuation), paving the way for next-generation thermoelectric materials for mid to high-temperature power generation applications in this work.

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keywords: thermoelectric materials, mobility engineering, waste heat recovery, half-Heusler

Electric field induced second-order anomalous Hall transport in unconventional Rashba system

Ankita Bhattacharya and Annica M. Black-Schaffer

Recent times have witnessed a surge of interest in the quantum geometry of electrons, due to the pivotal role it has been shown to play in different branches of physics. As a key example, the quantum geometric tensor (QGT) [1], defined in a parameterized Hilbert space and determining the geometry of eigenstate space, has been shown to play an indispensable role in transport properties of materials, both through its real part labeled as the quantum metric (QM) and its imaginary part, the Berry curvature (BC). Besides determining the topological characteristics of quantum materials, the BC emerges in various Hall effects [2], including leading to a linear anomalous Hall effect in solids with broken time-reversal symmetry (TRS) [2], while the QM has been shown to be essential in nonlinear transport theory [3].

Recently, Sodemann and Fu [4] proposed a second-order anomalous Hall effect in *noncentrosymmetric time-reversal-invariant* systems where instead of the BC, the dipole moment of BC over the occupied states, known as the Berry curvature dipole (BCD) is the key ingredient. Subsequently, BCD-assisted nonlinear transport have been detected experimentally in several nonmagnetic materials [5, 6]. However, a major caveat is that the BCD follows a strict symmetry constraint: the maximum symmetry allowed is the presence of a single mirror line in the transport plane [4]. This means the BCD is still zero in many high-symmetry but still inversion-broken systems. In these cases additional material engineering, such as interlayer twisting, applying strain or an electric field, is required to lift the symmetry constraint to observe BCD-assisted Hall effect. In particular, using an electric field utilizes the presence of another band geometric quantity, the Berry connection polarizability (BCP) [3], which is also the so-called band-normalized QM. This intrinsic band geometric quantity in the presence of an electric field provides a field-induced BCD, even in systems where the native BCD (and BC) are absent by symmetry [7]. An additional experimental advantage is that the field-induced BCD is linearly proportional to the applied electric field, and therefore, the Hall response can easily be tuned externally.

In our work, we study one of the most common inversion-broken but time-reversal invariant systems in 2D: the Rashba spin-orbit coupled system. We show how an electric field induced second-order anomalous Hall effect is present even in some Rashba systems as soon as they possess *unconventional* Rashba bands[8]. The main dissimilarity of unconventional Rashba systems compared to standard Rashba systems is that, by simply tuning the chemical potential, it is possible to achieve two spin-split Fermi surfaces of the same spin chirality. The spin-momentum-locked band structure of all Rashba systems provide a finite QM, but field induced BCD-assisted transport is not possible in conventional Rashba systems because contributions from different bands cancel. We show that this cancellation is lifted for unconventional Rashba bands without breaking TRS and without requiring additional materials engineering, and thereby we are able to find a highly tunable electric field induced second-order anomalous Hall transport in probably the simplest system in 2D, which should be uncomplicated to verify experimentally due to multiple materials already being proposed.

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Fate of many-body localization in an Abelian lattice gauge theory

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(Dated: October 18, 2024)

We address the fate of many-body localization (MBL) of mid-spectrum eigenstates of a matter-free $U(1)$ quantum-link gauge theory Hamiltonian with random couplings on ladder geometries. We specifically consider an intensive estimator, $\mathcal{D} \in [0, 1/4]$, that acts as a measure of elementary plaquettes on the lattice being active or inert in mid-spectrum eigenstates as well as the concentration of these eigenstates in Fock space, with $\mathcal{D}$ being equal to its maximum value of $1/4$ for Fock states in the electric flux basis. We calculate its distribution, $p(\mathcal{D})$, for $L_x \times L_y$ lattices, with $L_y = 2$ and 4, as a function of (a dimensionless) disorder strength α ($\alpha = 0$ implies zero disorder) using exact diagonalization on many disorder realizations. Analyzing the skewness of $p(\mathcal{D})$ shows that the finite-size estimate of the critical disorder strength, beyond which MBL sets in for thin ladders with $L_y = 2$, increases linearly with L_x while the behavior of the full distribution with increasing L_x at fixed α shows that $\alpha_c(L_y = 2) > 40$, if at all finite, based on data for $L_x \leq 12$. $p(\mathcal{D})$ for wider ladders with $L_y = 4$ show their lower tendency to localize, suggesting a lack of MBL in two dimensions. A remarkable observation is the resolution of the (monotonic) infinite temperature autocorrelation function of single plaquette diagonal operators in typical high-energy Fock states into a plethora of emergent timescales of increasing spatio-temporal heterogeneity as the disorder is increased even before MBL sets in. At intermediate and large α, but below $\alpha_c(L_y)$, certain randomly selected initial Fock states display striking oscillatory temporal behavior of such plaquette operators dominated by only a few frequencies, reminiscent of oscillations induced by quantum many-body scars.

Manipulation of materials at the nano-to-atomic scale for tuning the electronic properties and interactions at the solid-liquid interface during hydrogen generation

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Abstract:

Precise manipulation of the size and shape of nanocrystals is known to display interesting electronic properties that can be used for a wide range of functional applications. In this line, recent research efforts have been directed to push the limit and develop materials of few atomic clusters and even up to a single atom size. However, the development of such precisely controlled materials is extremely challenging. In this talk, I shall discuss some of our recently developed electronically tuned materials, like ordered/disordered atomic clusters, and single-atoms stabilized over suitable support, which we have used as catalysts to generate green fuel hydrogen by splitting water. Electrolytic water splitting involves the interaction of adsorbate species with solid catalytic materials, and the energy uphill engaged in the process can be minimized through proper electronic tuning of atomic clusters/single-atoms and synergists with their supports. The electronic origin of the exceptionally high efficiency in water splitting of the developed catalysts will be discussed from the density functional theory (DFT) perspectives.

Computational Roadmap of Emerging Materials: Implications of Piezochromism and Rashba Physics

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ABSTRACT: In this talk, I will start with the brief introduction of first principles electronic structure calculations in perovskite materials, and how it could be connected to the Computational Screening for achieving highly efficient and stable solar cell materials [1, 2]. Next, I will delve into the fundamentals and possible implications of Rashba phenomena in both hybrid and inorganic perovskite materials [3-5]. The electronic and optical properties along with the Rashba splitting and spin texture are systematically observed in noncentrosymmetric one-dimensional zigzag chain structure, (3AMP)BiI_5 within the thermodynamic limit under compression equivalent to 9.6 GPa [4]. 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. 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. The rest of the talk would be devoted to theoretical understanding of piezochromism, where hydrostatic pressure could be employed as an effective tool, giving rise to novel crystal structures and optical properties, while it has proven to be an alternative to chemical pressure [6-7]. Therefore, new functional materials with intriguing properties can be designed by exerting external pressure and strain. I will end my talk touching upon our recent successful endeavour of pre-intercalation mechanism in Li-ion battery, which appeared in Nature Materials [8].

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Title:
Theoretical analysis of multi-spin Excitations in 2D Antiferromagnet probed by Resonant Inelastic X-ray Scattering (RIXS)

Abstract:
In recent experiments, indirect Resonant Inelastic X-ray Scattering (RIXS) has emerged as a powerful tool for probing fundamental low-energy excitations within solids. RIXS can generate spin conserving (SC) ($\Delta Sz=0$) and spin non-conserving (NSC) ($\Delta Sz\neq0$) excitation and yield experimental signatures much more sensitive than Inelastic neutron Scattering.

We study a nearest and next nearest neighbor spin model relevant to High-TC cuprate for analyzing RIXS data of recent experiments [1]. These Cu L-edge (2p-3d transition) experimental studies indicate the possibility of multi-magnon spin excitations.

We compute the RIXS cross-section within the ultra-short core-hole lifetime expansion of the Kramers-Heisenberg scattering amplitude, allowing perturbative solution inverse in core-hole lifetime within linear spin wave theory (LSWT) [2]. Within the LSWT, we show that three-magnon excitation (in the NSC channel) can qualitatively capture observed experimental data for L-edge RIXS in La2CuO4; in addition, we also reproduce usual one and bi-magnon contributions. We confirm the validity of the LSWT result by exact diagonalization. I will conclude with primary steps aimed at uncovering damped magnon excitations (paramagnon) due to hole doping.

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Non-volatile electrically switchable spintronics properties in MXenes based heterostructures

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Materials that exhibit both ferroelectric and ferromagnetic properties, known as multiferroics, provide an excellent platform for studying magnetoelectric coupling. In such systems, it is possible to achieve electrically controlled magnetic behavior and magnetically controlled electric behavior. However, intrinsic multiferroics are limited. According to the d^0 rule for ferroelectricity, empty d-orbitals are required. On the other hand, for magnetism to exist, the d-orbitals must be partially filled. These contradictory conditions make it difficult to realize intrinsic multiferroics in single materials.One way to overcome the limitations of intrinsic multiferroics is by constructing heterostructures. In these systems, the ferromagnet couples with both polarization states of the ferroelectric material. By adjusting the polarization state, the magnetic and electronic behavior of the ferromagnet can be controlled. The polarization states of the ferroelectric material can be altered by applying an electric field, and this switching is entirely reversible and nonvolatile. As a result, the control over the ferromagnets is also fully nonvolatile.In this work, using Density Functional Theory (DFT) calculations, we constructed a 2D multiferroic heterostructure with H-VSe_2 as the ferromagnetic component and Sc_2CO_2 as the ferroelectric component. We demonstrated that the electronic band structure of the heterostructure can be reversibly switched between semiconducting and half-metallic states by changing the polarization state of Sc_2CO_2. Finally, we proposed two applications for this heterostructure: a transistor and a low-cost, power-efficient multiferroic memory device. The results and conclusions presented in this paper could be beneficial for developing next-generation spintronic devices.

Universality of quantum phase transitions in the integer and fractional quantum Hall regimes

Simrandeep Kaur, Tanima Chanda, Kazi Rafsanjani Amin, Kenji Watanabe, Takashi Taniguchi, Unmesh Ghorai, Yuval Gefen, G. J. Sreejith, Aveek Bid

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

Multifunctional properties of non-collinear antiferromagnet Mn_3Sn

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Antiferromagnetic materials are considered a promising alternative to conventional ferromagnets for spintronic applications. They are resistant to external magnetic interference, have very fast spin dynamics, produce minimal magnetic stray fields, and exhibit unique magneto-optical and magneto-transport properties. However, these inherent characteristics also pose challenges for their manipulation and for reading their magnetic states, which need to be addressed in order to make antiferromagnets a practical choice for spintronic applications.

In the first part of my talk, I will discuss a new mechanism to manipulate the magnetic states of Mn_3Sn that goes beyond a simple SOT mechanism[1]. The mechanism involves the setting of the antiferromagnetic domain configuration at the interface of Mn_3Sn with a heavy metal layer in which a spin-current 'seeds' the subsequent setting of the domain configuration of the entire antiferromagnet. The process also involves bringing the temperature of the antiferromagnet above its ordering temperature and then cooling it in the presence of the SOT provided by the spin current. We substantiate our hypothesis by nanosecond magnetization switching experiments in which we show that current pulses whose fall time is too short do not allow for switching of the entire antiferromagnetic layer.

In the second part, I will discuss generating robust spin currents in epitaxial thin films of the chiral antiferromagnet Mn_3Sn. Temperature-dependent spin-torque ferromagnetic resonance reveals that the Mn_3Sn layer's antiferromagnetic order generates an in-plane polarized spin current[2]. In contrast, the out-of-plane spin-polarized spin current originates from scattering at the Mn_3Sn/permalloy interface. This conclusion is supported by experiments with several other non-magnetic metals, all of which exhibit out-of-plane polarized spin currents due to the spin-swapping effect.

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Theory of Polar Skyrmions in Layered Structure of Ferroelectric Perovskites

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Discovery of polar skyrmions on the $(PbTiO_3)_n$ /$(SrTiO_3)_n$ superlattice in the absence of any known interaction which can orient electric polarizations at an angle between neighboring atoms is enigmatic. We show that the coupling of the electric polarization and strain at each layer is responsible for orienting polarizations. We formulate coupled Euler equations for electric polarization and displacement vectors and solve to find skyrmion solution for a range of electric fields with unique topological number in each layer. The type of skyrmions vary from Neel to Bloch depending on the position of the layers in the superlattice, as observed in the experiments.

Impact of antiferroelectric moiré domains on a graphene field-effect transistor

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Emergent phenomena enabled by moire´ patterns in an artificial two-dimensional superlattice have been a topic of great interest with the most recent being interfacial ferroelectricity in near-parallel twisted bilayers of transition metal dichalcogenides [1, 2]. The interlayer charge transfer driven emergent out-of-plane dipole moment in alternately polarized triangular domains, presents an exotic antiferroelectric system [3] in the moire´ length scale. Here, we study the impact of a moire´ induced fluctuating electric field using near-parallel twisted bilayer WSe_2 at 2.1^0 twist angle, placed in contact with a graphene field-effect transistor. Our experimental observations show emergent inhomogeneity and non-locality in graphene resulting from a disordered potential landscape. The 'disorder' or inhomogeneity itself is a tuneable emergent property arising from anti-ferroelectric nature of the underlying substrate. A quantitative analysis connecting the non-locality and channel inhomogeneity suggests non-local transport in an emergent valley Hall insulating phase in graphene confined within finite-size domains, providing a new parameter to exploit valley current in graphene. The twist angle regime ~ 2.1^0, lies at the cross-over of antiferroelectric-dielectric and is unique because the length scale of the polarization fluctuations across successive moire´ domains approach a few lattice spacings, thereby potentially impacting the valley symmetry of the graphene channel. This work furthers the understanding of the effects of ultrathin 2D ferroelectrics when embedded in a 2D field-effect architecture for emerging all-2D ferroelectric devices.

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Spin U(1) quasi-symmetry and quantized spin Hall effect in puckered lattice materials

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Abstract: 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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Reversible quantum phases in magnetic topological insulator

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Magnetic ordering in topological insulators disrupts time-reversal symmetry, transforming the topologically non-trivial surface state into a massive Dirac fermionic state. In the two-dimensional limit, $MnBi_2Te_4$, an intrinsic magnetic topological insulator, emerges as an intriguing candidate for exploring controllable topological phase transitions, from an axion insulator to a Chern insulator. While such phase transitions have been experimentally demonstrated, they are typically restricted to temperatures below 2 K and require significant magnetic fields above 9 Tesla. This talk will explore various methods for controlling topological phases without relying on high magnetic fields. The results are derived within first-principles calculations, supported by Hamiltonian modeling and Monte Carlo simulations.

Trends in magnetic interactions of transition-metal trilayers under electric fields

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Abstract: The electric current driven control is a widely used technique to manipulate the magnetic topological quasiparticles such as skyrmions in transition-metal based ultrathin films. However, it is accompanied by two serious drawbacks, namely, the skyrmion Hall and Joule heating effects, which have restricted the realization of skyrmion-based devices in spite of a decade long intensive research. Recently, the electric-field driven manipulation has been demonstrated as a successful technique to control skyrmions locally avoiding the two obstacles. Nevertheless, a comprehensive understanding across a variety of materials is required before it becomes a widely accepted technique. To address this, we have studied the impact of electric fields in a series of freestanding transition-metal trilayers on the magnetic interactions, which stabilize the skyrmions, and understand the origin of their field induced variation.

We calculate magnetic interactions in freestanding trilayers composed of a single Fe or Co atomic layer sandwiched between 4*d* and 5*d* transition-metal layers under various external electric fields using first-principles based density functional theory method. Furthermore, we have uncovered the general trends in magnetic interactions and explain their variation under electric fields from electronic structures. These analyses helps us to identify promising freestanding trilayers for thin film on surface calculation under electric fields for deeper physical insight into the mechanism of electric-field induced skyrmion manipulation.

Speaker: Prof. Ramesh Chandra Nath

Title: Field induced magnetic transition in the double trillium lattice antiferromagnet KBaCr2(PO4)3

R. Kolay, Qing-Ping Ding, Y. Furukawa, A. A. Tsirlin, and R. Nath

Abstract:

Frustrated magnets where configurations of localized magnetic moments do not satisfy pair-wise interactions simultaneously often have large ground-state degeneracy and realize exotic phases at low temperatures. Trillium lattices formed by corner-shared triangular units provide an ideal platform for magnetic frustration in three dimensions. In this talk, I would like to present the structural and magnetic properties of a Cr-based (S = 3/2) double trillium lattice system $KBaCr_2(PO_4)_3$ studied by thermodynamic and ^{31}P nuclear magnetic resonance (NMR) measurements complemented by theoretical calculations. Magnetization, heat capacity, and ^{31}P NMR measurements reveal the magnetic transition at $T_{N1} \simeq 12.5$ K in zero field followed by another transition (T_{N2}) at low temperatures in weak applied fields. These two transitions result in a complex phase diagram with magnetic field. The spin lattice of $KBaCr_2(PO_4)_3$ comprises two crystallographically nonequivalent ferromagnetic sublattices that are coupled antiferromagnetically, thus eliminating frustration in this trillium network and leading to weak ferrimagnetism in the vicinity of T_{N1}.

Tuning the robust magnetic properties in MPS3 (M = Mn, Fe, and Ni)

Suvodeep Paul , Devesh Negi , Saswata Talukdar , Saheb Karak, Shalini Badola, Bommareddy Poojitha, Manasi Mandal, Sourav Marik, R. P. Singh, Nashra Pistawala, Luminita Harnagea , Aksa Thomas, Ajay Soni, Subhro Bhattacharjee, and Surajit Saha

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Abstract

We have demonstrated the possibility to control the otherwise robust magnetic properties of transition-metal phosphorus trisulfides (Mn/Fe/NiPS3) in their heterostructures with Weyl semimetallic MoTe2 which can be attributed to the Dzyaloshinskii-Moriya (DM) interactions at the interface of the two materials. While the DM interaction is known to scale with the strength of the spin-orbit coupling (SOC), we demonstrate using experiments on heterostructures with a variety of substrates (underlayers) hosting variable SOC and electronic density of states (DOS) that the effect of DM interaction strongly varies with the electronic DOS of the SOC-hosting layer as well as the spin orientation and degree of anisotropy associated with the magnetic layer.

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$MnBi_2Te_4$ (MBT), an antiferromagnetic topological insulator, is an excellent platform for investigating the topological properties alongside magnetic characteristics. The magnetic phase transitions in the MBT family materials have been well explored using transport measurements. Using nanoelectromechanical devices, we study the intrinsic magnetism in MBT thin flakes through their magnetostrictive coupling. We investigate mechanical resonance signatures of magnetic phase transitions from antiferromagnetic (AFM) to canted antiferromagnetic (cAFM) to ferromagnetic (FM) phases versus magnetic field at different temperatures. The magnetic transitions are revealed by frequency shifts in mechanical resonance. We employ a magnetostrictive model to correlate the frequency shifts with the spin-canting states. Our work demonstrates a technique for studying magnetic phase transitions, magnetization, and magnetoelastic properties of the magnetic topological insulator.

Title: Emergent topology and its signatures in dissipative dynamics of topological condensed matter.

Suraj S.Hegde(IISER-Tvm), Toni Ehmcke(TU-Dresden,Germany), and Tobias Meng(TU-Dresden,Germany)

Abstract: Topological characterisation of quantum phases of matter has been well studied both theoretically and experimentally for low-energy states of closed condensed matter systems. Dissipation and decoherence are sometimes considered as a hindrance or as an external perturbation that affect the topological features. In this talk, I present how we need to rethink the notion of topology for open quantum systems. Taking a paradigmatic example of a topological phase, a Chern insulator under going a dissipative evolution under Gorini-Kossakowski-Sudarshan-Lindblad equation, I show how the notion of spectral winding/topology of the damping generator gives rise quantum channels localised only at an edge and undergoing extremal damping. These damping channels are robust against perturbations, symmetry-protected and could be of use in quantum technologies. Further, the dynamics show signatures of ‘non-Hermitian exceptional points’ which have no counterparts in Hermitian topological phases. I also discuss how these effects are already being probed in experiments on photonic lattices and also how dissipative boundaries of Hermitian topological phases can harbour such unique phenomena.

Solution of a Spin-1/2 Trimer Chain and Experimentally Verifiable Quantities

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We explicitly solve a Hamiltonian of a spin-1/2 trimer chain with J1-J2 antiferromagnetic interaction where J1 is the nearest neighbor intra-trimer and J2 in the inter-trimer excange intercations. The solution is in the form of three nonidentical fermionic bands. We further calculate dynamical spin structure factor, specific heat, and Raman scattering intensity due to simultaneous excitation of a pair of fermions. Some of the theoretical results are compared with the numerical simulations and the experiments reported in literature.

Magnon interactions, spectral renormalisation and potential phase instabilities in some pyrochlore spin models.

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Abstract

The pyrochlore lattice has been the host for the manifestation of many intensely investigated phases in spin models, from classical and quantum spin liquids to topological magnons. We present results from our ongoing study of the effect of spin wave interactions on the magnetically ordered phases of some pyrochlore spin Hamiltonians. We consider All-in-All-out (AIAO) and ferromagnetically ordered phases in a class of spin models with Heisenberg exchange and Dzyaloshinskii-Moriya interactions.

We find that the AIAO phase undergoes substantial spectral renormalisation and can potentially become unstable for small spin quantum numbers when the leading order corrections involving magnon interactions are accounted for. We present a survey of our results on the spectral renormalisation, spectra widths and two magnon continua for this class of models. We comment briefly on the effects of magnon interactions on the topological nature of band structures associated with these Hamiltonians.

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V. V. Jyothis, Kallol Mondal, Himanshu Mavani, Haraprasad Dhal, V. Ravi Chandra (work in progress)
V. V. Jyothis, Bibhabasu Patra, V. Ravi Chandra, J. Phys.: Condens. Matter 36 185801 (2024)

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Engineering flux-controlled flat bands and topological states in a Stagome lattice

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We present the Stagome lattice, a variant of the Kagome lattice, where one can make any of the bands completely flat by tuning an externally controllable magnetic flux. This systematically allows the energy of the flat band (FB) to coincide with the Fermi level. We have analytically calculated the compact localized states (CLS) associated to each of these flat bands appearing at different values of the magnetic flux. We also show that, this model features nontrivial topological properties with distinct integer values of the Chern numbers as a function of the magnetic flux. We argue that this mechanism for making any of the bands exactly flat could be of interest to address the FB superconductivity in such a system. Furthermore, we believe that the phenomenon of photonic flat band localization could be studied in the Stagome lattice structure, designed for instance using femtosecond laser induced single-mode waveguide arrays.

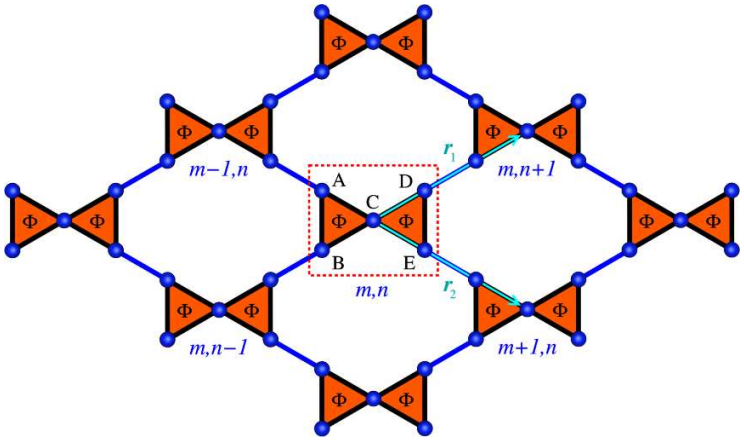

Fig. 1: Schematic diagram of a Stagome lattice geometry. The unit cell of the lattice is marked by the red dotted box. Both the triangular plaquettes in each cell are pierced by a uniform external magnetic flux Φ directed in the anticlockwise direction.

QMAT – 2024, IIT Guwahati

Non-Hermitian Many-Body Localization and Skin Effect

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Abstract: The Hermiticity of a Hamiltonian guarantees its real eigenvalues and orthogonaleigenstates. Last few years have witnessed a surge of interest in non-Hermitian physics of non-conservative systems which has led to novel and unprecedented phenomena and applications. One fascinating phenomenon that has no Hermitian counterparts is the non-Hermitian skin effect (NHSE) which describes the anomalous localization behaviour of eigenstates of a lattice with open boundaries. I will show the interplay of NHSE with the localization of a spinless fermionic lattice in the presence of a quasiperiodic potential. We examine a set of eigenstate and dynamical properties to characterize the distinction between two localization behaviours. The MBL states residing in the low-energy spectrum remain robust to non-Hermiticity, whereas the suppression in entanglement entropy indicates a strong sensitivity for the extended states. Furthermore, the time dynamics of imbalance clearly separates the two localization behaviours of a non-Hermitian many-body system. Our work presents the experimentally accessible diagnostics to realize the intriguing localization phenomena of non-Hermitian systems in quantum many-body experiments.

Frequency-selective amplification of nonlinear response in strongly correlated bosons

Aditya Prakash, Debamalya Dutta, Arko Roy, Kush Saha

In this talk, we present a protocol to generate enhanced non-linear responses of incident pulses in the density wave phase within the extended Bose-Hubbard model using the concept of resonance-induced amplification (RIA). This method enables the selection of an incident pulse frequency to amplify the desired harmonic order. We characterize the enhancement of the non-linear harmonic spectra under various frequencies and field strengths of the incident pulses, and demonstrate that an optimal field strength is necessary to realize our protocol.

Interplay of external drive and long-range hopping in the PLRBM model.

Auditya Sharma

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Indian Institute of Science Education and Research Bhopal
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We examine the impact of a time-periodic and aperiodic field on the power-law random banded matrix (PLRBM) model where variation in the power-law exponent yields a delocalization- to-localization phase transition. The transport study of the periodically driven system demonstrates that a suitably tuned time-periodic electric field induces logarithmically slow dynamics in the localized phase of the undriven system, while in the delocalized phase, we observe diffusive transport after an initial ballistic transport. Extending our analysis to the aperiodic Thue-Morse driving, we find that tuning driving parameters in a specific manner allows for exact dynamical localization in a disordered-free long-range model regardless of the long-range parameter.

Non-Equilibrium Dynamics of Ultracold Bosonic Gases: Insights from Cluster Mean-Field Theory

Deepak Gaur[1,2], Hrushikesh Sable [1,2] and D. Angom[3]

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[2] Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar - 382355, Gujarat, India
[3] Department of Physics, Manipur University, Canchipur - 795003, Manipur, India

Recent advancements in quantum technologies have been significantly influenced by the ability to dynamically control quantum states, highlighting the importance of studying out-of-equilibrium many-body dynamics. Quantum quenches, which involve altering system parameters, are a key tool for driving systems out of equilibrium and exploring new phenomena, such as quench-induced topological defects [1,2]. In this study, we analyze the non-equilibrium dynamics of ultracold atomic bosonic gases trapped in an optical lattice using the Bose-Hubbard model [3]. We investigate the dynamics of an initial Mott insulator state, subjected to a continuous quench across the quantum phase transition. Our theoretical approach employs the cluster mean-field theory to capture local quantum correlations while managing computational complexity for large systems [4]. Our calculations for a range of quench rates show evidence of critical scaling behavior consistent with the Kibble-Zurek mechanism (KZM) [1,2]. Notably, our cluster mean-field theory reveals non-trivial dynamics in the impulse domain of KZM, a feature not observed in single-site mean-field approaches [5]. Additionally, we estimate the critical exponents of the Mott-insulator to superfluid transition and explore how these exponents vary with cluster size, demonstrating that larger clusters provide more refined estimates. Our findings highlight the strength of cluster mean-field approach in a better description of non-equilibrium quantum many-body dynamics.

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Weak topological Anderson insulator in two-dimensional chiral symmetry class

Naba P. Nayak[1], **Soumya Bera**[1]

[1] *Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India*

Chiral symmetric systems in two dimensions lack conventional topological characteristics but exhibit weak topological phases induced by SSH-like staggering bonds. These phases remain stable under symmetry-preserving disorder. We explore the impact of this topology on the Anderson localization transition in the Chiral class, where localization occurs at different critical values depending on the direction, leading to an intermediate quasi-localized phase. Furthermore, this topology induces anisotropy in the transport properties of these systems. To illustrate this, we examine a bond-dimer model that features a weak-topological Anderson insulator phase alongside a trivial localized phase and a metallic phase, creating a diverse phase diagram that effectively demonstrates the interplay between topology and the Anderson transition. We also discuss the universality of this localization transition within the Chiral class.

The work is built from our recent work [1]:

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Commensurate supersolids and re-entrant transitions in an extended Bose-Hubbard ladder

Ashwath N Madhusudan, Gopal Chandra Santra, Inderpreet Kaur, Weibin Li, Rejish Nath

We discuss the ground state phases of an extended Bose-Hubbard ladder of unit filling via the density-matrix-renormalization-group method and, in particular, the effect of rung-hoppings. In contrast to a single-chain, a commensurate supersolid emerges, and based on the Luttinger parameter, we classify them into two types. The latter leads to a reentrant gapless behavior as the onsite interaction is increased while keeping all other parameters intact. A reentrant gapped transition is also found as a function of nearest-neighbor interactions. Further, we show that the string order characterizing the Haldane phase vanishes for a finite inter-chain hopping amplitude, however small it is.

Full distribution of local observables in an exactly solvable current carrying steady state of a driven XXZ chain

Sandipan Manna, G J Sreejith

Current carrying steady states of interacting spins chains exhibit rich structures generated through an interplay of current induced correlations and energetic constraints from the Hamiltonian. The XXZ spin chain when coupled to maximally polarizing Lindblad terms admits an exact solution in a matrix product state (MPS) form. We use this exact solution to study the correlations and distributions of simple local spin observables in the non equilibrium steady state (NESS). We present exact expressions for spin correlators, entropy per site, cumulant generating functions for distributions of local observables in the XX limit (Ising anisotropy $\Delta=0$). Further, we use the exact MPS solution in systems with $\Delta>0$, to numerically exactly calculate the entropy, correlations, as well as distributions of spin observables in blocks as large as $n\sim200$ sites allowing an estimation of the rate functions. The z magnetization distribution is consistent with short range spin correlations in the z direction while the x-magnetization shows a double peak structure at larger Δ suggesting short range ferromagnetic ordering. We find that the distribution of z-magnetization sharpens for parameters where the current is maximized.

Scar-induced imbalance and anomalous mid-spectrum zero modes in Rydberg ladders with staggered detuning

Mainak Pal, Krishnendu Sengupta, and Arnab Sen
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Madhumita Sarkar
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(Dated: August 15, 2024)

We consider quench dynamics in a kinetically-constrained Rydberg ladder model Hamiltonian [1], with zero and staggered detuning (Δ), and find that it exhibits weak violation of the eigenstate thermalization hypothesis (ETH), due to presence of quantum many-body scars (QMBS). The system fails to thermalize under it's own unitary evolution starting from simple high energy initial states $|\mathbb{Z}_2\rangle$ ($\Delta = 0, 1$) and $|\text{vac.}\rangle$ ($\Delta = 1$), for a time independent Hamiltonian. By studying the evolution of Shanon entropy and (von Neumann) entanglement entropy, we find that for specific parameter regimes, the nature of the revivals appear to be very different than the paradigmatic PXP model [2]. In particular near $\Delta = 1$, we find that the initial states $|\mathbb{Z}_2\rangle, |vac\rangle$ bounce back to the initial state from a non-classical state. We also find that the infinite time average values of various imbalances in longitudinal and transverse magnetizations, which are dominated by the presence of exact zero-modes, differ significantly from the expected thermal values at infinite temperature for a broad regime of parameters, implying a violation of diagonal ETH. Furthermore, significant off-diagonal matrix elements of these imbalance operators between zero and non-zero eigenmodes, lead to long lived oscillations and signal the breakdown of off-diagonal ETH.

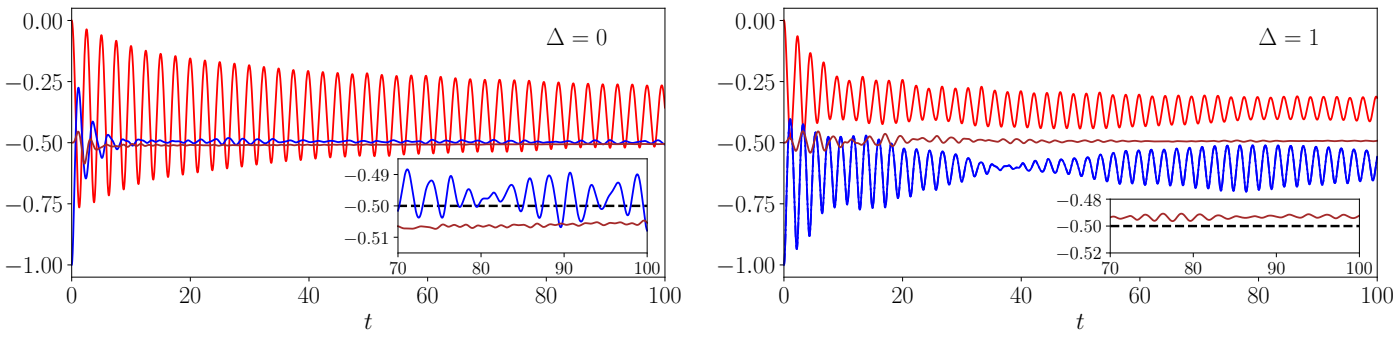

FIG. 1. Time evolution of site averaged longitudinal magnetization $\langle M_z(t)\rangle = \langle\psi(t)|\hat{M}_z|\psi(t)\rangle$ starting from simple initial states $|\mathbb{Z}_2\rangle$ (red), $|\text{vac.}\rangle$ (blue) and $|\mathbb{Z}_4\rangle$ (brown) for (a)$\Delta = 0$ and (b)$\Delta = 1$ in Rydberg ladder with $N = 32$ atoms.

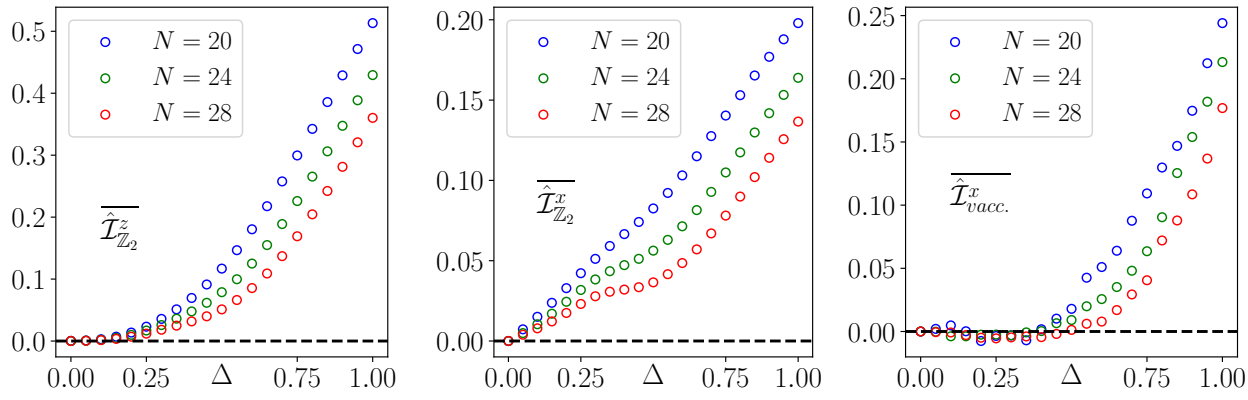

FIG. 2. Infinite time average value of local imbalances $\hat{\mathcal{I}}^z_{\mathbb{Z}_2}$, $\hat{\mathcal{I}}^x_{\mathbb{Z}_2}$ and $\hat{\mathcal{I}}^x_{vac.}$ for increasing values of Δ for $N = 20, 24, 28$.

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Temperature-induced supersolidity in spin-orbit-coupled Bose gases

Rajat, Ritu, Arko Roy, Sandeep Gautam

Close to the superfluid plane-wave (PW) - supersolid stripe (ST) phase transition point of a zero temperature quasi-one-dimensional spin-orbit-coupled Bose gas, we find that an increase in temperature induces a phase transition to the supersolid phase with a broken translational symmetry from the superfluid plane-wave phase. We use the Hartree-Fock- Bogoliubov theory with the Popov approximation to investigate the effect of thermal fluctuations on the collective excitation spectrum and investigate the softening of the spin- dipole mode corresponding to the shift in the quantum critical point. This is in stark contrast to the PW-ST phase transition in a homogeneous system where non-zero temperatures facilitate the melting of the stripe phase.

Sunday, 22nd December, 2024: [Day2]

List of Posters

Study on Exchange Bias effect in double perovskite Sm_2FeCrO_6 owing to structural deformation-induced multiple magnetic phases

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Abstract:

Recently, among other double perovskites, compounds based on A_2FeCrO_6 have shown interesting magnetic characteristics due to the presence of two 3d transition elements, namely Fe and Cr. In this present investigation we have synthesized the polycrystalline Sm_2FeCrO_6 (SFCO) sample using conventional solid-state reaction method for the first time. The single-phase monoclinic structure with a P21/n space group is identified by the Rietveld refinement of the XRD pattern recorded at room temperature. FESEM micrographs of the gold-coated pelletized sample are displayed, and the average particle size of the system is estimated by plotting the histogram with a Gaussian fit. The existence of mixed valence states of Fe and Cr ions is confirmed by X-ray photoelectron spectroscopy. Temperature dependent resistivity data under 0 kOe and 60 kOe magnetic field reveals the semiconductor like behavior of the SFCO system in the temperature range of 160 K to room temperature. To provide the explanation of electron hopping from this resistivity data, the density of localized states $(N(E_F))$, hopping energy (W) and hopping range (R) are estimated by fitting the VRH model and the activation energy (E_a) is also estimated by fitting the Arrhenius law. In addition, the temperature-dependent dc magnetization data of the sample shows that the zero-field cooled (ZFC) and field cooled (FC) curves begin to diverge significantly below 250 K. At 15 K, the ZFC curve exhibits a cusp-like behavior that is indicative of an antiferromagnetic, Néel transition. More interestingly, Non-saturation like behavior of the M-H curve at around 8 K and the low value of M_s has been observed which indicates the presence of multiple magnetic phases at lower temperature. A signature of the conventional Exchange Bias effect has been noticed with different cooling field and the maximum peak shift of 4 kOe is observed with 50 kOe cooling field. We have also reported the corresponding Training effect study of the sample here.

Integrability and Periodic Driving in Quantum Metrology

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Abstract:

Quantum metrology aims to improve the precision with which we estimate a parameter of interest. While the shot noise limit bounds classical metrology, that is not true for its quantum counterpart. However, quantum metrology has predominantly concentrated on leveraging quantum enhancements in integrable systems. Systems are frequently prepared to achieve these enhancements in non-classical states, notably entangled or squeezed states. However, recent research suggests the largely untapped potential in exploring periodically driven quantum-chaotic systems that could revolutionize the sensitivity and robustness of quantum sensors [1, 2].

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Designing higher-order saddle points and flat bands by long range hopping in kagome lattice

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We investigate the two-dimensional tight-binding model of kagome lattice incorporating nearest neighbor, next nearest neighbor, and second next nearest neighbor hopping integrals. Introducing a second next neighbor hopping parameter can not only induce flat bands in the band structure but also generate twofold degenerate flat bands. Additionally, by systematically tuning the next nearest neighbor hopping, higher-order van Hove singularities can be achieved. These singularities exhibit a power-law divergent density of states, leading to interesting phenomena such as atypical superconductivity and strong electron correlation. Our theoretical proposals aim to inspire experimentalists to design two-dimensional model systems where higher-order van Hove singularities coexist with flat bands.

Title : Localization transition in non-Hermitian quasicrystals with long-range hopping

Abstract : In this study, we examine the effect of long-range hopping in a one-dimensional non-Hermitian Aubry-Andre model with a generalized quasiperiodic potential. It has been already shown that in the absence of long-range hopping the system exhibits a re-entrant delocalization transition along with real-complex and spectral topological transitions as a function of the non-Hermiticity parameter in the model which is the complex phase in the quasiperiodic potential. Here we show that when long-range hopping is introduced, the reentrant delocalization and real-complex-real transitions linked to reentrant PT symmetry are disrupted, leading to a complex-to-real transitions. The fraction of delocalized states, which can be separated from localized or multifractal states, varies with the choice of the quasiperiosity in the model. Additionally, the entanglement entropy of non-interacting many-body ground states follows the area law in the localized region, but logarithmically violates this law in the delocalized region.

Electronic and magnetic properties of Sr_2FeTiO_6 implementing ab initio density functional theory

Debarghya Dutta
Center for Research in Nanotechnology and Science,
Indian Institute of Technology Bombay, Maharashtra - 400076

Abstract

3d transition metal-based double perovskites present a rich platform for exploring the effects of electron correlation (U) and Hund's coupling (J_H). Sr_2TiFeO_6 is a notable compound in this category, featuring magnetic Fe^{4+} and nonmagnetic Ti^{4+} ions occupying the B/B' sites. In this study, we performed a theoretical investigation of the ground state structure, electronic, and magnetic properties using Density Functional Theory (DFT). The Hubbard U parameter was included to accurately represent the correlation effects within the Fe d orbitals. Our electronic density of states (DOS) calculations reveal that the FM state exhibits metallic behavior, with distinct contributions from the two Fe atoms indicating mixed valence states of Fe^{3+} and Fe^{4+}. This underscores the crucial role that Fe d-states play in determining the electronic and magnetic characteristics of Sr_2TiFeO_6. Furthermore, the calculation of exchange interactions suggests a predominant antiferromagnetic interaction between Fe atoms, complemented by a weaker ferromagnetic component. This nuanced interplay between magnetic interactions emphasizes the complexity and richness of the magnetic behavior in Sr_2TiFeO_6.

Tuning Optical Phonons: An approach to achieve ultralow lattice thermal conductivity in $TlIn_{0.5}Ga_{0.5}Te_2$

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We investigate the microscopic mechanism of ultra-low lattice thermal conductivity in $TlGaTe_2$ and $TlInTe_2$ by combining first-principles density functional theory and Wigner framework based unified theory of lattice heat transport which considers the contributions arising from both particle-like phonon propagation and wave-like phonon tunnelling[1-2]. The particle-like phonon contribution is calculated from the diagonal elements of heat-flux matrix, which is exactly same as the Pierels-Boltzmann transport equation (PBTE) and the wave-like phonon is calculated using the off-diagonal (OD) elements of the heat flux matrix. We show that Ioffe-Regel limit in space is more accurate than Wigner-limit in time to represent the nonsharp particle-wave crossover of phonons. The calculated thermal conductivities of $TlGaTe_2$ and $TlInTe_2$ are 0.736 and 0.537 W/mK considering normal 3-ph scattering, Umklapp scattering, OD terms and the additional grain boundary scattering, which agree well with previous experimental reports[3-4]. We found that optical phonons dominate in heat transport in both the materials, which is very unusual. For example, In $TlInTe_2$, the contribution of acoustic phonons is only 38% and optical phonons contribution is 62%. So, the challenge was tuning optical phonons to reduce the lattice thermal conductivity. We substitute 50% Ga in $TlInTe_2$ and find the reduction of optical phonon frequencies and the contribution of acoustic phonons has been increased to 52%. The lattice thermal conductivity of $TlIn_{0.5}Ga_{0.5}Te_2$ also reduced to 0.482 W/mK at 300 K. The origin of lower lattice thermal conductivity in $TlGa_{0.5}In_{0.5}Te_2$ coming from the avoided crossing in the phonon dispersion due to two separate atoms at same lattice site. Our analysis reveals that though particle-like phonon propagation dominates in this class of compounds but there is a 24-34% contribution of wave-like phonon at 800 K and it increases with the temperature. We found the contribution of wave-like phonons increased to 34% in $TlIn_{0.5}Ga_{0.5}Te_2$ from 27% in $TlInTe_2$, which is a clear evidence of more disordered nature of $TlIn_{0.5}Ga_{0.5}Te_2$. We suggest a strategy to reduce lattice thermal conductivity by tuning optical phonons adding avoided crossings by substituting a different atom at the same lattice site.

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Exploring microscopic origin of ferroelectric and magnetic properties in Lu_2CoMnO_6

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Off late Double perovskites are receiving significant attention in recent research due to their variety of applications [1]. Derived from simple perovskite structure ABO_3 (where A is a large electropositive cation and B is a small transition metal ion), these classes of materials have diverse chemical and physical properties, ranging from insulating to metallic electronic structures and several magnetic orderings, including antiferromagnetic, ferromagnetic, and frustrated states. This versatility is due to the structural and compositional flexibility of the perovskite framework [2,3]. With the advent of spin frustrated multiferroics, where in ferroelectricity is driven by exotic magnetic ordering rather than non-centro-symmetric crystal structure, understanding rare earth based double perovskites ($RE_2B'B''O_6$) becomes crucial where partial or complete cation substitution at different degrees at R and B', B" sites provide more flexibility to tailor the physical properties [4]. Thus, exploring and innovating magnetic materials like double perovskites is crucial for advancing material science, as they provide exceptional solutions for efficient, sustainable, and high-performance technologies.

Here, we present synthesis and characterization of Lu_2CoMnO_6 double perovskite by employing ceramic route where high purity constituent oxides were mixed in stoichiometric ratio then grinded and calcinated at appropriate temperature. Phase formation was confirmed by powder x-ray diffraction (XRD) employing Benchtop x-ray powder diffraction system. The figure 1 shows Rietveld [5] fitted x-ray diffractogram, which confirms the compound crystallizes in monoclinic structure with $P2_1/n$ space group and refined lattice parameters are a = 5.1808(9)Å b = 5.5635(5)Å c = 7.4361(1)Å and β = 90.359(2)° along with 7.5 % of CoO and 0.76 % of Lu_2O_3 secondary phases which can be eliminated by sintering at appropriate temperature. We are in process of carrying temperature dependent magnetization along with isothermal magnetization and dielectric study to understand magnetic interactions, and electric properties. We will then perform temperature dependent neutron diffraction studies to microscopically explore role of antisite disorder in magnetic structure and correlate ferroelectric and structural parameters.

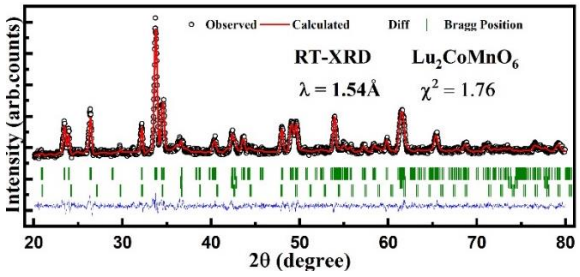

Figure 1: Room temperature Rietveld fitted x-ray diffractogram of Lu_2CoMnO_6.

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Title: "Investigating Topological Ferromagnetism in RMn_6Sn_6 (R = Lu, Mg) Kagome Lattices: Impact of Dimensionality Reduction"

Abstract: Over the past decade, research has increasingly focused on topological materials with non-trivial geometric phases and correlated systems with robust interactions, marking a cutting-edge frontier in quantum matter studies. A major challenge is the minimal electron-electron correlations in many topological materials, which can be addressed by increasing the density of states near the Fermi level. The Kagome lattice, with its unique electronic structures like flat bands and van Hove singularities, has emerged as a promising candidate for enhancing these correlations. Recent efforts have shifted to three-dimensional Kagome systems where layers are combined with other atomic layers, aiming to preserve the Kagome layers' characteristic properties through weak coupling. Transitioning to slab Kagome structures offers a versatile platform for exploring fundamental physics and novel engineering functionalities. The disruption of symmetries, such as inversion (IV), Time reversal (TR), mirror symmetries, has been pivotal in revealing various topological phases. Kagome ferromagnets, incorporating magnetism and spin-orbit coupling, can host diverse phenomena such as Dirac cones, Weyl chirality, and exotic quantum phases like spin liquids. These properties make them valuable for applications in spintronics, quantum computing, and energy conservation. Using ab-initio Density Functional Theory in our study of the inter-metallic RMn_6Sn_6 Kagome compound, which features a combination of ionic and valence bond characteristics, we find that the Mn bi-layers exhibit antiferromagnetic (AFM) spin orientation with respect to each other for R=Lu and ferromagnetic (FM) for R=Mg as Nearest neighbour effective Heisenberg Spin Hamiltonian is being solved for the energy equation of (G-AFM, C-AFM, A-AFM & FM) all possible magnetic configuration. Then the Charge density Contour plot was introduced where valence electron cloud overlap is a measure of bond strength. With the motivation of dimensionality reduction we obtain ferromagnetic ordering regardless of its bulk's magnetic nature. Out of the pair RMn_6Sn_4 , RMn_6Sn_8 the later is an Sn rich FM slab. In the vicinity of the Fermi level E_F which is particularly relevant for the metallic region of interest, significant characteristics such as flat bands, linear crossings, and subsequent phenomena like anti-crossing and band inversion induced by spin-orbit coupling (SOC) were observed using both the PBE and PBE_sol functionals (GGA approximation). The inclusion of the on-site Coulomb interaction energy U resulted in noticeable modifications in the flatness of bands near the Fermi level, emphasizing its influence on the electronic structure within this energy range. To calculate the topological properties, maximally localised Wannier functions for each structure were computed to derive a tight-binding model from ab-initio calculations using WANNIER90 code. In the investigation of the topological properties of the spin-split bands in the metallic system, after TR symmetry breaking (applying SOC) we specifically began by computing Berry curvature(BC) by Kubo formula and the Chern number by integrating the BC using pair of bands forming the anti-crossing to assess their nontrivial nature. For those pairs, subsequently we analysed Nodal points with opposite chirality projected in the first Brillouin zone and also calculated Anomalous Hall Conductivity (AHC) (which is reduced while going from bulk to slab of Mg based) . Their low (AHC) enables efficient spin current manipulation, reduces energy dissipation, and supports rapid data operations, making them ideal for low-power MRAM and magnetic domain-wall memory. Additionally, they enhance MRI capabilities, improve diagnostic contrast, and facilitate efficient energy conversion for thermo-electric generators and energy harvesting devices. 'Chemistry vs Structure' comparison between Lu and Mg based bulk and slabs, shows that integrating constituents of Mg-based and Lu-based compounds into each other's lattice parameters while preserving the magnetic state reveals that the stability of the resulting magnetic state is primarily influenced by chemical composition rather than lattice parameters. In conclusion the take home message is that this observation underscores the significant role of chemical interactions in determining magnetic stability, suggesting that magnetic behavior is intricately linked to chemical environment rather than structural framework alone.

Quantization of Thermal Hall Conductance under Edge Reconstruction

Amulya Ratnakar, Sampurna Karmakar and Sourin Das

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Four-terminal charge and thermal conductance [1] are of special significance in quantum Hall physics, as they carry topological signatures. Although one might expect the quantization of conductance to break down in the presence of backscattering across the bulk, we aim to demonstrate that a finite amount of backscattering does not alter the quantization in a four-terminal geometry. However, when edge reconstruction is coupled with backscattering, significant deviations of the conductance from quantized values can occur; in some cases, these deviations continue to reflect a topological invariant, while in others, they do not. In this talk, we'll explore this phenomenon in light of recent advancements in accurately measuring thermal Hall conductance in quantum Hall systems. Building on the insights from Ref. [2], which examines the effects of interedge backscattering on electrical Hall conductance in the integer quantum Hall regime, we theoretically investigate the robustness of four-terminal thermal Hall conductance in the integer quantum Hall system under various edge reconstruction scenarios [3, 4]. Our analysis extends to systems with varying numbers of upstream and downstream modes, including both charge and neutral modes. I will present results showing that when upstream charge and neutral modes are present in a quantum Hall system, the corresponding Hall conductance deviates from the expected bulk topological value, shifting to distinct plateau levels based on the specific set of edge modes transmitting through the quantum point contact.

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Title: Study of interaction-driven phases in the half-filled Two-Dimensional Su-Schrieffer-Heeger model

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Abstract:
Topological states of matter have been widely studied as being driven by an external magnetic field, intrinsic spin-orbital coupling, or magnetic doping in various lattice systems and the discovery of Quantum anomalous hall (QAH) state with time-reversal symmetry (TRS) breaking in the absence of a magnetic field is one of the cornerstone. Recently alternative routes of realizing QAH have been explored in which Interaction-induced spontaneous TRS breaking provides a distinct route to realizing QAH states in correlated matter. Such QAH orderings have been argued to exist in two-dimensional semimetals with trivial topology with vanishing (Dirac band crossing) as well as finite density of states (Quadratic band crossing, QBT) at the Fermi level in mean-field calculations. Although the former case is quite controversial, several exact diagonalization calculations have proposed conflicting viewpoints against mean field calculation in the context of the presence of the QAH phase in Dirac band touching systems. The presence of the QAH phase in QBT systems is unequivocally established by several exact calculations. Here We study the quantum phases driven by interaction in a semimetal with a quadratic band touching at the Fermi level in a 2D spinless SSH model with an extended fermion-Hubbard interaction at the mean-field level. We have found TRS broken QAH like phase and we will discuss various interesting charged order phases emerging out of interactions.

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

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

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Modulation of Structural and Electronic Phases in Two-dimensional $PdSe_2$

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Tuning the ambipolar behaviour in charge carrier transport via defect-engineering is crucial for achieving high mobility transistors for nonlinear logic circuits. Here, we present the electric-field tunable electron and hole transport in a microchannel device consisting of highly air-stable van der Waals (vdW) noble metal dichalcogenide (NMDC), $PdSe_2$, as an active layer. Pristine bulk $PdSe_2$ offers ambipolar transfer characteristics with a slight electron dominance recorded in field-effect transistor (FET) characteristics showing an ON/OFF ratio < 10 and electron mobility ~21 $cm^2/(V.s)$. However, transfer characteristics of $PdSe_2$ can be tuned to a hole-dominated transport while using hydrochloric acid (HCl) as a *p*-type dopant. On the other hand, the chelating agent EDTA, being a strong electron donor, enhances the electron-dominance in $PdSe_2$ channel. In addition, *p*-type behaviour with a 100 times higher ON/OFF ratio is obtained while cooling the sample down to 10 K. μ-focused angle-resolved photoemission spectroscopy also resembles the *p*-type band structure of $PdSe_2$ single crystal at low temperature. In addition, the pressure-induced structural modulation associated with metallization were also investigated by high pressure X-ray diffraction and Raman spectroscopy study. $PdSe_2$ exhibits anomalous in-plane expansion under hydrostatic pressure. Around 4.7 GPa, it undergoes an orthorhombic to pyrite (cubic) structural transition with a significant reduction of the interlayer vdW gap resulting in a 3D network. Raman spectroscopy and *ab initio* electronic structure calculations at the transition pressure regime reveal anomalous phonon mode softening with the weakening of Se-Se dimer bonds and interlayer charge transfer followed by a semiconducting to metallic transition. Also, around 9 GPa, a new low symmetric phase evolves and coexists with the cubic phase. Such an anisotropic and puckered vdW architecture may open up new possibilities towards next-generation electronics as well as exotic superconducting phases under external perturbation.

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Stain induced evolution of band edge alignment and excitonic lifetime in vdW heterostructure: A case study of $CrMo_3S_8/CrW_3S_8$

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Abstract:

In this study, we present the first-principles calculations to investigate the excitonic properties and band edge alignment of the $CrMo_3S_8/CrW_3S_8$ van der Waals heterostructure, with a particular focus on the impact of strain. Firstly, Density functional theory (DFT) based first-principles electronic structure calculations is conducted on the heterostructure, enabling us to examine the band edge alignment. Due to the crucial role of excitonic effects in optoelectronic devices we calculate the exciton energies and its strengths by GW-Bethe Salpeter Equation(BSE) method. This information allows us to further determine the exciton radiative lifetime.
The influence of lateral strain on the heterostructure is then systematically explored.We analyse how strain modifies the band edge alignment, potentially altering the charge transfer dynamics. Additionally, we examine the strain-induced changes in exciton radiative lifetime. The ability to predict and control radiative lifetimes in these 2D materials through strain offers promising avenues for their application in solar energy conversion and other optoelectronic technologies. By understanding the interplay between strain, band alignment, and excitonic behaviour, we aim to contribute to the development of advanced, tunable devices based on van der Waals heterostructures.

Keywords: *Density Functional Theory; Exciton Radiative Lifetime; GW-BSE; Band edge alignment; heterostructures*

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Theoretical quest for type-II band edge alignment and higher excitonic radiative lifetime of $KBi(PS_3)_2/NaSb(PS_3)_2$: An insight from strain manipulation

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Our theoretical investigation attempts to envisage the electronic and optical properties, band edge alignment, Power Conversion Efficiency(PCE) and the excitonic radiative lifetime for the chalcophostates - $KBi(PS_3)_2/NaSb(PS_3)_2$. We aim to explore different possible stacking constructed from monolayers of $KBi(PS_3)_2$ and $NaSb(PS_3)_2$ and consider the structure with the minimum ground state energy for further calculations using first principles Density Functional Theory (DFT). The band structures of chalcophosphates which are semiconductors with a reported band gap of ~2 eV are aligned according to the vacuum level in order to check their band edge alignment. The absorption spectra and excitonic lifetime are computed based on the GW-BSE method. Strain is a useful stimulus in tuning the electronic as well as optical properties. Our investigation explores the response of the chalcophosphates with increasing strain with a focus on the possible changes in it's band gap, optical behaviour, notably the optical absorption spectra and the effective mass of the charge carriers. We also observe the variation of excitonic lifetime with strain. The responses of the chalcophosphates under varying strain proves it to be a potential candidate for photovoltaic devices that can have significant impact in designing novel optoelectronic devices.

Keywords: DFT, Band Edge Alignment, Excitonic lifetime, PCE, Strain.

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Transport properties of the 2D SSH in Quantum Hall Regime

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In this study, we investigate the transport properties of a two-dimensional Su-Schrieffer-Heeger (2D SSH) model in the quantum Hall regime using the non-equilibrium Green's function (NEGF) formalism. The device Hamiltonian, where the 2D SSH model serves as the channel, is constructed using a nearest-neighbour tight-binding model. A perpendicular magnetic field is introduced, and its effects are incorporated into the contacts via Peierls substitution. By varying the magnetic field, we observe that a transition is induced from a gapped phase to a regime showing flat band at the zero energy. This transition is characterised by emergence of highly localised states in the bulk, as observed by local density of states (LDOS) calculations. Moreover, transmission measurements indicate a shift from insulating to metallic behaviour, driven by the magnetic field when analysed along kx POBC. By studying the energy spectra, we observe the formation of Landau levels. Our results reveal that the non-degenerate and degenerate landau levels (transmission modes) vary as integers or odd integers depending on the strengths of diagonal, intercell, and intracell hopping. Additionally, when transport properties are analysed for the ky POBC, we observe that edge modes play a crucial role in facilitating ballistic transport.

Effect of Rashba Spin orbit coupling on monolayer and bilayer graphene

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Key Words: Graphene monolayer, Rashba Spin-orbit coupling, staggered potential

Graphene is an emerging material to study spintronics as it has low spin-orbit coupling strength, high electronic charge mobility and negligible hyperfine interaction. We are studying the effect of extrinsic spin orbit coupling on monolayer graphene. This extrinsic effect is done using Rashba spin orbit coupling (RSOC) by applying external electric field perpendicular to the plane of graphene or interaction with the substrate. Also, the modification occurs in the band structure of graphene on applying staggered potential along with RSOC. We can further study the trigonal wrapping (TW) on graphene [1] which shows results that are analogous to bilayer graphene. This TW can be seen with in a contour plot with a finite strength of Rashba coupling constant. Further, we also investigate the energy band spectrum of bilayer graphene and observe the properties similar to monolayer graphene. But within low energy approximation, it was found that there is formation of chiral quasiparticles instead of Dirac fermions in bilayer graphene due to the parabolic nature of energy band spectrum [2].

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Universal properties of single-particle excitations across the many-body localization transition

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Understanding the nature of the transition from the delocalized to the many-body localized (MBL) phase is an important unresolved issue. To probe the nature of the MBL transition, we investigate the universal properties of single-particle excitations produced in highly excited many-body eigenstates of a disordered interacting quantum many-body system. In a class of one-dimensional spinless fermionic models with random disorder, we study the finite-size scaling of the ratio of typical to average values of the single-particle local density of states and the scattering rates across the MBL transition. Our results indicate that the MBL transition in this class of one-dimensional models of spinless fermions is continuous in nature. For various ranges of interactions in the system, the critical exponent ν with which the correlation length ξ diverges at the transition point W_c, $\xi \sim |W - W_c|^{-\nu}$, satisfies the Chayes-Chayes-Fisher-Spencer(CCFS) bound $\nu \geq 2/d$ where d is the physical dimension of the system. We also discuss why the critical exponent obtained from finite-size scaling of the conventional diagnostic of many-body localization, the level-spacing ratio, strongly violates the CCFS bound while the single-particle density of states and scattering rates are consistent with the CCFS criterion.

Jana, Chandra, Garg Phys. Rev. B **109**, 214209 (2024)

Abstract

Combining transport and magnetization measurements, we discover the emergence of a tricritical point connecting the antiferromagnetic, metamagnetic and paramagnetic region in $MnBi_2Te_4$, a magnetic topological insulator candidate which can potentially exhibit axion electrodynamics. We observe a unique magnetic field driven phase diagram where the second order antiferromagnetic to paramagnetic phase boundary bifurcates into two first order lines at the tricritical point. The two first-order lines enclosing the metamagnetic phase eventually terminate at the quantum critical end points with the application of magnetic field.

Combining transport and magnetization measurements, we discover the interplay of both on the chiral orbital currents developed in $Mn_3Si_2Te_6$, a ferrimagnetic nodal line semiconductor which shows colossal magnetoresistance. We observe that with doping the Te atoms with Se, the chiral orbital currents become weaker and thus affect the magnetoresistance of the sample. We see that the easy axis which previously do not portray any colossal magnetoresistance starts showing considerable drop in resistance on application of magnetic field.

Abstract

The Aharonov-Bohm (AB) caging effect describes the extreme localization of particles in certain tight-binding lattices when subjected to a magnetic field. Traditionally, AB caging is associated with non-interacting particles; however, interactions typically disrupt this caging, allowing particles to escape. In this study, we show that under specific conditions, interactions can actually restore AB caging. We analyze a system of two ultracold bosons on a diamond lattice, which are subject to both onsite and nearest-neighbor interactions in the presence of an artificial gauge field. Our results indicate that when these interactions are of comparable strengths, AB caging is reinstated. Additionally, we find that this restoration of AB caging in interacting particles can lead to an inverse Anderson transition in the presence of onsite disorder. These insights could pave the way for realizing AB caging and inverse Anderson transitions in interacting particle systems via quantum gas experiments.

Planar Hall Effect in Quasi-Two-Dimensional Materials

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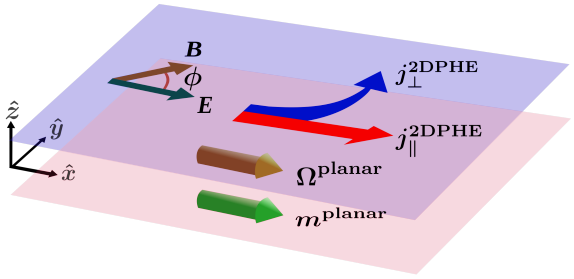

FIG. 1. Schematic for 2D planar Hall effect (2DPHE). Layered 2D materials host hidden planar Berry curvature ($\boldsymbol{\Omega}^{\text{planar}}$) and planar orbital magnetic moment ($\boldsymbol{m}^{\text{planar}}$) arising from inter-layer tunneling. The $\boldsymbol{\Omega}^{\text{planar}}$ and $\boldsymbol{m}^{\text{planar}}$ combine with the in-plane electric and magnetic field to induce a longitudinal and transverse current in the 2D plane.

The planar Hall effect (PHE) is the generation of longitudinal and transverse voltages in the plane of the applied electric ($\boldsymbol{E}$) and magnetic fields ($\boldsymbol{B}$). In 3D materials, PHE generally originates from the coupling of the Berry curvature (BC) and orbital magnetic moment (OMM) to the band velocity and in-plane magnetic field. However, the Berry curvature-induced conventional planar Hall effect is forbidden in 2D systems as the out-of-plane Berry curvature cannot couple to the band velocity of the electrons moving in the 2D plane. The only resort to this issue is having a planar component of BC and OMM, and thereby in our letter we raise the question: do the planar BC and OMM really vanish in quasi-2D system? The answer is affirmative: a quasi-2D system might have a finite interlayer tunneling induced nonzero planar components of BC and OMM; provided the system possess either of broken inversion or time-reversal symmetry.

The linear ($\sim \boldsymbol{E}$) planar current can be expanded in powers of $\boldsymbol{B}$ and written into the form

$$j_a = \tau\chi_{ab;c}E_bB_c + \tau\chi_{ab;cd}E_bB_cB_d \ , \tag{1}$$

where, τ is the electron scattering time, $\{a,b,c,d\} \in \{x,y\}$ are the 2D Cartesian coordinates, and the Einstein summation convention is used. Following semiclassical Boltzmann transport formalism, we provide the detailed expression of each of these response tensors, and segregated them into three parts based on distinct quantum geometric origin: i) first part involves BC only, ii) second part involves only OMM, and iii) third part is composed of mixed terms involving both BC and OMM. Alongside the fundamental $(\mathcal{P},\mathcal{T})$ symmetry analysis, we also study a complete 2D crystalline symmetry restrictions. Based on our symmetry analysis, we choose uniaxially strained bilayer graphene to demonstrate the 2DPHE in a real sample. The results are depicted in Fig 2. Interestingly, as one may note, the 2DPHE being a Fermi surface phenomenon peaks around the band edges where the Van Hove singularities exist. In BLG, the Van Hove singularities also correspond to topological Lifshitz transitions. Thereby, 2DPHE may be employed as an essential probe to detect topological Lifshitz transitions in quasi-2D materials.

Our proposed 2DPHE is an important addition to the different fascinating observations in topological 2D materials and ignites further exploration of hidden planar band geometry-induced 2DPHE and related transport phenomena for innovative applications.

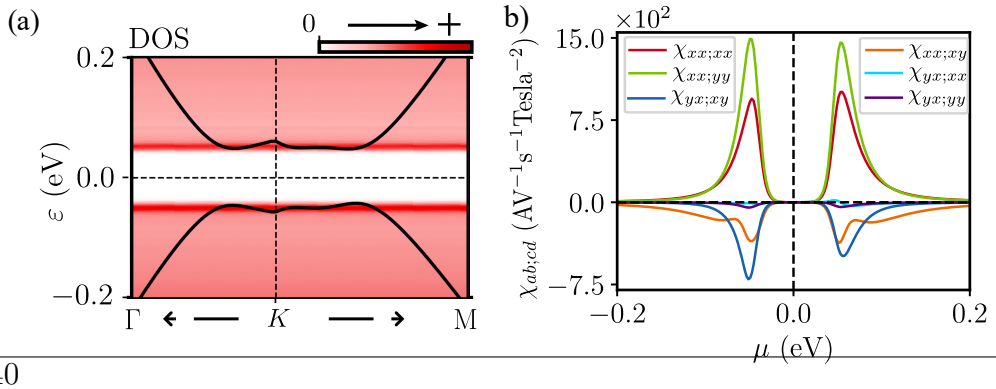

FIG. 2. (a) Electronic band structure of strained BLG around the K point, with the background color showing the density of states (DOS). (b) Different components of 2DPHE response tensors $\chi_{ab;cd}$ as a function of μ evaluated at temperature $T = 50$ K.

Abstract for poster presentation

Origin of resistive state switching in titanate spinel with low threshold electric-field

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Material systems exhibiting a transition from a Mott insulating to conducting state under the application of a small threshold current/electric field are extremely promising for a plethora of potential applications in the field of electronic devices and memory technology. Furthermore, they can provide unique platform to study the non-equilibrium phenomena and underlying microscopic mechanism in such systems. However, manifestation of resistive switching with very small threshold field have rarely been achieved in transition metal spinel oxides. Only a few transition metal oxides/chalcogenides systems have been found to exhibit such a resistive-state transition with a typical threshold electric field (E_{th}) ~ several kV/cm. Mott breakdown with a small threshold field (E_{th}) has recently been identified in the family of spinel oxides, more precisely in V-doped $MgTi_2O_4$ with E_{th} ~ 40 V/cm at 50 K. High-current-induced charge transfer from Ti^{3+} to V^{3+} softens the Jahn-Teller(JT)-effect-driven structural transition, which gives rise to metallicity. Here, we have investigated the resistive switching properties of magnesium titanate oxides. The system undergoes the breakdown at a much smaller threshold field (~ 60 V/cm at 40 K) than the Zener breakdown limit (~kV/cm). The electric-field induced low resistive state is metastable and the system returns to its initial high resistive state when the applied field or voltage is turned off manifesting volatile resistive switching (VRS) or threshold switching as coined the other way. Interestingly, our system demonstrates a forming free and stable threshold switching with negligible cycle to cycle variations in switching voltages. Further, systematic investigations predict a non-thermal origin for the observed switching phenomena. Also the very low threshold field requirement in our system will benefit in terms of low power consumptions. Our study underlines that the current- or electric field-induced phase transition provides useful pathways to create tunable resistors/selectors based on titanate spinels for low-temperature applications. Threshold switching devices also have shown potentials in imitating the imperative neural characteristics to be implemented as artificial neurons in the neuromorphic engineering.

Keywords: Threshold field, Volatile resistive switching, Forming free switching, Selectors, Artificial neurons.

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Evolution of Structural and Magnetic Properties in $Fe_2Cr_{1-x}V_xAl$ ($0 \leq x \leq 1$) Alloys

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Abstract:

Existence of disorder in crystal structure can be significant in deciding physical properties, thus microscopic understanding of disorder is crucial for investigating novel phenomenon. Few iron based full Heusler compounds are theoretically predicted to be half-metallic [1] which have tremendous applications in spintronics [2]. The present study investigates the evolution of structural and magnetic properties in the $Fe_2Cr_{1-x}V_xAl$ ($0 \leq x \leq 1$) alloy series, with a focus on understanding the role of disorder in establishing intriguing magnetic behavior. Previous literature reports that Fe_2VAl stabilizes in the $L2_1$ structure without structural disorder. However, substituting Cr at the V site introduces anti-site disorder, particularly between the Fe & Al and Cr & Al sites [3]. We synthesized Fe_2CrAl using arc melting, and the phase purity was confirmed through x-ray and neutron diffraction analyses. Magnetization studies revealed that Fe_2CrAl undergoes a magnetic transition across a range of temperatures, indicating complex magnetic behavior. Remarkably, distinct magnetic properties were observed both below and above the ordering temperature, suggesting a nuanced and intricate magnetic behavior [2]. Further analysis through neutron diffraction at various temperatures (3 - 300 K) confirmed the presence of anti-site disorder between the Cr and Al sites in Fe_2CrAl. We are currently conducting temperature-dependent neutron diffraction studies on other compositions within the $Fe_2Cr_{1-x}V_xAl$ series. This work aims to establish the degree of anti-site disorder and its correlation with the observed magnetic properties, providing deeper insights into the structure-property relationships in these materials.

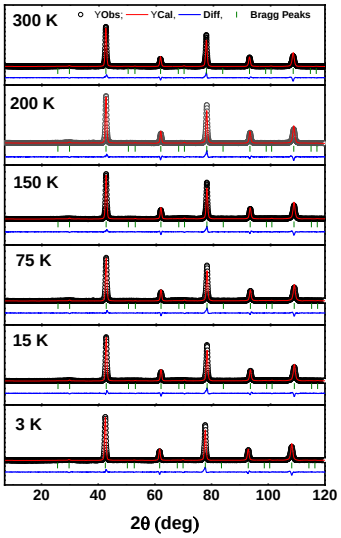

Figure: Temperature dependent neutron diffraction of Fe_2CrAl.

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Signature of criticality in angular momentum resolved entanglement of scalar fields in $d > 1$

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ABSTRACT: The scaling of entanglement entropy with subsystem size fails to distinguish between the gapped and the gapless ground states of a scalar field theory in $d > 1$ dimensions. We show that the scaling of the angular momentum resolved entanglement entropy S_ℓ with the subsystem radius R can clearly distinguish between these states. For a massless theory with momentum cut-off Λ, $S_\ell \sim \ln [\Lambda R/\ell]$ for $\Lambda R \gg \ell$, while $S_\ell \sim R^0$ for the massive theory. In contrast, for a free Fermi gas with Fermi wave vector k_F, $S_\ell \sim \ln [k_F R]$ for $k_F R \gg \ell$. We show how this leads to an "area-log" scaling of total entanglement entropy of Fermions, while the extra factor of ℓ leads to a leading area law even for massless Bosons. At finite temperatures, we find that there is a crossover in the scaling of S_ℓ from the $T = 0$ logarithmic scaling to a high T linear scaling $S_\ell \sim \pi T R/3$. The logarithmic scaling exists for larger subsystem sizes for larger values of ℓ. We provide estimates of temperatures and subsystem sizes where this critical scaling can be seen in experiments on ultracold atoms.

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Magnetization and neutron characterization of Kagome compound $Nd_3Sb_3Mg_2O_{14}$.

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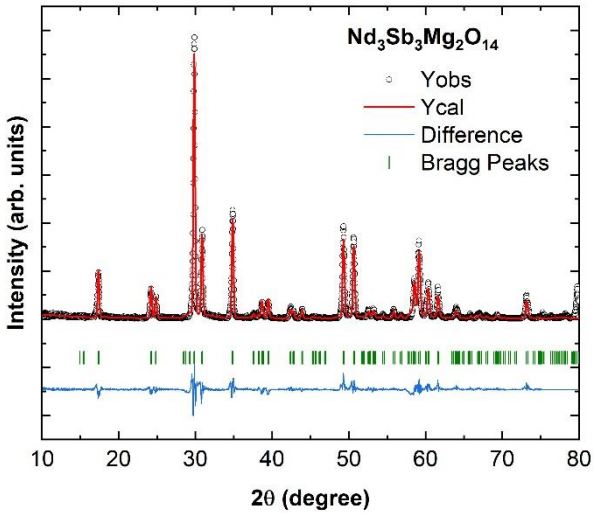
Our work is focused on investigating physical properties, as well as the crystal and magnetic structures, of the Kagome compounds that exhibit geometric frustration.

One promising class of materials in the material science research are the derivatives of pyrochlore compound with general formula $RE_3Sb_3A_2O_{14}$, (RE = Rare earth, A = Zn, Mn, Mg etc.) which are theoretically predicted to exhibit quantum spin liquid (QSL) behavior. Pyrochlore lattices, characterized by their arrangement of A3B and B3A layers, form a Kagome lattice when non-magnetic ions are introduced at the A site. This Kagome lattice provides an isolated two-dimensional (2D) triangular geometry that leads to frustration, a condition where spins tend to stay entangled and do not settle into a conventional ordered state down to absolute zero temperature. This makes such materials strong candidates for QSL behavior [1], which have potential application in intriguing research area like quantum computation, data storage and several others.

In our work, we report on $Nd_3Sb_3Mg_2O_{14}$, synthesized via a ceramic route. We used high-purity (≥99.9%) precursors, which were sintered at 1350°C for 48 hours with intermediate grindings. Structural analysis via X-ray diffraction confirmed the formation of a single phase. We have also prepared other samples in this series, including $Ho_3Sb_3Zn_2O_{14}$ and $Pr_3Sb_3Zn_2O_{14}$, with results for the former expected to be detailed in an upcoming manuscript. Our preliminary findings are encouraging and suggest that further investigation is needed to confirm QSL behavior [2,3]. Future experiments like neutron diffraction and specific heat in milli-Kelvin temperatures will be crucial for verifying the quantum spin liquid characteristics of the compound in question [4].



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Quantum Otto engine using Kitaev clusters

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In small-sized clusters, we study the four-stroke Otto engine. The clusters consist of a few sites, and there are spin-spin interactions among the sites. In the background of Kitaev interaction, we consider the presence of Heisenberg and Γ interaction, along with a finite magnetic field in the $\hat{z}$-direction. We see this engine, depending on the parameter values, can operate in four different modes: heat engine, refrigerator, heat accelerator, and heat distributor. We find that these regions are almost cluster-size independent. We investigate in detail, how the performance depends on the cluster size and whether the non-Kitaev interactions have any advantage on the engine performance. We notice that there is a significant enhancement of efficiency of a heat engine when competing Kitaev and Heisenberg interactions are present, instead of just the Kitaev one; efficiency decreases when they are of the same sign. The presence of Γ on top of Kitaev interaction seems to have no significant advantage on efficiency. We found that work delivered by the engine depends linearly on the size of the system. Finally, we study the engine for larger spin-S, and show that, depending on the parameter values, the quantum engine may have dimensional advantage/disadvantage.

Longitudinal and transverse conductivity measurements across the Verwey transition in Fe_3O_4 thin film

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The Fe_3O_4, an inverse spinal compound, also known as magnetite has received a lot of attention due to the combination of several interesting properties, such as high spin-polarized current [1], and high Curie temperature ~ 858 K etc. It exhibits a first order metal-insulator transition, which is widely known as Verwey transition (VT), T_V, at ~ 120 K [2]. The VT is linked to the charge ordering of the Fe^{2+} and the Fe^{3+} ions, as well as a structural transition (high temperature cubic to low temperature monoclinic structure), and electron-phonon coupling [2, 3]. It has been reported that, the Fe_3O_4 exhibits a strong correlation between longitudinal conductivity and anomalous Hall effect (AHE). A. Fernández-Pacheco *et al.*, reported the universal scaling behavior, $\sigma_{xy} \propto \sigma^{1.6}_{xx}$, over four decades of the longitudinal conductivity [4]. The scaling suggested a common underlying mechanism for electrical, electronic and magnetic properties in this compound and the origin of the AHE may include contributions from skew scattering, and side jump. However, understanding of the relation between longitudinal and transverse conductivity across Verwey transition, and contributions of the electrical, electronic and magnetic properties in the same, is still an open problem. Here, we report longitudinal conductivity and AHE measurements on pulsed laser deposition grown single crystalline Fe_3O_4 thin film (on LAO substrate). Grown thin film exhibits T_V ~ 120 K, and about three orders of magnitude change in resistivity across T_V, confirming the high-quality of the sample. The AHE data at room temperature is consistent with previous reports [4]. However, AHE signal does not scale with magnetization when approaching T_V, moreover, transverse conductivity measurements across T_V reveals that the carrier type changes from electron to electron and hole both.

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Floquet-Engineered Valley-Topotronics in Kekulé -Y Bond Textured Graphene Superlattice

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August 26, 2024

Abstract

The increasing need of data storage or computer logic systems endeavours the condensed matter research to exploit all possible degree of freedom (DOF) in a quantum material. One such DOF's are the "valley-pseudospins" giving rise to the valleytronics (analogous to the spin degree of freedom in spintronics). In a valleytronics material, we look for a scope to exploit the carrier's valley DOF for the purpose of encoding quantum information. The Kekulé -Y (Kek-Y) 2D graphene superlattice is one such stucture with an entirely modified valleys. Experimental realization of this Kek-Y distorted 2D graphene superlattice has been confirmed by Gutierrez *et al*[1]. The exquisite distortion in a Kekulé -Y (Kek-Y) superlattice[2] merges the two inequivalent Dirac cones (from the K- and the K'- points) into the highest symmetric Γ-point in the hexagonal Brillouin zone. We report that UV circularly polarised light not only opens up a topological gap at the Γ-point but also lifts the valley degeneracy at that point. Endowed with Floquet dynamics and by devising a scheme of high-frequency approximation, we have proposed that the handedness (left/right) in polarised light offers the possibility to realize the valley-selective circular dichroism in Kek-Y shaped graphene superlattice. Also, the non-vanishing Berry curvature and enumeration of valley resolved Chern number $\mathcal{C}_K/\mathcal{C}_{K'} = +1/-1$ enable us to assign two pseudospin flavors (up/down) with the two valleys. Thereby, the above observations confirm the topological transition, suggesting the ease of realising the valley quantum anomalous Hall state within the photon-dressed Kek-Y. These findings further manifest a non-zero optical valley polarisation which is maximum at the Γ-point. Our paper[3] thus proposes an optically switchable topological valley filter which is desirous in the evolving landscape of valleytronics.

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BKT phase transition in mildly disordered superconducting anti-dot films of NbN

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Abstract

Berezinski-Kosterlitz-Thouless (BKT) phase transition has earlier been explored primarily in extremely thin or highly dis-ordered superconducting films. In these systems, the intrinsic inhomogeneity of the films often obscures the transition due to broadening. Herein, we present a study of the Berezinski-Kosterlitz-Thouless (BKT) transition in anti-dot films of superconducting NbN. Films with moderate dis-order and of thickness between 15 - 5 nm were grown on nano-porous anodic aluminium oxide membranes with two different pore diameters. Superfluid stiffness (J_s) was measured using current-voltage and penetration depth measurements. J_s was observed to decrease substantially in the anti-dot films for a given thickness which was beyond that expected due to changes in geometry. Clear and distinct BKT transitions were seen in them accompanied by increase in the vortical fluctuation regime. Monte Carlo simulations on a two-dimensional XY model was done which explained the experimental results. Finally, our results demonstrate that owing to the large decrease in J_s in the anti-dot films, the BKT transition becomes sharper even for films with moderate dis-order, thereby making them a good model system to probe the BKT physics.

Topological Phases of Conduction Band Modified p-wave Periodic Anderson Model

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The p-wave Periodic Anderson Model (p-PAM) was introduced by Alexandrov and Coleman in 2014 [1] to investigate topological properties of heavy-fermion materials.
In this study, we investigate the topological properties of modified p-PAM, wherein the conventional conduction band is substituted with a Su-Schrieffer-Heeger (SSH) type conduction band. Our model exhibits a topological phase transition driven by the continuous change in the ratio of the intra-lattice and inter-lattice hopping of conduction electrons. Additionally, a topological to trivial phase transition can be induced by changing the ratio of non-local hybridization between conduction and impurity electrons, from positive to negative via zero.
Our current analysis focuses on the non-interacting *f* electrons. Further, we employ the Density Matrix Renormalization Group (DMRG) technique and slave-particle based mean-field theory to explore the role of electron interactions in the localized *f* band on the topological phase transitions. Preliminary results indicate that these interactions could significantly influence the topological phases and transitions in our model.

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Theoretical study of the electronic, magnetic and transport properties of 3d transitional metal (Fe,Co) doped Bi_2Te3 using first-principles

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Abstract

We studied the electronic, magnetic, and transport properties of Fe and Co-doped Bi_2Te_3 [$Bi_{2-x}TM_xTe_3$ (TM=Fe,Co)], using the spin-polarized Korringa-Kohn-Rostoker (SPR-KKR) coherent-potential approximation (CPA) method within the atomic sphere approximation (ASA) [1] framework. Our objective is to investigate the residual resistivity of the doped alloys as a function of doping concentration. The charge self-consistent calculations, done at lattice parameters obtained from fully relaxed, full-potential [2] calculations, were carried out for 8% and 36% Fe-doped Bi_2Te_3, and 8% and 20% Co-doped Bi_2Te_3, respectively. The Fe-doped system is found to be non-magnetic, while the Co-doped system turns out to be magnetic. Furthermore, we find that the local magnetic moment of the Co-doped alloy increases with increase in Co concentration, in disagreement with experiment [3]. This mismatch may be due to the differences in the experimental and optimized unit cell volumes by around 6%. Using the Heisenberg model, we have calculated the Ruderman-Kittel-Kasuya-Yosida interaction which are found to dominate over other exchange interactions. Finally, the calculated residual resistivity of Fe and Co-doped Bi_2Te_3 alloys are in good agreement with earlier experimental values of residual resistivity [2, 3].

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Coexistence of Electron and phonon topology in Perovskite $SrRuO_3$

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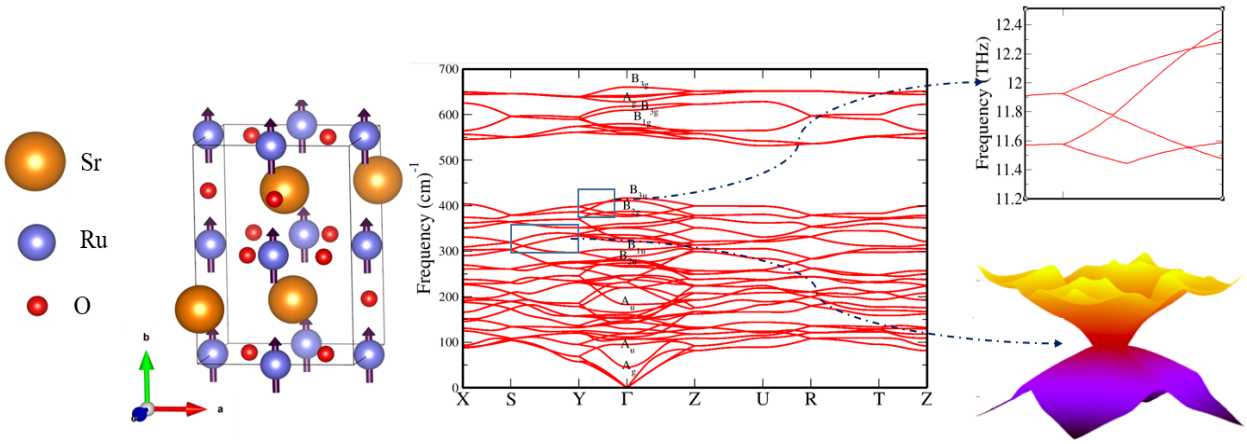
$SrRuO_3$, a perovskite-type ruthenate, is well known for its remarkable electrical and magnetic properties. It possesses good thermal and chemical stability favouring excellent lattice match with various functional oxides. In the present work we try to address the structural, vibrational, electronic and topological properties of $SrRuO_3$ using first principles calculations. We do see the intersection of electron and phonon topology in $SrRuO_3$, which crystallizes in the orthorhombic symmetry with space group *Pnma* (62). The analysis reveals three orthogonal two-fold screw rotations ($\{C_{2x}|\frac{1}{2},\frac{1}{2},\frac{1}{2}\}$, $\{C_{2y}|0,\frac{1}{2},0\}$, $\{C_{2z}|\frac{1}{2},0,\frac{1}{2}\}$) and three glide symmetries ($\{\mathcal{M}_{100}|\frac{1}{2},\frac{1}{2},\frac{1}{2}\}$, $\{\mathcal{M}_{010}|0,\frac{1}{2},0\}$, $\{\mathcal{M}_{001}|\frac{1}{2},0,\frac{1}{2}\}$). $SrRuO_3$ exhibits semiconducting behaviour with a narrow band gap of 0.68 eV and demonstrates four-fold degenerate bands with Dirac crossings near the Fermi level. Phonon calculations using a 2×2×2 supercell reveal that the phonon bands along the X-U-R-S-X, S-R-T-Y-S, and U-R-T-Z-U paths are two-fold degenerate, indicating the presence of three nodal surface phonons on the ki = ±π (i = x, y, z) planes. Notably, two doubly degenerate nodal lines along the Y-T-S path merge into a single four-fold degenerate nodal line along the S-R path. This four-fold degeneracy reflects multiple Dirac nodal line phonons, highlighting the unique topological nature of phonons in $SrRuO_3$. The appearance of the Dirac nodal line phonons can be determined from the aspect of symmetry. The present work suggest that the investigated compound is interesting for its fascinating topological features.



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Structural and Magnetic Properties of $SmAg_2Ge_2$ Single Crystal

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We have investigated the structural, magnetic and heat capacity properties for the inter-metallic $SmAg_2Ge_2$ compound. $SmAg_2Ge_2$ single crystal crystallizes in the $ThCr_2Si_2$-type tetragonal structure (space group *I4/mmm*). Sm moments in $SmAg_2Ge_2$ order antiferromagnetically at T_N = 9.2 K. From isothermal magnetization strong non-linearity and meta-magnetic transition are observed at critical fields B_{m1} = 8 T and ending at B_{m2} = 11 T for $SmAg_2Ge_2$ at 8 K, 8.5 K, and 9 K temperatures along the B perpendicular to c. The heat capacity and resistivity also show anomaly at T_N in zero-filed, which broadens and moves to lower temperatures in an applied magnetic field. The extracted entropy at the transition temperature is consistent with the theoretical value R ln(2S + 1) for S = 7/2 of the Sm^{3+} ion. High-quality single crystals of $SmAg_2Ge_2$ were grown using the AgGe flux. The 3N-Sm, 5N-Ag, and 5N-Ge starting materials were taken in the ratio 1:16.25:6.75 ratio and placed in a high-quality recrystallized alumina crucible. The single crystals were grown by heating the quartz ampoules to 1150°C at 60 °C/h, held for three weeks, and then slowly cooled to 750°C at 2°C/h. The crystals were separated from the flux by centrifugation at that temperature. We obtained several shiny platelike crystals of typical size 5 × 3 × 0.3 mm^3 for $SmAg_2Ge_2$. A small slab of the crystals was ground to make fine powder and then the sample was mounted on a glass slide at room temperature for x-ray diffraction (XRD) to check the phase purity. X-ray diffraction (XRD) data accession was performed at room temperature with a PANalytical x-ray diffractometer mounted with a Cu-K_α monochromatic source with wavelength λ = 1.5406Å. We also determined the structural refinement parameter for $SmAg_2Ge_2$ with Rietveld refinement of the XRD data using the Full-Prof package. The obtained single crystals of $SmAg_2Ge_2$ were oriented along the principal crystallographic direction of Laue diffraction using a polychromatic X-ray source. The crystals were cut into desired shapes using a spark erosion electric discharge machine. The elemental chemical composition of $SmAg_2Ge_2$ was studied by energy-dispersive x-ray spectroscopy (EDX) semi-quantitative chemical analysis. SEM scans were taken on cleaved surfaces of the crystals which documented the single-phase nature of the crystals. The composition of each plate-like crystal studied here was measured at six or seven positions on each of the two basal ab-plane faces, and the results were averaged. Good chemical congruity was found for each crystal. Temperature and field-dependent DC magnetic measurements were performed on a superconducting quantum interference device vibrating sample magnetometer (SQUID-VSM), Quantum Design, USA with the field along the principal crystallographic direction. We made electric contacts using the silver paste with a gold wire diameter of 40 μm on a $SmAg_2Ge_2$ crystal surface. Magnetic field dependence electrical resistivity (ρ) of $SmAg_2Ge_2$ and thermal transport were measured by the standard four-probe in a Quantum Design Physical Property

Measurement System (PPMS). The sample with a mass ~ of 12 mg we attached with GE varnish to a 12 µm diameter Chromel Constantan thermocouple, and heated with light at a frequency of 16 Hz. The size of the temperature oscillations is inversely proportional to the sample's heat capacity plus the addenda (smooth plus thermocouple). While with this method it is possible to measure a very small single-crystal it is not possible to judge the absolute value of the specific heat. The heat capacity was measured as a function of the different fields. Electrical resistivity and magnetoresistance as a magnetic field and temperature function were studied using a standard four-probe technique in a Quantum Design Physical Property Measurement System (PPMS).

Unveiling the phonon topological features of inter-alkali metal sulphides RbXS (X=Li, Na)

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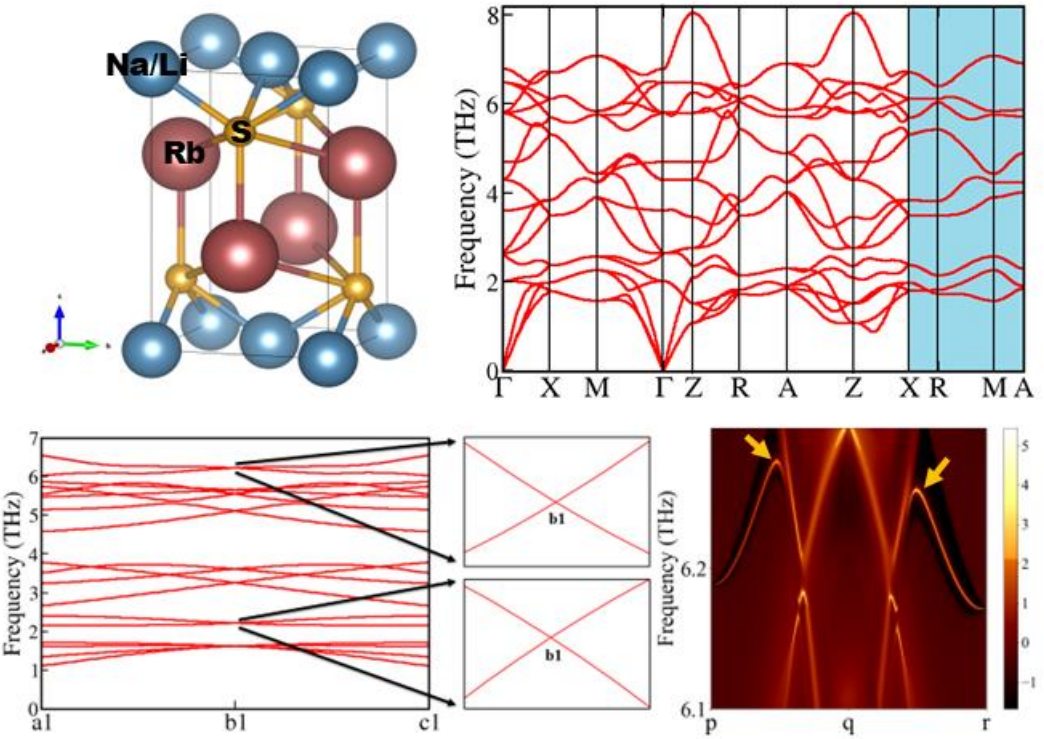
A theoretical approach to unveil the phonon topological characteristics of RbXS (X=Li, Na) were carried out using density functional theory (DFT). The above compounds crystallize in tetragonal structure with *P4/nmm* space group. RbXS possesses non-symmorphic symmetry including glide plane characterized by $\{M_z \mid \frac{1}{2},\frac{1}{2},0$, screw axes $\{C_{2x} \mid \frac{1}{2},0,0\}$, $\{C_{2y} \mid 0,\frac{1}{2},0\}$, along with time-reversal $\{T\}$ symmetries. The occurrence of two-fold degeneracies along M-X-R-A in both RbLiS and RbNaS imply the presence of nodal surface along the $k_y=\pi$ plane. The focus of our investigation is on the exotic phonon drumhead surface states emerging in multi-directions along high-symmetry points in the Brillouin zone. These also exhibit topological features, including linear dispersion and flower-like nodal lines, that are robust and protected by the bulk properties. The findings presented here not only contribute to the fundamental understanding of topological phonon states but also



open up possibilities for leveraging these properties in practical applications.

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Performance Parameters of Infra-red and Visible-active MXene Photocatalysts for Water Splitting

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August 29, 2024

Abstract

Water splitting reactions through photocatalysis is an efficient and sustainable technique for the generation of green energy. The photocatalyst's ability to effect simultaneous generation of hydrogen and oxygen, along with efficiency in utilisation of charged carriers, conversion of solar energy to hydrogen, fast migration, and low recombination rates of carriers, are the parameters to decide its suitability in water splitting. In literature, comprehensive calculation and analysis of all these performance parameters for a potential photocatalyst are rare. In this work, we have performed first-principles-based computations to find new efficient photocatalysts from the family of Janus MXenes and assessed their performance parameters. Strain engineering has been invoked in search of new materials. Out of 14 studied materials, we find 5 materials: Sc_2COS, Zr_2COS, Hf_2COS, and $ZrHfCO_2$ under zero or finite tensile strain and Hf_2COSe at 6% tensile strain meeting the requirements of simultaneous reactions to split water. The computations of various efficiency-related parameters demonstrate that Zr_2COS, Hf_2COS, and Hf_2COSe have excellent efficiencies, significantly better than the well-known photocatalysts. The origin of such performances lies in their electronic and optical properties, which are analysed systematically.

Magnetic Compensation and Frequency Dispersion in Dynamical Susceptibility of Distorted Honeycomb Lattices

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Abstract

Magnetoelectric (ME) phenomena in honeycomb lattices are the subject of intense research activity because it is pivotal in understanding the multiferroic nature of the compounds that have potential applications in the field of magneto-electronics [1-4]. Usually, materials exhibiting ME phenomena possess robust magnetic ordering and electric polarization, where both order parameters are strongly coupled with each other [5,6]. In this context, here we report the magnetic properties of a few distorted honeycomb lattices having the general formula $A_4B_2O_9$ (e.g. $Ni_4Nb_2O_9$ space group *Pbcn*) that exhibit the ME effect. Our studies reveal two distinct crystal-field environments experienced by the divalent Ni ions due to which the compound exhibits ferrimagnetic ordering around 76 K (T_{FN}) and the imbalance in spin-moments ($\mu_{\text{-Ni-1}} = 1.7\mu_B$ and $\mu_{\text{-Ni-2}} = 2\mu_B$) occurs. Interestingly, such long-range ordering collapses just below the T_{FN}, and the system experiences negative magnetization along with the magnetic compensation effect across 33 K (T_{CMP}). The spin dynamics reveal the dispersive nature of the transition across T_{FN} (Fig.1) within a narrow temperature window as small as 1 K (ΔT), revealing the frozen-spins structure instead of a perfect canonical spin-glass state having Mydosh parameter $\Omega \sim 3.4\times10^{-4}$. These observations are further supported by the analysis based on the empirical scaling laws such as: (*i*) Vogel-Fulcher Law $\tau = \tau_0 exp\left[\frac{E_a}{k_B(T-T_0)}\right]$ and (*ii*) Power-law of critical slowing down, $\tau = \tau_0\left[\left(\frac{T-T_F}{T_F}\right)^{-z\nu}\right]$.

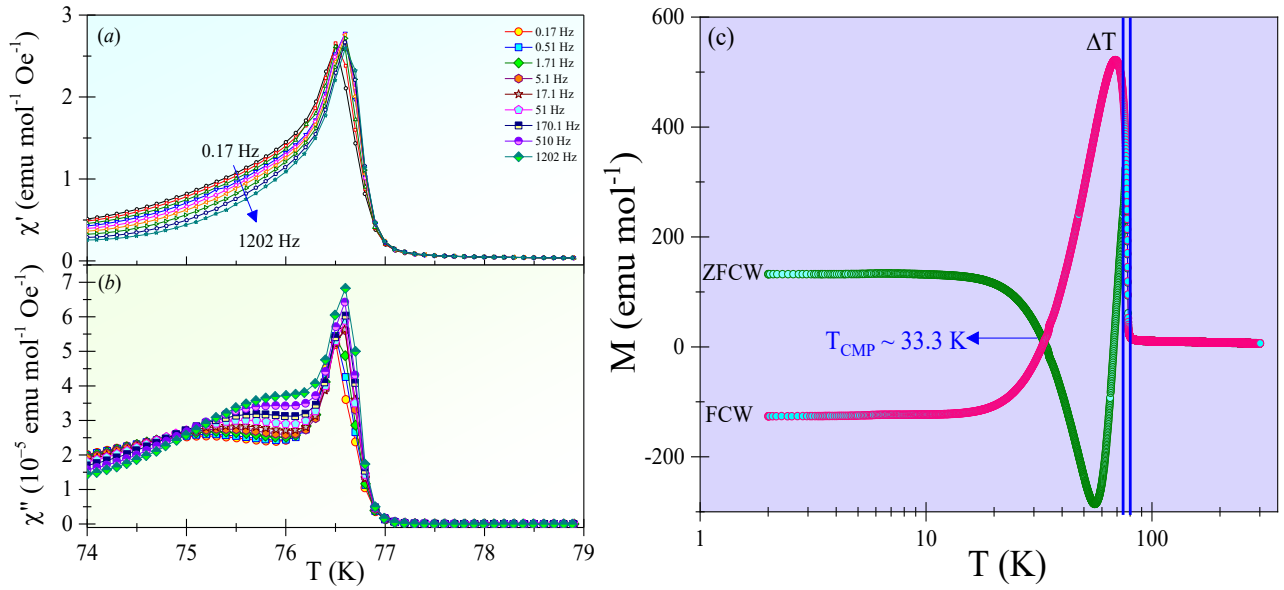

Figure 1. Frequency dispersion of the ac-magnetic susceptibilities (a) real-part component, χ' (T), and (b) imaginary-component χ'' (T). (c) Magnetization (M) Vs. Temperature (T) showing the compensation point (T_{CMP}) below T_{FN} with temperature window (ΔT) under both zero-field-cooled (ZFC) and field-cooled (FC) conditions.

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Ergotropy, bound energy and entanglement in 1D long range Kitaev model

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Recently, a connection between quantum thermodynamics and quantum information theory was established by showing a linear relationship between the product of bound energy of the subsystem with the system size and the square of its entanglement entropy in the ground state for a free fermionic chain with nearest-neighbor hopping, with a conjecture that this linearity holds for any model with conformal symmetry. Motivated by recent experiments where long-range interactions that decay as a power law with distance can be realized using trapped ions and neutral atoms coupled to a photonic mode of a cavity, and by the fact that such interactions naturally emerge in a wide range of physical systems, including atomic, molecular, and optical systems, we investigate the possibility of extending the connection between quantum thermodynamics and quantum information theory to a long-range interacting model, where conformal symmetry is broken due to the long-range nature of these interactions [1]. In particular, we consider a 1D Kitaev model with a pairing interaction term that decays with distance as a power law with an exponent α. In this model, conformal symmetry is broken for $\alpha < 3/2$. We analytically show that for $\alpha = 1$, the linear relationship between bound energy and the square of entanglement entropy persists with the same slope as in the $\alpha \to \infty$ case, where the long-range Kitaev model is mapped to the XY model via the Jordan-Wigner transformation and can be described using conformal field theory.For $\alpha = 1$, we observe an additional $\log(\log(N))$ correction term in the entanglement entropy of the subsystem in the ground state, in addition to the dominant $\log(N)$ term, where N represents the system size. We further show that this linearity holds even for $\alpha \lesssim 1/4$. The presence of long-range interactions enhances work extraction (ergotropy). We analytically show that the subsystem ergotropy scales linearly with the system size for $\alpha = 0$, logarithmically for $\alpha = 1$, and saturates for $\alpha \to \infty$ in the large N limit.

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Magnetic properties of a rare-earth dichalcogenide compound, $TbSe_2$

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Abstract

Transition metal dichalcogenides have been attracting considerable interest due to their unique structure and excellent electrical and thermal properties. We report here the magnetic property of a rare-earth based layered dichalcogenide $TbSe_2$, crystallising in a tetragonal structure with space group P4/nmm. This compound exhibits a long-range antiferromagnetic nature with two magnetic transitions at 6.8 K and 5.4 K respectively. The compound exhibits multiple steps like features in the isothermal magnetization, which could arise from the field induced spin reorientation transitions in this compound. The multiple magnetic features in magnetic susceptibility shows the presence of a complex magnetic ground state in $TbSe_2$.

Abstract for Poster

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Flat bands could be engineered in one-dimensional fermionic models [1]. These flat bands have supertranslation symmetry, and this theory is ultralocal. The inclusion of Hubbard interaction with supertranslation symmetries makes the model integral but exhibits a richer phase diagram. However, the small perturbation in the Hamiltonian breaks the Carroll. Still, the ultralocal feature survives in one of the phases, which could be shown numerically using DMRG beyond the perturbative regime.

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Characterization of superconducting thin films using Planar Microwave resonator

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A planar superconducting resonator is a powerful technique in quantum information science, allowing us to explore various material properties at low energy scales. We use NbN thin films with critical temperature up to 16 K, featuring different thickness and levels of disorder, deposited by DC magnetron sputtering. The planar resonator structure is designed with a UV laser writer, and the pattern is etched using ion milling. The microwave properties of NbN thin films have been investigated between 2 GHz and 20 GHz using coplanar transmission line resonators and stripline resonators. We got the loaded Quality factor about 7000 at 2.6 K temperature. We obtained information on the magnetic penetration depth, surface resistance, and surface reactance from temperature and power dependence measurements of the quality factor and resonance frequencies. The stripline structure of NbN can be applied to bulk samples, such as Pb, and allows for the direct calculation of surface resistance.

QMAT 2024 Conference

Unveiling the photophysical properties of Mn-doped $FAPbI_3$ perovskites via a First-Principles Study

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Abstract: Perovskites, specifically organic-inorganic lead halide perovskites, have demonstrated remarkable promise for application in various optoelectronic devices. Of particular interest is Formamidinium Lead Iodide ($\mathrm{FAPbI_3}$) perovskite, which is being extensively researched for its use as an active layer in photovoltaic devices due to its broad absorption spectrum, optimal band gap, excellent optoelectronic properties, cost-effectiveness, and high power conversion efficiency. However, the practical benefits of these perovskites are often constrained by lead toxicity and their susceptibility to instability when exposed to moisture and oxygen. To explore resolutions to these challenges, a study of Mn doped $\mathrm{FAPbI_3}$ perovskite is being undertaken here. First-principles calculations based on DFT (Density Functional Theory) are employed to analyse and compare the various photophysical properties of $\mathrm{FAPb_{1-x}M}n_x\mathrm{I_3}$ by varying *x* over a range of values between 0 and 1. The bandgap energy and charge-transfer mechanisms are impacted while doping the crystal.

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Nitrogen vacancy defects in diamond as a promising candidate for quantum sensing

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Diamond is gaining increasing attention as platform for quantum technologies thanks to the properties of its defects, namely nitrogen vacancies. The nitrogen-vacancy (NV) center is a defect in which a nitrogen atom replaces a carbon atom and the adjacent site in diamond's tetrahedral lattice is vacant. In its negatively charged state, the NV center gains an extra electron from the lattice, forming a ground-state spin system that can be polarized with 532-nm light, even at room temperature. One of the spin states fluoresces much more brightly than the others so that fluorescence can be used for spin-state readout. At the same time, the NV's electron spin states are sensitive to magnetic and electric fields through the Zeeman and Stark effects, respectively. These properties make NVs in diamond very attractive for quantum information systems and for high sensitivity electromagnetic field quantum sensors. A key aspect for both quantum information systems and quantum enabled electric and magnetic field sensing is the possibility of realising an integrated and scalable platform in diamond, exploiting the NV as an optically detecting atomic probe[1]. Here we present an integrated magnetometry platform that utilizes femtosecond-laser-written type-II waveguides and shallow nitrogen vacancy centers in diamond for enhanced quantum sensing of magnetic field and temperature sensing. Unlike bulk NV centers, which are located deeper within the diamond, these NV centers are implanted just a few nanometers below the diamond surface, fully overlapping with the waveguide's mode field. This setup optimizes photon routing, leading to efficient detection of magnetic resonance signals and enabling high-sensitivity measurements of magnetic fields, temperature, and strain[2]. We perform simulation for optical waveguiding to understand the coupling efficiencies of waveguides with NV centers for efficient sensing strategies.

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Developing quantum architectures for laser inscribed SiV based integrated quantum photonics in diamond

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Silicon vacancy (SiV) centres have emerged as promising candidates for quantum technologies, particularly in the fields of quantum computing and quantum communication. They are point defects in the crystal lattice of diamond, where a silicon atom replaces two adjacent carbon atoms. These defects act as isolated, atom-like systems embedded within the diamond matrix, exhibiting unique optical and spin properties. However, optical qubit manipulation, operating temperature and scalability are the key technological challenges. Enabling precise control over light fields at the single-photon level represents a critical hurdle for emerging quantum technologies which can be overcome through integrated quantum photonics on a scalable platform. Recently, femtosecond laser writing has been utilized to form integrated photonics in diamond coupled with ion implanted SiVs for single photon operations [1,2]. Laser-written diamond photonics offers 3D fabrication capabilities and large mode-field diameters compatible with fiber optic technology. Here, we propose novel architectures for quantum algorithms consisting of non- local gates such as Hadamard and CNOT via entanglement, simulated using python based QISKIT. By applying these concepts, we propose experimental circuits in diamond for few qubits quantum teleportation, superdense coding and travelling salesman problem. We also discuss the experimental viability of the proposed architectures.

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Strain induced electronic and magnetic transition in S=3/2 antiferromagnetic spin chain compound $SbCrS_3$

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The study of two-dimensional (2D) magnetic materials and their pressure driven electronic and magnetic transitions are growing research field in modern condensed matter physics. In this context, recently antiferromagnetic Cr-based compounds such as $FePS_3$, CrI_3, $CrBr_3$ have been investigated experimentally and theoretically for their possible spintronics applications. Here, we theoretically studied the electronic and magnetic properties of a relatively less explored Cr-based chalcogenide, namely $SbCrS_3$ where 2D layers of magnetic Cr^{3+} ions form a triangular lattice. In this work, we employed density functional theory including Hubbard U (DFT+U approach) in conjunction with constrained random-phase approximation (cRPA) where the later was used to estimate the strength of U. Our findings at ambient pressure show that the system exhibits an semiconducting antiferromagnetic ground state with a gap of 0.5 eV and large Cr moments that corresponds to nominal S=3/2 spin-state. To understand the nature of magnetism, we calculated the inter-site magnetic exchange coupling strength using magnetic force theorem. The exchange interaction calculation shows, 1st nearest-neighbor (NN) interatomic exchange coupling (J_1) is found to be strongly antiferromagnetic (AFM), while 2nd NN coupling (J_2) are relatively weaker ferromagnetic (FM), making this system a candidate for 1D non-frustrated antiferromagnetic spin-chain family of materials. Based on orbital resolved interactions, we demonstrated the reason behind two different types of interactions among 1st and 2nd NN despite their very similar bond lengths. We observe a significant spin-orbit coupling effect, giving rise to a finite magneto crystalline anisotropy, and Dzyaloshinskii-Moriya (DM) interaction. Further, we found that by applying uniaxial tensile strain along crystallographic a and b-axis, $SbCrS_3$ exhibits a magnetic transition to an semi-conducting FM ground state and give rise to novel phenomenon angle dependence of exchange coupling. We also showed that the Neel temperature of AFM ground state could be significantly enhanced by applying compressive strain. Thus, our findings can enrich the versatility of $SbCrS_3$ and make it a potential application.

**This work has been carried out in collaboration with Dr. Swarup Kr. Panda (Bennett University, Greater Noida, India).*

Enhanced Negative Magnetization in Ferrimagnetic Cobalt-Orthotitanate: Role of Jahn-Teller Active $^2D_{5/2}$–Cu

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ABSTRACT

Strongly correlated aspects of Cobalt-Orthotitanate, Co_2TiO_4 at low-temperatures has been the subject main focus in recent years in the field of magnetism because the longitudinal ferrimagnetism and re-entrant transverse spin-glass components coexist leading to some exotic phenomena such as bipolar exchange bias (H_{EB}~−20 kOe at 10 K) and spin-liquid state (<20K) [1,2]. In the current work we report the enhanced negative magnetization in Ferrimagnetic (FiM) Co_2TiO_4 with a special focus on the Cu (ground state: $^2D_{5/2}$) substitution at the tetrahedral low-spin Co-sites (Fig.1a,b). Overall two different compositions ($Co_{1.8}Cu_{0.2}TiO_4$, and $Co_{1.6}Cu_{0.4}TiO_4$) have been investigated including the pristine system Co_2TiO_4 all of which were stabilized with cubic-structure of *Fd-3m* space group having the lattice parameters 8.45 Å. The two magnetic sublattices contains unequal magnetic moments and different temperature dependence due to which FiM ordering arises in these systems. For the pristine case the FiM Néel temperature T_{FN} occurs 47.2 K below which the two-sublattice magnetizations balances with each other resulting compensation effect at T_{CMP} = 32 K (Fig.1a). However, such compensation phenomena vanish with the incorporation of Jahn-Teller active Cu^{2+} ions and a large negative moment emerges below 40 K. Also, the effective magnetic moment (μ_{eff}) decreases from μ_{eff} = 6.5 μ_B (for Co_2TiO_4) to 5.55 μ_B (for $Co_{1.6}Cu_{0.4}TiO_4$). Moreover, the T_{FN} was found to be decreasing from 47.2 K (for Co_2TiO_4) to 45 K (for $Co_{1.6}Cu_{0.4}TiO_4$). Along with the major transition T_{FN}, we also noticed a low-temperature maximum (T^*) in the differential susceptibility (d(χT)/dT) across 43 K (for $Co_{1.8}Cu_{0.2}TiO_4$) and 41 K (for $Co_{1.6}Cu_{0.4}TiO_4$), which may be due to the short-range correlations below T_{FN}.

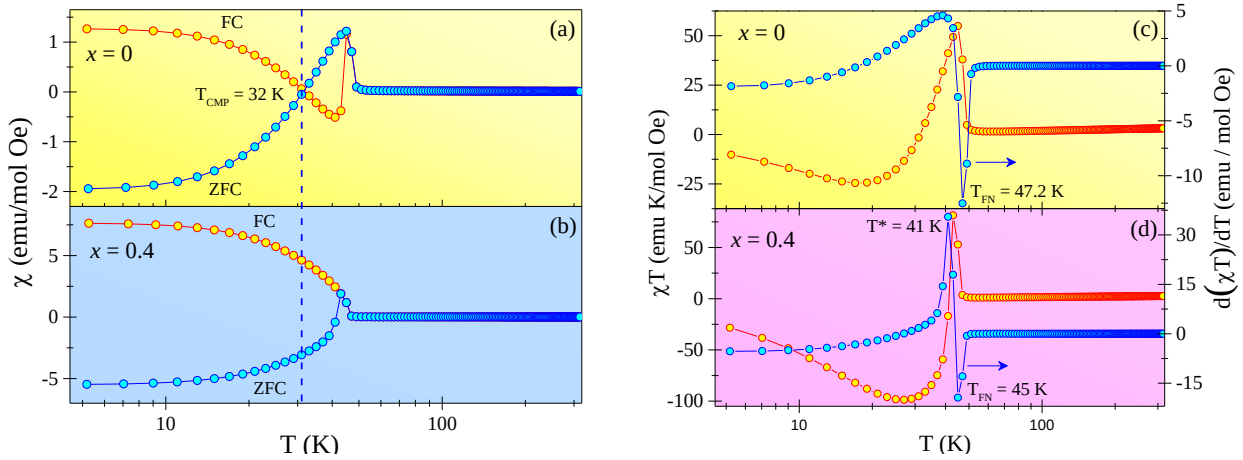

Figure 1: (a,b) Temperature dependence of magnetic susceptibility χ(T) measured under both ZFC and FC modes for Co_2TiO_4 (x = 0) and $Co_{1.6}Cu_{0.4}TiO_4$ (x = 0.4), and (c,d) Differential susceptibility d(χT)/dT Vs. T and the product χT Vs. T for x = 0 (Co_2TiO_4) and x = 0.4 ($Co_{1.6}Cu_{0.4}TiO_4$) depicting the inflection points across T^*, T_{CMP} and T_{FN}.

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Influence of Ni^{2+} Substitution on Microwave X-Band Radiation Losses in Y-Type Hexaferrites

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Abstract: Y-type strontium hexaferrite is attractive material for various applications, such as high frequency antennas and RF devices, because of its interesting magnetic properties. Ni substituted strontium hexaferrite with varying concentration of nickel were prepared using chemical co-precipitation methods for tuning its structural and magnetic properties. The structural properties were characterized by X-Ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and the morphology and size distribution of the particles have been studied using high resolution field emission scanning electron microscopy (FESEM). Thermogravimetric analysis (TGA) was performed to find the stability of the sample by comparing the weight changes at a given temperature. Magnetic properties were determined using a vibrating sample magnetometer (VSM). The study on the radiation losses X band were performed by means of vector network analyzer (VNA) and indicated that the samples show reflection loss of -29.63(99.9% loss) at frequency 9.05 GHz and the results show that both the complex dielectric constant and dielectric loss decrease as measuring frequency increases. The low reflection loss makes these Y-type hexaferrites a potential candidate for high-frequency absorbers in the microwave region.

Keywords: Strontium hexaferrrite, microwave absorber, nanoparticle.

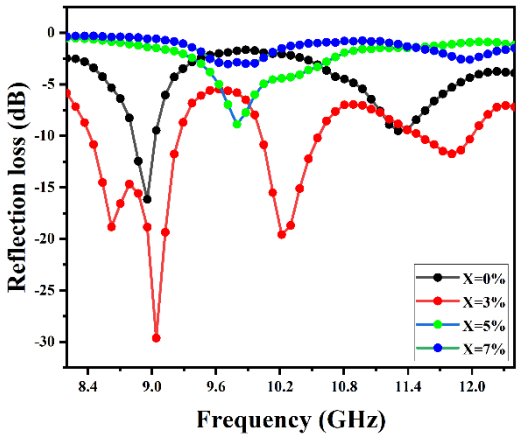

Figure 1: Measured reflection loss of strontium hexaferrite (x= 0%, 3%, 5%, 7%).

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Anisotropy and Dipolar interaction tunable $CuFe_2O_4$ nanoparticle for Magnetic Hyperthermia Application

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The ability of magnetic nanoparticles (MNPs) to self-heat in the presence of an Alternate magnetic field (AMF) is a unique characteristic that makes them useful for biomedical applications, particularly magnetic hyperthermia. Anisotropy and dipolar interaction of nanoparticles are two prominent metrics that frequently spark controversy regarding how they influence heating efficiency. In this work, we have tuned the anisotropy of $CuFe_2O_4$ MNPs through site-specific substitution with Cobalt ions at three different concentrations using the coprecipitation method. In the synthesized $Cu_{1-x}Co_xFe_2O_4$ (x=0,0.1,0.3,0.5) NPs, the dipolar interaction has been tuned by giving a SiO_2 coating which reduces the agglomeration between the MNPs. Swapping Cu^{2+} ions with highly anisotropic Co^{2+} ions in the octahedral site of the crystal disrupts the cation distribution and also increases the effective anisotropy of the system with an increase in cobalt concentration from x=0 to x=0.5. The induction heating analysis done under an AMF of frequency 337 KHz, shows the temperature rise in 900 s increases from x=0 to 0.5. This highlights how anisotropy influences the self-heating efficiency of MNPs. The x=0.5 sample showing the maximum heat release of 47°C proves to be a potential candidate for magnetic hyperthermia application.

Symmetry lowering through surface engineering and improved thermoelectric properties in Janus Mxenes.

Himanshu Murari, Subhradip Ghosh

Abstract

Despite ample evidence of their influence on the transport properties of two-dimensional solids, the interrelations of reduced symmetry, electronic and thermal transport have rarely been discussed in the context of thermoelectric materials. With the motivation to design new thermoelectric materials with improved properties, we have addressed these by performing first-principles density functional theory based calculations in conjunction with semi-classical Boltzmann transport theory on a number of compounds in the MXene family. The symmetry lowering in parent M_2CO_2 (M = Ti, Zr, Hf, Mo) MXenes is achieved by replacing the transition metal M on one surface, resulting in Janus compounds MM‘CO_2 (M = Ti, Zr, Hf and M′ = Mo, Zr, Hf; M ≠ M′). Our calculations show that the thermoelectric figure-of-merit can be improved significantly by such surface engineering. We discuss in detail, both qualitatively and quantitatively, the origin behind high thermoelectric parameters for these compounds. Our in-depth analysis shows that the modifications in the electronic band structures and degree of anharmonicity driven by the dispersions in the bond strengths due to the lowering of symmetry, an artefact of surface engineering, are the factors behind the trends in the thermoelectric parameters of the MXenes considered. The results also substantiate that the compositional flexibility offered by the MXene family of compounds can generate a complex interplay of symmetry, electronic structure, bond strength and anharmonicity which can be exploited to engineer thermoelectric materials with improved properties.

Role of Spin-Orbit coupling in topological candidates: A Case Study of $Pb_{2-x}Bi_xPd$

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The concurrence of non-trivial band structure and superconductivity can host a novel phase called topological superconductivity [1]. A typical host of non-trivial band structures is topological semimetals, a class of gapless electronic phases showing topologically stable intersections of energy bands [2]. Searching for superconductivity in intrinsic and doped topological semimetals offers a great platform to come across topological superconductivity. Conventional superconductors host phonon-mediated Cooper pairs that can flow through a material without scattering. In contrast, the topological superconductor, a kind of unconventional superconductor, contains other quasiparticle excitations called Majorana fermions at the surface [3]. The band topology and superconducting properties are certainly altered by spin-orbit coupling (SOC), which leads to unconventionality in the system [4]. However, despite various noteworthy efforts, the exact superconducting pairing mechanism still needs to be resolved for these systems.

I will present my recent work on the interplay between two topological superconductor candidates, Pb_2Pd and Bi_2Pd. My current research highlights single crystal growth, characterization, and superconducting properties of the $Pb_{2-x}Bi_xPd$ series. I will discuss the series' structural transformations and superconducting phase diagram. The trends observed in mixing two high SOC elements (Pb and Bi) may pave a path towards understanding the ground state properties and pairing mechanism in our future work.

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Luminescent metal halide perovskite nanocrystals, their stability and applications

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Abstract:

Metal halide perovskites have emerged as a promising building block for optoelectronic applications due to their remarkable and adjustable photophysical properties such as high photoluminescence, color tunability, excellent charge carrier properties, narrow emission spectra, defect tolerance, multi-photon absorption, easy solution processability and much more. However, these capable applications are facing a major challenge of stability due to the low formation energy of perovskite materials. These materials are sensitive to high humidity, temperature, polar solvents, halide exchange process, ion migration, and so on, leading to poor stability which greatly hampers the commercialization of perovskite-based devices. Many novel strategies have been instigated (such as surface ligand engineering, ion doping, core-shell structure, etc.) to improve the stability and luminescent intensity of perovskite nanocrystals. In our work, a facile synthesis method is adapted to tackle instability issues of perovskite nanocrystals which proved to be a potential candidate for WLED and sensing applications.

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Superconductivity in In-Sn system

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The recent discovery of superconductivity in topological materials, such as topological semimetals and insulators, represents a significant advancement in the field of quantum materials, opening new avenues for exploration [1]. Topological superconductors (TSCs) are unconventional superconductors characterized by a fully gapped superconducting bulk and conducting gapless surface states. These surface states host Majorana fermions, particles that are their own antiparticles, which are considered potential candidates for quantum qubits [2]. However, only a few intrinsic topological materials exhibit superconductivity, highlighting the need to discover new superconducting topological materials. Bimetallic superconducting alloys, which are less explored, offer a promising platform to realize topological superconductivity due to their strong spin-orbit coupling and non-trivial band structures [3].

I will present the synthesis and detailed study of the structural and superconducting properties of In-Sn bimetallic alloys, specifically In_3Sn and $InSn_4$, using X-ray diffraction (XRD), transport, magnetization, and heat capacity measurements. These measurements indicate type-II, fully gapped superconductivity in the weak coupling limit. Additionally, these materials provide insight into the effects of spin-orbit coupling and topologically non-trivial surface states on superconducting properties, which is crucial for understanding topological superconductivity.

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New Auxiliary Model Approach Towards Studying Correlated Electrons

Insights on pseudogap regime and non-Fermi liquid at ½-filling

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Understanding the mechanism of high-temperature superconductivity in strongly correlated materials is a long-standing problem in quantum condensed matter physics. Within cuprate superconductors and some of their cousins, the most challenging aspects of superconductivity involve its normal phases - the pseudogap regime and the strange metallic phase. It is not well understood whether the pseudogap phase (characterised by partial gapping of spectral weight near the Fermi surface) involves any symmetry-broken long-range order. Similarly, the strange metal phase, where resistivity scales differently from the expectations of Fermi liquid theory down to very low temperatures, remains mysterious. The mechanisms underlying either phase are still unclear. At a deeper level, it remains to be understood why a variety of strongly correlated materials display broadly universal phase diagrams.

In this work, we develop a new auxiliary model-based method to study electronic models of strong correlation. Specifically, the method allows us to study a Hubbard-Heisenberg model (lattice model) by solving a simpler quantum impurity model (auxiliary model). As part of the method, we derive relations connecting the Hamiltonians, eigenstates, and Greens functions from the auxiliary model to the lattice model. The method reveals, among other things, a phase diagram at half-filling involving a partially gapped phase sandwiched between a Mott insulator and a Fermi liquid. Studies of the spectral function, self-energies, and low-energy effective Hamiltonians reveal that the gapless excitations within the pseudogap phase are of the non-Fermi liquid kind. We shed more light on the mechanism of pseudogapping by computing static correlations and entanglement measures within the phase. Our approach opens the door to similar studies of various other challenging models.

Optimized Memristors Using Mixed Cation Perovskite $FA_{0.90}Cs_{0.10}PbI_3$ with High On-Off Ratio and Low Power Consumption

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ABSTRACT

Perovskite materials have emerged as promising candidates for next-generation memristors due to their unique tunable properties and compatibility with low-cost fabrication techniques. In this study, we explore the integration of a mixed A-site cation perovskite, $FA_{0.90}Cs_{0.10}PbI_3$, into memristor devices, focusing on the optimization of switching behavior and stability. Our memristor demonstrates an impressive on-off ratio of 10^5, combined with excellent switching speed and low operating voltage, achieving high endurance and stable performance over extended cycles. The memristive behavior in perovskites is largely attributed to ion migration, which enables dynamic resistance switching and contributes to the reliable operation of the device. This characteristic of perovskite material makes it as a strong contender for replacing traditional materials in memory technologies. Having already revolutionized optoelectronic devices, perovskites are now showing significant potential in the field of memristors, offering advantages such as low power consumption, scalability, and the ability to be fabricated on flexible substrates. Our findings suggest that these perovskite-based memristors can be effectively utilized in applications such as neuromorphic computing, non-volatile memory, and future wearable electronics, paving the way for advancements in both performance and integration of electronic devices.

KEYWORDS

Perovskite memristors; ion migration; endurance; on-off ratio; non-volatile memory.

Measuring quantum efficiency of Photo-Carnot Engine via vanishing quantum coherence in a lossy cavity

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Quantum heat engines (QHE) have been the subject of intense investigation since the proposal of the first QHE by H. E. D. Scovil and E. O. Schulz-DuBois in 1959[1]. In this work, we investigate the quantum Carnot engine in which the working medium is a photon gas inside the cavity with perfectly reflecting walls. The thermal baths that supply heat to the radiation field consist of a stream of three-level atoms passing through the phaseonium fuel, with atomic coherence between two degenerate lower levels. Notably, The phase (ϕ) of atomic coherence is a novel and fascinating control parameter that may be changed to enhance the temperature of the radiation field[2]. Furthermore, we are considering the relevant losses from the cavity like "Ohmic" loss, leakage from cavity and loss due to the spontaneous emission with the quantum field theoretic approach of the field to determine the quantum efficiency and output power of the Photo-Carnot QHE. Our findings shed light on the intricate interplay between the quantum field theoretical approach of field, cavity loss and the quantum efficiency, offering new avenues for theoretical investigation and experimental verification.

Keywords: Quantum heat engine, Atomic coherence, Loss mechanism, Phaseonium fuel.

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Exploiting Two-Dimensional Bi_2Te_3 Topological Insulator Metamaterials for Advanced Terahertz Applications

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In recent years, there has been growing interest in exploring the potential of two-dimensional materials as a metamaterial in the terahertz (THz) regime. Metamaterials are artificially structured materials engineered to control electromagnetic waves in ways that are not possible with natural materials. Here, we have used Bi_2Te_3 topological insulator as a meta surface. It is known for its robust surface states that are protected by time-reversal symmetry. These surface states can host massless Dirac fermions and exhibit spin-momentum locking, making them promising for various applications in spintronics, quantum computing, and optoelectronics. To harness the capabilities of Bi_2Te_3 as a THz metamaterial, we conducted simulations to optimize the design of periodic structures for different applications in the THz regime, particularly as a filter. The mechanism involves exploiting the unique electronic properties of the surface states, which exhibit high mobility and low scattering due to their topological protection. These surface states interact strongly with THz radiation, leading to enhanced electromagnetic responses, such as high tunability and low energy dissipation. We employed techniques such as lithography for precise patterning and thermal deposition for uniform thin film growth, enabling the creation of these structures with high accuracy and ensuring the desired electromagnetic properties. Specifically, the design includes periodic arrays that can manipulate THz waves through resonances and interference effects. All the results will be presented. The integration of 2D Bi_2Te_3 as a metamaterial in the THz regime not only enhances the performance of existing THz devices but also opens new avenues for innovative applications. The robustness of the surface states, combined with the flexibility in designing the electromagnetic response of the metamaterial, makes Bi_2Te_3 an excellent platform for advancing THz technology.

Keywords: Terahertz; Metamaterial; Topological Insulator; Resonance and Lithography.

Defect-Engineered Bi_2Te_3 Ultrathin Film-based Optoelectronic Synapses for Neuromorphic Computing

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ABSTRACT

Optoelectronic synapses (OES), inspired by biological neuromorphic systems, have garnered significant attention as a potential solution to the von Neumann bottleneck in traditional computing. Various materials, including two-dimensional (2D) materials, have been employed to fabricate OES devices, achieving varying degrees of success. Among these, topological insulators exhibit promising properties, and Bi_2Te_3, with its Te vacancies commonly found in epitaxially-grown samples, emerges as a noteworthy candidate for constructing an OES system. These vacancies, introduced during growth, effectively trap and release charges, resulting in persistent photoconductivity, which can be leveraged as the operating mechanism for OES. This study presents a Bi_2Te_3-based artificial optoelectronic synapse using an ultrathin layer grown via the Thermal evaporation method and post-annealing treatment. The device's performance has been modulated from photodetector to OES device by Te vacancies engineering in Bi_2Te_3 by varying post-annealing temperatures. We successfully demonstrate essential synapse characteristics, such as paired-pulse facilitation (PPF), short-term and long-term memory, spike-timing-dependent plasticity, spike-rate-dependent plasticity, and learning-relearning behavior. These metrics position Bi_2Te_3 as an exceptionally attractive and highly compelling candidate for artificial visual perception systems.

KEYWORDS
Optoelectronic synapse; neuromorphic computing; Bi_2Te_3; persistent photoconductivity; Defect-engineering.

We investigate the pressure induced flat bands in large angle twisted bilayer graphene (tBG). Under the zero external pressure the tBG show the first flat bands for the twist angle 1.08◦. The commensurate higher angle twisted bilayer graphene have large bandwidth lower energy bands when compared to the magic angle (1.08◦) twisted bilayer graphene. In this paper we demonstrate that under the uniaxial pressure (along the z-axis) between the twisted layers of graphene, the bandwidth of the lower energy bands decrease, and we got the flat bands for the higher angle (1.538◦, 2.004◦, 3.89◦, 6.008◦, 7.34◦, 9.43◦, 13.17◦ and 21.78◦) twisted bilayer graphene. Interestingly, the pressure required to have the flat bands increases with the increasing twist angle. We also show the clear evidence in reduction of the band with as a function pressure, and a sudden raise in the bandwidth after a critical pressure for given higher angle twisted bilayer graphene. The nature of the flat bands under the pressure is different than the flat bands at magic angle with no pressure. We demonstrate that the interplay between the interlayer coupling and the twist angles is the key role to obtain the flatlands.

High green index electromagnetic interference shields with semiconducting Bi_2S_3 fillers in a PEDOT:PSS matrix

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ABSTRACT

Conventional metallic EMI (electromagnetic interference) shields and newer 2D material-based shields typically satisfy the shielding effectiveness (SE) requirements for most applications. However, their performance is largely driven by the reflection of incoming electromagnetic waves due to their high electrical conductivity, which can lead to secondary pollution. This issue is becoming more pronounced with the increasing density of electronics and communication networks in modern society. Therefore, there is a growing need for EMI shields that primarily absorb incoming radiation. Such shields would exhibit a high green index, defined as the ratio of absorbance to reflectance, ideally close to or exceeding one. For nonmagnetic materials, an effective approach to minimize the impedance mismatch is by reducing the effective permittivity of the shielding material. In this work, we introduce a novel EMI shield utilizing a semiconducting Bi_2S_3 filler within a conductive PEDOT:PSS polymer matrix, in place of conventional conductive fillers, to lower the effective permittivity. Our findings demonstrate that even with a modest filler loading of 10% Bi_2S_3, the shield achieves a high SE of over 40 dB with a green index of 0.75. Increasing the Bi_2S_3 content to 15 wt% brings the green index close to unity, though the SE decreases to 30 dB. The underlying shielding mechanism is elucidated through electromagnetic parameter measurements and supported by density functional theory (DFT) calculations. This study establishes a basis for developing lightweight, ultrathin EMI shields that minimize secondary pollution while maintaining high performance.

KEYWORDS:

Electromagnetic interference shielding, Green index, Semiconducting filler, Conducting polymer, DFT.

Rahsba spin-orbit coupling induced quantum valley anomalous hall phases in pseudospin-1 dirac fermions

Puspita Parui

Abstract of the poster

We theoretically investigate the topological properties of a pseudospin-1 Dirac fermionic system under the influence of Rashba spin-orbit coupling (RSOC), magnetic exchange interaction, and staggered potential. The momentum-locked spin texture of the lowest-energy nearly flat bands, dominated by exchange coupling, is fully spin-polarized, unlike the pseudospin-$\frac{1}{2}$ Dirac system, which exhibits a helical spin texture across the Brillouin zone. These fully spin-polarized bands contribute to a quantum anomalous Hall effect with a quantized Hall conductivity of $2e^2/h$. The system exhibits a bulk band gap, with the nanoribbon geometry revealing two pairs of gapless chiral edge modes at opposite edges of the system, confirming the quantum anomalous Hall phase. Further, introducing a sublattice-dependent staggered potential leads to a quantum valley anomalous Hall (QVAH) phase, characterized by unequal valley contributions, resulting in a single pair of chiral edge

Field-derivative Torque Induced Magnetization Reversal in Antiferromagnets and Ferrimagnets

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Understanding the mechanism of spin switching in antiferromagnets and ferrimagnets via the excitation of THz pulses holds the promise for future generation magnetic memory devices. Such spins switching can be accomplished by the Zeeman torque exerted by the THz pulses on the magnetic spins [1]. Theoretical and experimental works have established that the field-derivative of terahertz pulse also exerts a torque – field-derivative torque (FDT) [2,3]. Here, we investigate the role of the FDT in the spin switching in antiferromagnets and ferrimagnets using computational approach. Our results foresee that the using a single THz pulse, the spin switching in presence of FDT requires rather less THz magnetic field compared to the spin switching without the FDT. Using successive THz pulses, we observe that the dynamics of Néel vector can be switched on and off depending on the time delay between two THz pulses. To this end, we make a comparison of switching time in antiferromagnets and ferrimagnets. These results not only shed light on the significance of the FDT in magnetization switching but also suggest materials where this switching effect is pronounced.

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Magnon mediated spin pumping by coupled ferrimagnetic garnets heterostructure

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Keywords: Ferrimagnet, Spin Pumping, Magnons, Coupling, Thin Film

ABSTRACT

Spin pumping has significant implications for spintronics, providing a mechanism to manipulate and transport spins for information processing. Understanding and harnessing spin currents through spin pumping is critical for the development of efficient spintronic devices. The use of a magnetic insulator with low damping, enhances the signal-to-noise ratio in crucial experiments such as spin-torque ferromagnetic resonance (FMR) and spin pumping. A magnetic insulator coupled with a heavy metal or quantum material offersa more straightforward model system, especially when investigating spin-charge interconversion processes to greater accuracy. This simplicity arises from the absence of unwanted effects caused by conduction electrons unlike in ferromagnetic metals. Here, we investigate the spin pumping in coupled ferrimagnetic (FiM) $Y_3Fe_5O_{12}$ (YIG)/$Tm_3Fe_5O_{12}$ (TmIG) bilayers combined with heavy-metal (Pt) using the inverse spin Hall effect (ISHE). It is observed that magnon transmission occurs at both of the FiMs FMR positions. The enhancement of spin pumping voltage (V_{sp}) in the FiM garnet heterostructures is observed. The plausible reason might be the interfacial exchange coupling between FiMs. The modulation of V_{sp} is achieved by tuning the bilayer structure. Further, the spin mixing conductance for these coupled systems is found to be around 10^{18} m^{-2}. Our findings describe a novel coupled FiM system for the investigation of magnon coupling providing new prospects for magnonic devices.

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Annual Conference on Quantum condensed matter

Canted antiferromagnetic order in $MnBi_4Te_7$ single crystals

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One of the most exciting areas in condensed matter physics is the investigation of the correlation between topology and magnetism in quantum materials. This field is greatly affected by the Quantum Anomalous Hall Effect (QAHE), which was first observed in MBE grown Cr and V doped $(Bi, Sb)_2Te_3$ thin films [1]. This novel state with full quantization has only been detected at extremely low temperatures (~1K or below) thus far. For any practical application, this effect must be realized at room temperature, which requires a detailed knowledge and exact control of the topological insulating state with long range magnetic order. A workable method for achieving this control is provided by canted antiferromagnetic topological system [2,3]. Where a small canting of the spins leads to a net magnetization that is essential for breaking time-reversal symmetry.

In this work, we synthesize high-quality single crystals of $MnBi_4Te_7$, a member of the intrinsic magnetic topological MBT family. The crystals quality and phase are confirmed by the detail structural characterisation and compositional investigation. Our systematic magneto transport data showed a sharp antiferromagnetic transition at approximately 12.9 K. Our experimental findings highlight the important role of spin canting in influencing the magneto-transport properties of magnetic topological insulators (MTIs) by revealing the existence of a canted antiferromagnetic state below the transition temperature. Our AC susceptibility results further support the canted spin texture characteristic. Furthermore, the bulk crystal exhibits an AHE which we attribute to the reorientation of magnetic domains and the effects of spin canting on resistive states in which hysteresis results in distinct transport properties that vary depending on the direction of the applied magnetic field.

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Glassy behaviour and correlated magnetic properties enhanced with Bi substitution at A-site in La_2NiMnO_6

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Abstract

Structural and magnetic properties of $La_{1.5}Bi_{0.5}NiMnO_6$ (LBNMO) has been reported with first principle calculation for ground state electronic and magnetic properties. The synthesized sample is crystallized in Pbnm space group. The 25 % substitution of Bi at A-site in La_2NiMnO_6 leads to the Ni and Mn ordering which can be observed from the larger magnetic moment in thermal and field variation of magnetization measurement compared to La_2NiMnO_6 polycrystal [1]. A long range weak ferromagnetic (WFM) ordering is observed at 236 K which is less than that observed in the parent sample [2]. Frequency variation of alternative current (AC) magnetic susceptibility measurement shows a shift near to 118 K towards the higher temperature regime signifying glassy type of behavior confirmed from the magnetic memory effects and thermal relaxation analysis. The presence of antisite disorder (ASD) due to presence of Mn^{3+}/Mn^{4+} and Ni^{3+}/Ni^{2+} is confirmed from the X-ray photoelectron spectroscopy measurement.

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Ultrahigh SERS Sensitivity of Niobium Pentoxide Nanoparticles Enabled by Oxygen Vacancy Engineering: Theoretical and Experimental Insights

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Oxygen vacancy engineering in metal oxide-based semiconductors has emerged as a promising research direction for sensing applications like Surface-enhanced Raman scattering (SERS) and gas sensing, offering the potential to replace costly and unstable noble metal substrates in the future. However, enhancing the SERS sensitivity in semiconductor-based substrates remains a significant challenge. In this study, we demonstrate that oxygen vacancy engineering in Niobium pentoxide (Nb_2O_5) nanoparticles can achieve ultrahigh SERS sensitivity. Oxygen vacancies were introduced and controlled in the Nb_2O_5 nanoparticles through a straightforward high-energy ball milling method followed by post-growth oxygen annealing. This approach resulted in a substantial enhancement factor (EF) of 5.15×10^7 for the detection of Methylene Blue (MeB) molecules, with a minimum detection limit of 10^{-8} M - two orders of magnitude lower than the pristine Nb_2O_5 substrate. A thorough analysis of the experimental results, combined with theoretical calculations, revealed that the SERS performance is directly correlated with the concentration of oxygen vacancies in the Nb_2O_5 nanoparticles. Density functional theory (DFT) calculations indicated a strong coupling of vibronic states and an increased charge transfer (CT) efficiency within the Nb_2O_5–MeB complex, facilitated by the trap states introduced by oxygen vacancies in the defective Nb_2O_5 structure. Additionally, finite element method (FEM) simulations indicated a field enhancement factor of approximately 4.17 $\times 10^2$, contributing to the overall SERS EF. The remaining enhancement, approximately 1.23

× 10^5, is attributed to the oxygen vacancy-mediated charge transfer, which is the highest reported value to date. These findings provide valuable insights into the design and fabrication of defect-engineered, cost-effective semiconductor-based SERS substrates for various applications, including trace dye detection. This research paves the way for the development of advanced sensing platforms with improved performance and broader applicability.

Development of 3-axis a low-cost compact cryogenic nanopositioner for low temperature scanning probe microscopy and point contact spectroscopy

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Precision nanopositioning is essential for a wide array of advanced technologies, including microscopy, superconductors, semiconductor testing, and optics. Here, we present the development of a compact low-cost, home-built inertial nanopositioner operating on the slip-stick principle, along with computer-controlled drive electronics. The nanopositioners have a modular design where individual modules for movement in the horizontal and vertical directions can be stacked above one another for motion along three orthogonal directions with a minimum step size of ~100 nm. We have tested our nanopositioners by fabricating a fully automated point contact Andreev Reflection setup operating down to 2 K. Our nanopositioners can also be easily integrated into various low-temperature scanning tunneling microscopes.

(All designs presented here are open source and available for anyone who wants to replicate.)

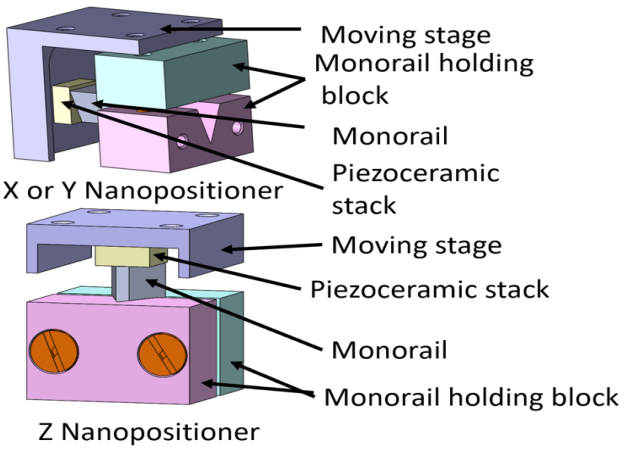

Fig 1. Design of X and Z nanopositioner

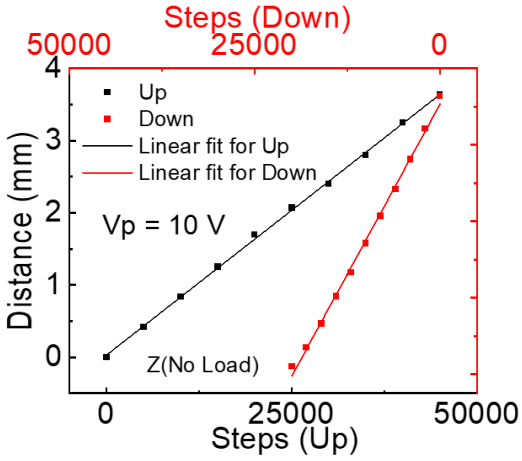

Fig 2. Distance vs Step size of Z nanopositioner for moving up and down at 50 V. Fitted with line of slope of 80.23 nm/ step and 177.86 nm/ step for up and down respectively.

Magnetic properties of non-collinear Heusler antiferromagnet Ru_2MnSi

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The field of antiferromagnetic spintronics has experienced significant growth in recent years and has potential applications in various spintronics technologies. These materials exhibit a large anomalous Hall effect, magneto-optical Kerr effect, large tunnelling magneto-resistance, etc., despite having zero net magnetization. However, the non-collinear antiferromagnetic family is currently limited to Mn_3X (X = Sn, Ge, etc.) and Mn_3AN (A = Sn, Ni).

In this study, we investigated a new family of non-collinear antiferromagnets. We synthesized the Heusler alloy Ru_2MnSi using the arc melting technique, which involves melting the high-purity individual elements, namely Ru, Mn, and Si. The composition of the alloy, as determined by energy-dispersive X-ray spectroscopy, is found to be 57:13:30. This study reveals that the alloy is not stoichiometric. Additionally, the X-ray diffraction technique has been employed to study the crystal structure of Ru_2MnSi, which shows a predominant phase of polycrystalline Ru_2MnSi and a minor phase of hexagonal Ru. Furthermore, temperature-dependent magnetization and magnetic hysteresis measurements confirm the antiferromagnetic ground state, consistent with theoretical predictions.

Keywords— Spintronics, noncolinear antiferromagnet, Heusler alloy

Parsing skin effect in a non-Hermitian spinless two-orbital model and its circuit realization

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Abstract

We examine a non-Hermitian (NH) tight-binding system comprising of two orbitals per unit cell and their electrical circuit analogs. We distinguish the PT-symmetric and non-PT symmetric cases characterized by non-reciprocal nearest neighbor couplings and onsite gain/loss terms, respectively. The localization of the edge modes or the emergence of the topological properties are determined via the maximum inverse participation ratio, which has distinct dependencies on the parameters that define the Hamiltonian. None of the above scenarios exhibits the non-Hermitian skin effect. We investigate the boundary modes corresponding to the topological phases in a suitably designed electrical circuit by analyzing the two-port impedance and retrieving the admittance band structure of the circuit via imposing periodic boundary conditions. The obtained results are benchmarked against the Hermitian version of the two orbital model to compare and discriminate against those obtained for the NH variants.

Keywords: Non-Hermitian quantum mechanics, Topological insulators, PT symmetry, Electrical circuits.

Competition between Entanglement and Symmetry Breaking in Kondo Effect under the Influence of local Magnetic field

Debraj Debata, Abhirup Mukherjee, Siddhartha Lal

Abstract:
A Kondo spin-$\frac{1}{2}$ impurity in local magnetic field shows a $T = 0$ quantum phase transition from the Kondo singlet phase to a field-aligned local moment as the magnetic field strength is tuned. We observe the breakdown of Kondo screening and the destabilization of the entangled singlet state due to tuning the magnetic field close to the critical value. This is a transition from a quantum dynamical state to one with classical dynamics. Fermi liquid excitations lying just above the singlet are replaced by non-Fermi liquid excitations at the QCP. Spectral function and quasiparticle residue also show signatures of Kondo destruction. This system offers a toy model to investigate the decohering effects of an environment on a quantum system against that of a continuous observer.

Conduction Mechanism in Mott-Hubbard Insulator $LaTiO_3$

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(Dated: 31 August 2024)

Mott-Hubbard insulators, like $LaTiO_3$, are materials where strong electron-electron interactions cause insulating behavior, even when their band structure might suggest they should conduct. This study investigates the conduction mechanisms of $LaTiO_3$ over a frequency range from 100 Hz to 1 MHz. Analysis reveals that polaron hopping dominates the AC conductivity, while DC conductivity data indicate a variable range hopping mechanism. Analysis of DC conductivity using the Arrhenius equation provides activation energy and insights into the nature of hopping processes and polaron concentration. Additionally, the interactions between spin and lattice are explored. These findings advance the understanding of $LaTiO_3$ and underscore the broader significance of studying Mott-Hubbard insulators, which offer valuable insights into electron correlations and the design of advanced materials with unique electronic properties.

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Spinterface Mediated Magnetic Properties of $Co_{20}Fe_{60}B_{20}/Alq_3$ Heterostructures

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Organic spintronics aims to combine organic electronics and spintronics by bringing the organic semiconductors (OSCs) to the close proximity of various inorganic materials[1]. When organic molecules are deposited on a ferromagnet, a few monolayers of organics acquire magnetism because of the orbital hybridization and charge transfer at the hybrid interface, popularly known as "spinterface"[2]. Spinterface modifies the density of states of ferromagnet and tends to modulate several magnetic properties like magnetization reversal, domain dynamics, magnetic anisotropy etc. of the ferromagnet/organic molecule heterostructure [3-6]. A small π- conjugated molecule Tris(8-hydroxyquinolinato)aluminum commonly known as Alq_3 with the chemical formula $Al(C_9H_6NO)_3$ is an OSC widely used in organic electronics. It has a large spin-diffusion length making it favorable for spin transport thus making it suitable for spintronics applications [7].

In this study, the spinterface is formed when Alq_3 molecules are placed on the amorphous ferromagnet CoFeB. The magnetic domain size and form are considerably changed by the *π-d* hybridization in CoFeB/Alq_3, which also strengthens the coercive field. The Alq_3 molecules enhance the magnetic anisotropy (~86%) and reduce domain sizes of CoFeB upon the formation of the spinterface. The ferromagnetic resonance study reveals that the Gilbert damping gets reduced in the CoFeB/Alq_3 heterostructures. From this study, we can conclude that Alq_3 is a good candidate to tailor magnetic domains and anisotropy and is a promising candidate for developing spin-based electronic devices with potential advantages over traditional inorganic materials.

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QMAT 2024 Conference

Green-synthesis of Fluorescent Carbon Quantum Dots for application in sensing and ion detections

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Abstract: Detection of harmful ions in water is very important to keep people and the environment safe. Toxic ions like heavy metals, fluoride, and nitrates can cause serious health problems and also damage to the nature. Conventional methods used for the detection of these ions often involve complex, costly, and environmentally hazardous procedures. This study aims to deal with these challenges by synthesizing carbon quantum dots (CQDs) via a green, chemical-free method using natural precursors. Green synthesis reduces environmental impact and offers a sustainable alternative to conventional techniques. The synthesized CQDs are explored for their potential as effective, sensitive, and specific fluorescent markers for detection of harmful ions in water. The study further investigates the optimization of fluorescence response through pH and temperature adjustments, aiming to improve the detection capabilities of these green-synthesized CQDs. This research highlights the dual benefits of using eco-friendly materials and approaches for monitoring water quality, contributing to the development of sustainable technologies for environmental protection.

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Magnetic and magnetic-transport property of $NiCo_2O_4$ nanoparticles

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Transition metal oxides are currently a subject of great interest because of their significant magnetism, rich magneto-transport properties, and potential applications in energy storage and spintronics. Nickel cobaltite ($NiCo_2O_4$) shows promise as a material for use in supercapacitors, Li-ion batteries, electrocatalysts, fuel cells, and sensors. Recently, $NiCo_2O_4$ (NCO) thin films have demonstrated significant potential in spintronics applications due to their strong out-of-plane magnetic anisotropy, linear magnetoresistance, and robust anomalous Hall effect that persist above room temperature. However, the magnetic and magneto-transport properties of NCO bulk have not been explored.

Here, we aim to synthesize single-phase NCO nanoparticles using a cost-effective sol-gel auto-combustion method and study its structural, magnetic, and magneto-transport properties. The structural property of the synthesized nanoparticles has been characterized using powder X-ray diffraction (XRD). The XRD results confirm the pure spinel phase formation of the synthesized NCO nanoparticles. The average crystallite size of the sample is found to be ~ 12 nm using Scherrer's formula. The morphological and compositional properties are carried out using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX), respectively. The results from the EDX analysis indicate a Ni to Co ratio of approximately 1:2 in the synthesized NCO nanoparticles. The SEM micrograph reveals that the particles have a spherical morphology, and the average particle size is approximately 20-30 nm. The temperature dependence and magnetic hysteresis measurements show a ferrimagnetic ground state with the Curie temperature beyond 400 K. The saturation magnetization and coercivity are found to be 0.18 emu/g and 3042 Oe, respectively, at 5 K.

Keywords: Transition metal oxides, Sol-gel auto-combustion, Ferrimagnetism.

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Phonon Dynamics in Reconstructed Moire´ Superlattice of Engineered 2D Lateral Heterostructures

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) have received extensive attention owing to their exotic physical, electro-optical properties and applications for next-generation flexible and transparent optoelectronics. Co-integration of different 2D TMDs into heterostructure can evoke new functionalities and provide new ways to manipulate their electronic, optical, and excitonic properties. Though 2D heterostructures have been studied extensively in the past decades using mechanically exfoliated samples understanding fundamentals on directly synthesized TMDs is still missing and needs further investigation.. In this context, the chemical vapour deposition (CVD) method holds the optimized balance between high quality, controllability, and cost-effectivity [1]. Among others, the water-assisted one-pot CVD strategy is the most straightforward, robust, and highly controllable to grow electronic grade 2D LHS in situ with controlled thickness, layer number, and domain width using bulk TMDs as solid precursors in the presence of different carrier gases for the selective evaporation [2,3]. Using this strategy and manipulating precursor to substrate distance, growth temperature, time, and adatoms flux, we have fabricated monolayer, bilayer, and trilayer multi-junction MoS_2-WS_2, $MoSe_2$-WSe_2 LHS. Using the dry transfer method, we have transferred MoS_2-WS_2 LHS onto other 2D HS (Fig1). High-frequency and low-frequency Raman and photoluminescence spectroscopic measurements were carried out to understand the lattice reconstruction, interlayer interaction, optical characteristics, and charge transfer dynamics of these hybrid heterostructures with tunable moire´ periods. The stacking order-dependent formation of phonons, interlayer excitons, and their complexes was investigated in detail.

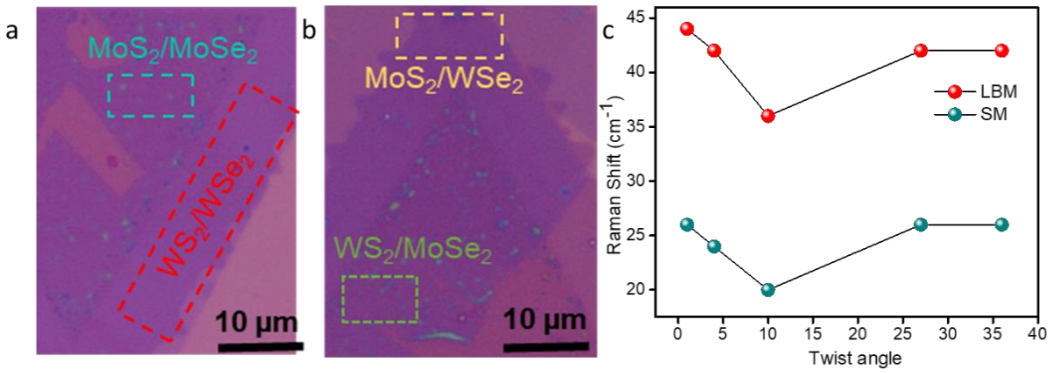

Figure: (a,b) Optical images of heterobilayers.(c) Twist angle dependence of Lower breathing and Shear modes for WS_2/WSe_2 heterobilayers

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A comprehensive exploration of the intriguing phenomena known as the spin Nernst effect (SNE) and the spin Hall effect (SHE) within the context of nonmagnetic strong topological insulator $ZnCu_2SnSe_4$, has been carried out employing first-principles calculations. Our theoretical calculations unveil significantly large intrinsic spin Nernst conductivity (SNC) and spin Hall conductivity (SHC) in the bulk topological insulator ZnCu2SnSe4. Delving deeper into the intricacies of our findings, we elucidate how the inverted band order in the topological materials drastically influences the spin Berry curvature, consequently exerting a profound impact on SHC and SNC. Detailed analyses reveal that the contribution from the bulk to the generation of pure spin current in a topological insulator is comparable to that of a surface. This underscores the potential role of topological insulators in the development of spin-switching devices. We present compelling evidence that $ZnCu_2SnSe_4$ holds immense promise as an optimal candidate for the generation of pure spin currents, achieved through the application of both thermal gradients and electric fields. This, in turn, opens up exciting avenues for its utilization in the realms of spin-caloritronics, spin-orbitronics, and spintronics.

Reference: *Shivam Sharma and Abir De Sarkar 2024 J. Phys.: Condens. Matter 36 445501*

Two-dimensional material-based printed optoelectronic synapse for next-generation neuromorphic application

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Abstract: Optoelectronic synapses, which integrate photodetection and synaptic functions in a single platform, offer a promising approach to mimic the visual processing capabilities of the human brain. These devices allow for simultaneous perception, processing, and memorization of visual information, making them ideal for advanced artificial vision systems with applications in robotics, autonomous vehicles, medical imaging, and surveillance. Recent research has focused on two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), which offer unique properties like tunable bandgaps, high light-matter interaction, mechanical flexibility, and ultrathin structures. These characteristics make 2D materials suitable for energy-efficient, flexible, and wearable devices. Despite their advantages, the fabrication of 2D material-based devices has predominantly relied on lithography-based techniques, which are costly, require cleanroom facilities, and involve high-vacuum systems. These limitations hinder the scalability of these devices for practical applications. Printing technology has emerged as a cost-effective, non-vacuum, maskless alternative for device fabrication, offering low-temperature processing. However, fully printed 2D material-based optoelectronic devices are rarely reported due to challenges like reduced photoelectric conversion efficiency and material degradation in printed thin films. In this work, we introduce a novel approach that combines chemical vapor deposition (CVD) of monolayer molybdenum disulfide (MoS_2) with printed electrodes to fabricate a high-performance optoelectronic synaptic device. This is the first reported integration of CVD and printing technologies for such devices. The resulting system demonstrates excellent synaptic behaviors, including excitatory postsynaptic current (EPSC), paired-pulse facilitation (PPF), short-term memory (STM), long-term memory (LTM), and spike-timing-dependent plasticity (STDP). This hybrid approach offers a scalable and cost-effective pathway for developing high-performance optoelectronic devices, opening new possibilities for artificial vision and neuromorphic computing applications.

Coherent population transfer with polariton states in circuit QED

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The stimulated Raman adiabatic passage (STIRAP) allows selective, coherent population transfer in a three-level quantum system by the adiabatic control of two suitably chosen envelopes and delayed laser pulses. However, the long operation time involved with the adiabatic protocols makes them more susceptible to decay and decoherence. A shortcut-to-adiabaticity technique, namely, counterdiabatic driving (CD), suppresses the decoherence-induced loss by speeding up the STIRAP process, thereby enhancing the efficiency and fidelity of population transfer. The superadiabatic STIRAP (saSTIRAP) method requires the application of a shortcut drive or CD pulse, which couples the coherently trapped states in a three-level quantum system. Hence, the closed-loop Λ system consisting of all electric dipole-allowed transitions is an essential requirement for saSTIRAP, which is rarely admissible in a natural atom. This paper theoretically investigates an experimentally feasible model for implementing saSTIRAP using a closed-loop Λ system with doubly dressed polariton states in a driven circuit QED system. We show a population transfer with efficiencies close to 80.75% and 98.10% with fidelities of 89.86% and 99.04% for the resonant STIRAP and saSTIRAP protocols, respectively, with experimentally feasible parameters. The efficiency of the population transfer can be further increased by improving the coherence times of the cavity and the transmon qubit. This work may be useful in designing fast, efficient quantum gates for applications in quantum technologies.

Keywords: Quantum optics, Stimulated Raman Adiabatic Passage, Circuit Quantum Electrodynamics
DOI: 10.1103/PhysRevA.110.023716

Artificial Intelligence and Machine learnings in Physics

Restricted Boltzmann Machine approach to solve Quantum Many-Body problems

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Category: Poster

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

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

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Impurities induced vortex lattice melting and turbulence in rotating Bose-Einstein condensates

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We investigate the impact of various impurities on rotating Bose-Einstein condensates confined within two-dimensional harmonic and optical lattice potentials. Without impurities, the rotating condensates display an organized square lattice pattern of vortices due to the influence of a square optical lattice. The introduction of impurity potentials disrupts this lattice structure, inducing a phase transition from an ordered state to a disordered state. Our analysis encompasses both static and dynamic types of impurities. The static impurities are implemented using a randomly varying potential with a spatially random amplitude. The transformation of the vortex lattice structure, in this case, relies on the strength and lattice constant of the impurity potential. For dynamical impurities, we employ a Gaussian obstacle that orbits around the condensate at a specific distance from its center. In this scenario, the vortex lattice melting occurs beyond a certain threshold radius and frequency of oscillation of the rotating obstacle. We characterize the melting of the vortex lattice due to impurities using various quantities, such as the structure factor and angular momentum. Notably, in the vortex-melted state, the angular momentum follows a power-law dependence with an exponent of approximately 1.73, regardless of the type of impurity. Finally, we demonstrate the signature of the presence of a turbulent state within the vortex-melted state generated by both static and dynamical impurities.

Non-equilibrium theory for pump-probe spectroscopy

Shivangi , Rajdeep Sensarma

Abstract

Condensed matter physics employs various techniques such as thermodynamic measurements, spectroscopy, and transport methods to investigate materials. Among these, pump-probe spectroscopy stands out as a non-equilibrium technique that excites a system with a pump pulse and monitors its response with a probe pulse. This method is particularly powerful for studying strongly correlated systems, where coherent behavior and interaction effects play crucial roles. Despite its utility, interpreting pump-probe features in these systems lacks a standardized "dictionary" due to the complex interplay of interactions. While semi-classical approaches are prevalent, they often fail to capture these interactions adequately. In contrast, Keldysh field theory offers a promising framework by incorporating interaction effects, potentially unveiling interaction-specific signatures in pump-probe measurements. This research aims to develop such a theoretical framework to understand pump-probe spectroscopy in non-interacting systems, setting the stage for future studies to investigate critical features and deeper understandings of the complex materials.

Effect of inter coulomb interaction on the transport properties of a single molecular transistor in the presence of electron-phonon interaction

Manasa Kalla, Ch. Narasimha Raju

Abstract— We study the effect of inter coulomb interaction on the quantum transport properties of a single molecular transistor in the presence of electron-phonon interaction using the Keldysh Green function technique. We use the Anderson-Holstein Model to describe the single molecular transistor that consists of a molecular quantum dot (QD) with two states (ground state and excited state) coupled to two metallic leads. The phonons are eliminated by the Lang-Firsov transformation and the effective Hamiltonian is used to study the effect of on the spectral density function, tunneling current, differential conductance and spin polarization of a single molecular transistor at zero temperature.

***Keywords*—**Quantum Dots, Anderson-Holstein Model, Inter and Intra coulomb interaction, electron-phonon interaction

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Volatile organic compounds (VOCs) emitted by food products are considered markers for assessing quality of food. In this work, first-principles Density Functional Theory (DFT) and Non-equilibrium Green's function (NEGF) methods have been employed to model chemo-resistive gas sensor based on two-dimensional silicene based nanosheets that can sense the six different VOCs emitted by standard food products. Our calculations with unpassivated and flourine passivated silicene(F-silicene) sheets as sensor materials show that flourine passivated silicene has significantly better sensitivity towards all six VOC molecules (Acetone, Dimethylsulfide, Ethanol, Methanol, Methylacetate and Toluene). Moreover, flourinated silicene sensor is found to be capable of separately recognising four VOCs, a much better performance than r-GO used in a recent experiment. We analyse the microscopic picture influencing sensing capabilities of un-passivated and fluorinated silicene from the perspectives of adsorption energy, charge transfer and changes in the electronic structure. We find that better sensing ability of fluorinated silicene nanosheet can be correlated with the changes in the electronic structures near the Fermi level upon adsorption of different VOCs. The results imply that passivated silicene can work better as a sensor than r-GO in case of generic food VOCs. The results are important since modelling of various two-dimensional nano-sensors can be done in the similar way for detection of more complex VOCs emitted by specific food products.

Majorana Qubits: Perspectives and Challenges in Quantum Computation

Abstract

Quantum computation emerges as a revolutionary field, offering the potential to solve problems intractable for classical computers. Condensed matter physics, with its rich variety of quantum phenomena, provides a promising platform for realizing quantum computational elements. Non-Abelian anyons, such as Majorana fermions, play a crucial role in quantum computation due to their unique braiding statistics, which can be harnessed for fault-tolerant quantum information processing. Majorana fermions emerge in various condensed matter systems, such as at the edges of topological superconductors. A notable example is the p-wave Kitaev chain, utilized in this study.

This work investigates the emergence of Majorana fermions in a p-wave Kitaev chain by analyzing the band spectrum and Berry phase, confirming the presence of Majoranas. It also exploits the symmetries inherent in the model to classify the system within the framework of the tenfold topological classification. This classification allows for the use of appropriate topological invariants to accurately count the number of emergent Majorana modes. Additionally, the study explores the non-Abelian statistics of Majorana fermions, where the exchange (or braiding) of these particles results in a transformation described by a unitary operator. This work constructs such a unitary operator essential for the exchange of two Majoranas, demonstrating the non-Abelian nature of their statistics. This research aims to provide insights into the behavior of Majorana fermions and lays the groundwork for their potential application in quantum computing.

Ultra-Broadband Terahertz Metamaterials for 6G and beyond

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Abstract: Our study presents a novel metamaterial design that enables ultra-wideband terahertz transmission while being insensitive to polarization. This is achieved by stacking a cross-shaped resonator on top of a square ring resonator separated by an optimized polyimide spacer. Our results indicate that stacking the resonators provides wideband terahertz transmission.

Introduction: Exploring the electromagnetic spectrum, the terahertz (THz) domain, spanning 0.1 to 10 THz, lies between the microwave and infrared regions and is largely untapped. This "terahertz gap" offers the potential for revolutionizing high-speed wireless communication, promising data transfer rates up to 1 Tbps. To harness this potential, the development of broadband THz devices like wave plates, switches, and filters is crucial for advancing THz photonics and communication systems [1]. Metamaterials (MMs), with their sub-wavelength structures, stand out for their ability to manipulate THz waves beyond conventional material capabilities. Despite progress, broadening the bandwidth of metamaterials, such as through planar metamaterial, remains challenging. In addressing this, we introduce a two-layer multi-stacked metamaterial configuration that comprises a cross-shaped resonator on the top of square ring structure spacing with a loss-free polyimide. We conduct rigorous simulations to investigate the broadband transmission response, focusing on the thickness of the spacer and positioning of resonators and the near-field coupling between them. Additionally, we employ a transmission line model to elucidate the broadband resonance mechanism of our proposed metamaterial. The finding of broadband enhancement can be useful in the THz photonics and next-generation wireless communications [2].

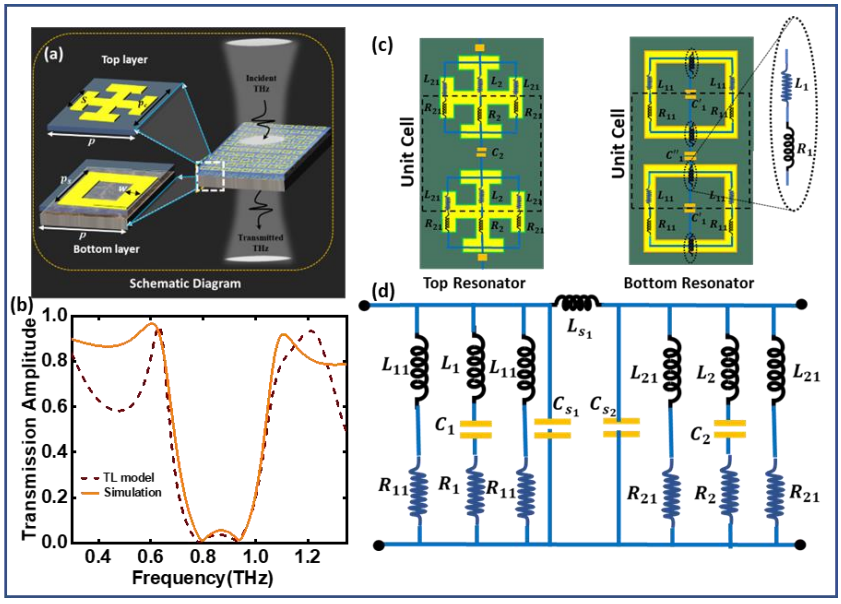

Figure 1: (a) Represents the unit cell of the metamaterial with different resonators. (b) Represents the transmission amplitude calculated from CST and TL line model. (c) Circuital representation of the unit cells. (d) Represents the coupled circuital model of the multistacked MM.

Ultra-broadband transmission of designed MM: The proposed metamaterial configuration, designed using

CST software, features a multi-stacked structure with a cross-shaped resonator placed on top of a square ring resonator, separated by a *50 μm* thick loss-free polyimide film. The square ring resonator, with a periodicity of *P=100* μm, lengths of P_c*=63 μm*, and a width of *w=7 μm*, is designed on a *30 μm* thick silicon substrate with *0.2 μm* thick aluminum resonators to prevent THz wave penetration. The cross resonator, with a length of P_s*=81 μm* and *S=20 μm*, is then placed on the ring resonator with the polyimide spacer. The permittivity of quartz and polyimide is chosen to be 4.4 and 3.5, respectively. Simulations utilized a frequency domain solver with tetrahedral meshing and a normally incident plane wave, accommodating both TE and TM polarizations (see Figure 1(a)).

Table 1: Circuit parameters for calculating the electromagnetic response of the TL models.

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
R_1(Ω)	05.0	R_2(Ω)	1	C_{S1} (fF)	1.70	R_{11}(Ω)	6.54	L_{21}(pH)	182
L_1(pH)	39.4	L_2(pH)	56.52	C_{S2} (fF)	1.19	R_{21}(Ω)	1.46	-	-
C_1(fF)	0.74	C_2(fF)	0.71	L_{S1} (pH)	41.36	L_{11}(pH)	140	-	-

Analyzing the transmission response of the metamaterial's resonators and their combined effect, we observed a substantial enhancement in transmission bandwidth. The square ring resonator alone showed a bandwidth (FWHM) of 0.22 THz, which enhanced to 0.35 THz upon integrating a cross resonator, marking a bandwidth increase of over 150% in the multilayered setup compared to a single layer. The design's orthogonal symmetry ensures uniform transmission for both TE and TM polarizations, enhancing its applicability. The broadband transmission is due to the superposition of individual resonances (positioned closely), with their convergence boosting the overall bandwidth, demonstrating the synergistic benefit of the multi-stacked approach.

To elucidate the broadband resonance mechanism of our multilayered metamaterial, we formulated a circuital model with coupled resonators [3]. This model employs a series combination of inductance (L), capacitance (C), and resistance (R) to mirror the CST simulation's transmission response, showcased in Figure 1(c) and (d). Table 1 outlines the parameters for L, C, and R. The transmission line (TL) circuit models for this dual-layered structure perfectly matches well validating the model's effectiveness in capturing interactions between the stacked resonators.

Conclusions: We designed polarization-insensitive broadband modulators using stacking of resonators. A FWHM of 350 GHz has been achieved for the multistacked MM, enhancing the bandwidth by over 150% compared to a single resonator. The transmission line model was employed to explain the coupling between the stacked resonators. The designed broadband metamaterial can be used as broad stopband filters and for functional broadband THz device applications.

Acknowledgements

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Active Tuning of Polarization-Insensitive Quasi-BIC Mode in THz Metasurfaces

*Note: Sub-titles are not captured in Xplore and should not be used

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***Abstract*— The practical application of symmetry-protected quasi-bound states in the continuum (quasi-BIC) mode is often constrained by their intrinsic polarization dependence, which arises from symmetry-breaking effects. In this work, we demonstrated the excitation of a polarization-independent, dynamically switchable quasi-BIC mode in a terahertz (THz) metasurface. This is achieved through the strategic integration of a graphene layer into the metasurface design. The incorporation of graphene enables dynamic control over the quasi-BIC mode by adjusting the fermi energy from 0.01 eV to 1 eV.**

Keywords—Terahertz, metasurface, quasi-BIC

I. Introduction

In recent years, bound states in the continuum (BIC) have emerged as a paradigm-shifting concept in the field of photonics and metamaterials, due to their high-quality factor(Q factor) nature. BIC is characterized by its ability to remain localized despite existing in the continuum spectrum of radiation modes. Many works have been reported in the context of the excitation of quasi-BIC modes for terahertz metasurfaces. Most of the reported studies are based on symmetry-protected quasi-BIC resonance, in which the structural symmetry is perturbed to transform the ideal BIC into a quasi-BIC mode[1], [2], [3]. However, a significant challenge in harnessing the full potential of BICs lies in their inherent sensitivity to polarization due to structural symmetry breaking of the metasurface unit cell. To surmount this obstacle, we have demonstrated an innovative method for achieving polarization-insensitive quasi-BIC resonances by utilizing two pairs of metallic ring resonators in a metasurface unit cell. We have further shown the active modulation of the quasi-BIC mode by utilizing the graphene layer in the metasurface. The fermi energy of the graphene can be changed by applying external biasing voltage which can change the quasi-BIC mode into a BIC mode[4].

II. Design and Modelling

We have used Finite Integration Technique-based CST microwave studio suite simulation software to design and model the metasurface design. The design is excited with a normally incident TE-polarized THz radiation. The boundary conditions are chosen as unit cell along X and Y directions to incorporate the periodic repetition of the unit cell block. The design is simulated under the frequency domain solver with fine tetrahedral meshing. Figure1 presents a schematic of the metasurface design, with structural parameters: $r_1 = 33\mu m$, $r_2 = 27\mu m, P = 200\mu m$ and width $(w) = 6\ \mu m$. The aluminum rings are designed on the top of a quartz substrate.

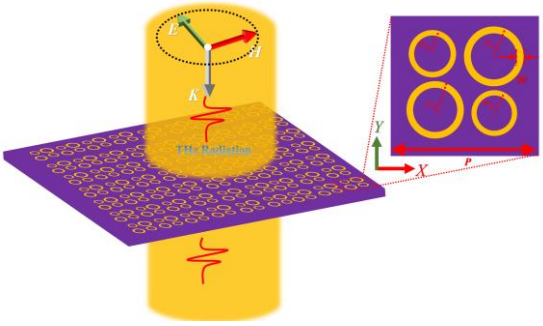

Figure 1: The schematic view of the planar metasurface design. The unit cell consists of four aluminum ring structures on the top of quartz substrate. The geometrical parameters are: $r_1 = 33\mu m$, $r_2 = 27\mu m, P = 200\mu m$ and width $(w) = 6\ \mu m$.

III. Discussion

To excite a quasi-BIC resonance mode in the structure we have introduced a structural symmetry breaking effect. Figure 2(a) shows the excited quasi-BIC mode with a symmetry perturbation parameter α=6.66%. Under the symmetry

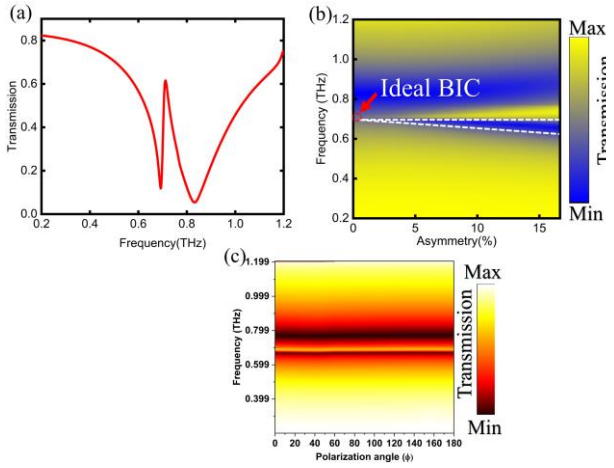

Figure 2: (a) The simulated transmission spectrum with an asymmetry parameter $\alpha = 6.66\%$ for a TE polarized incident radiation, (b) the colour contour plot showing evaluation of BIC to quasi BIC under symmetry breaking effect, (c) the contour plot depicting the variation of resonance mode with respect to the incident polarization angle.

breaking effect the usually uncoupled resonance mode couples to the free space radiation continuum with a net dipole moment. It is evident from fig2(b) that the asymmetric narrow linewidth resonance disappears from the spectrum as we make the structure symmetric. The contour plot depicts that the

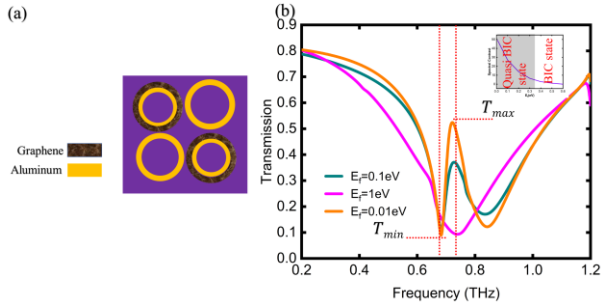

Figure 3(a) The schematic of the metasurface unit cell, when graphene is used for dynamic tunability, (b) the simulated transmission response with respect to varying fermi energy $E_f = 0.01\ eV, 0.1\ eV\ and\ 1\ eV$. The inset shows the switching behavior with the adjustment of E_f in terms of spectral contrast.

broad continuum still exists in a symmetric structure with α=0%, however as we increase the asymmetry the ideal BIC mode manifests as a finite linewidth quasi-BIC resonance mode. The proposed design also shows perfect stability under the polarization angle rotation of the incident wave as shown in Fig 2(c). To exploit the dynamic modulation of the existing quasi-BIC mode we have used a graphene layer surrounding the two metallic rings of radius 30 μm as shown in Fig 3(a). The conductivity of the graphene monolayer depends on the fermi level according to the Kubo formula[4], [5] :

$$\sigma_g(\omega) = \frac{e^2 E_f}{h^2 \pi} \frac{j}{(\omega - i\tau^{-1})} \quad (1)$$

where, τ is the relaxation time, e is the electronic charge and E_f is the fermi energy of graphene. The fermi energy can be tuned by an external biasing voltage according to a closed approximation relation[5]:

$$E_f = \hbar V_f \sqrt{\frac{\pi \epsilon_r \epsilon_0 V_g}{e t_{sub}}} \quad (2)$$

where, V_f is the fermi velocity and V_g is the external biasing voltage, t_{sub} is the thickness of the substrate. Equation 1 considers only the intra-band electron transitions under THz wave excitation, due to the low photon energy of THz frequency. Figure 3(b) depicts that by changing the graphene Fermi energy from 0.1 eV to 1 eV the resonance behavior of the metasurface can be transformed from quasi BIC to BIC. At $E_f = 0.1eV$ the graphene layer behaves as a semiconductor and hence the quasi BIC mode exists due to the effective symmetry breaking. As the Fermi energy increases to 1 eV graphene behaves as a conducting material and hence effective degree of perturbation in the system becomes zero. In such cases, the metasurface unit cell behaves similarly as symmetric structure and hence the quasi-BIC resonance disappears. To further depict the switching behavior from quasi-BIC to BIC, we have calculated the spectral contrast of the resonance mode as:

$$Spectral\ Contrast = \frac{(T_{max} - T_{min})}{(T_{mx} + T_{\min})} \times 100\%.$$

The inset in Fig. 3(b) shows the variation of the spectral contrast of the quasi-BIC resonance mode with the fermi energy of graphene. A zero spectral contrast depicts that the quasi-BIC resonance mode merges into the continuum and hence behaves as an ideal BIC mode.

IV. Summary

In summary, this study has successfully demonstrated a metasurface featuring a symmetry-protected quasi-bound state in the continuum (quasi-BIC) mode, which is independent of polarization. The quasi-BIC mode is excited by adopting an innovative symmetry-breaking approach. A layer of monolayer graphene was incorporated into one pair of metallic rings within a metasurface consisting of four ring resonators. This pair has a smaller radius compared to the other pair. This integration facilitates a dynamic transition from a quasi-BIC to an ideal BIC mode, triggered by alterations in the Fermi energy (Ef) from 0.1 eV to 1 eV. Such changes cause the graphene's conductivity to shift from semiconductor-like to metallic-like behavior. As a result, the quasi-BIC mode vanishes from the spectrum due to the absence of symmetry-breaking effects in its metallic state.

Acknowledgment

The author GK would like to acknowledge the financial support from the SERB, India (CRG/2021/002187).

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Monday, 23rd December, 2024

List of Abstracts – Talks

[Day3 Parallel Session -1]

Systematically compactifying the two-channel Kondo model: fermions to bosons and back in a consistent way

Nayana Shah*
Washington University in St. Louis

We revisit the compactification of the two-channel Kondo model and show that bosonization-debosonization (BdB) can be used as a systematic method for that purpose but only if we use a consistent BdB framework.

Non-Linear Hall Effect in Flatlands and Chiral Crystals

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Indian Institute of Science, Bangalore

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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Trade-off relations between quantum coherence and measure of many-body localization

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Saha Institute of Nuclear Physics, Kolkata

Quantum coherence, a fundamental resource in quantum computing and quantum information, often competes with localization effects that affects quantum states in disordered systems. In this work, we prove exact trade-off relations between quantum coherence and a measure of localization and many-body localization, namely, the inverse participation ratio (IPR). We prove that the l1-norm of quantum coherence and the relative entropy of coherence for a pure quantum state satisfy complementarity relations with IPR. For a mixed state, IPR and the l2-norm of quantum coherence as well as relative entropy of coherence satisfy trade-off inequalities. These relations suggest that quantum coherence, in disordered quantum systems is also an ideal characterization of the delocalisation to many-body localisation transition, much like IPR, which is a well-known diagnostic of MBL. These relations also provide insight into the unusual properties of bipartite entanglement entropy across the MBL transition. We believe that these trade-off relations can help in better understanding of how coherence can be preserved or lost in realistic many-body quantum systems, which is vital for developing robust quantum technologies and uncovering new phases of quantum matter.

Negative Capacitance for Stabilizing the Logic State in a Tunnel Field-Effect Transistor

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Negative capacitance (NC) in ferroelectric (FE) materials, typically unstable, can be stabilized by integrating a suitable dielectric (DE) in series with FE capacitors. Additionally, incorporating a FE capacitor into the gate stack of a metal oxide semiconductor (MOS) transistor enhances gate capacitance, especially in the NC region, acting as a step-up voltage transformer proportional to FE material polarization. Thus, negative capacitance field-effect transistors, or NCFETs, are promising device architectures for achieving improved performance in terms of on−off ratio, and power consumption. The present study investigates the influence of negative capacitance (NC) on the transfer characteristics of van der Waals (vdW) FET below and above a critical voltage (V_{th}) on the heterophase of the channel WS_2 and $CuInP_2S_6$-$In_{4/3}P_2S_6$ (CIPS-IPS) gate. Generally, $CuInP_2S_6$ (CIPS) is a 2D FE material that exhibits switchable polarization down to 4 nm at room temperature [1]. However, in cases of Cu deficiency in CIPS, the system experiences a chemical phase separation, leading to the formation of a paraelectric (PE) $In_{4/3}P_2S_6$ (IPS) phase alongside the FE CIPS phase. Additionally, Cu deficient CIPS-IPS is recognized for its significant electric-field-controllable macroscopic ionic conductivity. The interplay between this conductivity and ferroelectricity gives rise to ferroionic states. Notably, a less pronounced NC resulting from the spatial distribution of the FE-PE heterophase and an onset of ionic conductivity above V_{th} play a crucial role in stabilizing n-channel conductance of WS_2 by dual gate modulation [2]. This results in the emergence of a non-volatile logic state between the two binary states typical of conventional tunnel field-effect transistors (TFETs). Concerned study proposed NCTFETs based on ferroionic crystals as promising devices for generating a stable logic state below the coercive voltage. In addition, tunnelling and voltage pinning effects play a key role for enhancement of the transistor's on−off ratio.

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Abstract

Goniopolarity is a term which suggests that a material can behave either like an n-type or a p-type material depending on the crystal orientation. In this presentation we show goniopolarity using electrical and thermo-electric transport measurements in a kind material which has recently been dubbed as altermagnet. I will make a short introduction to goniopolarity and altermagnetism and by employing electrical and thermo-electric transport measurements and first principles calculations we will try to understand whether they are interconnected.

Sn0.06Cr3Te4: A Skyrmion Superconductor

Thirupathaiah Setti*
S. N. Bose National Center for Basic Sciences, Kolkata

Topological superconductors are an exciting class of quantum materials from the fundamental sciences and potential technological applications points of view. Here, we present the successful introduction of superconductivity in a ferromagnetic layered skyrmion system Cr3Te4, obtained by the Sn intercalation, below a superconducting transition temperature of 3.5 K. We observe several interesting physical properties, such as superconductivity, magnetism, and the topological Hall effect, simultaneously in this system. Despite the magnetism and Meissner effects being anisotropic, the superconductivity observed from the in-plane electrical resistivity is nearly isotropic, suggesting separate channels of conduction electrons responsible for the superconductivity and magnetism of this system, which is also supported by our spin-resolved DFT calculations. We identify two orders of higher carrier density in superconducting Sn0.06Cr3Te4 than the parent Cr3Te4. A jump in heat capacity around the Tc with a volume fractio.

Interplay of altermagnetism and pressure in hexagonal and orthorhombic MnTe

Nayana Devaraj,[1] Anumita Bose,[1] and Awadhesh Narayan[1]

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Alternative magnetic materials or "altermagnets", characterized by their non-relativistic, momentum-dependent spin-split states, represent a cutting-edge advancement in the field of magnetism, offering promising avenues for spintronic applications. Among these materials, hexagonal MnTe has emerged as a standout material candidate for its substantial spin-splitting. In this study, employing first-principles electronic structure calculations and spin group symmetry analysis, we delve into the interplay of altermagnetism and pressure in two main phases of MnTe. Our relativistic calculations demonstrate the presence of tunable anomalous Hall effect (AHE) in hexagonal MnTe. In addition, our results underscore the pivotal role of pressure as a tuning parameter for the alternative magnetic traits in the system. Furthermore, we identify another phase of MnTe with orthorhombic structure, namely γ-MnTe, hosting altermagnetic characteristics. We study, in detail, its response in AHE and spin-spliting due to magnetization and pressure variations, respectively. Our study highlights the substantial impact of pressure on the properties of alternative magnetic materials, particularly emphasizing the pronounced tuning effect observed in the hexagonal and orthorhombic MnTe.

Exploring the spin resolved fermi surface in an altermagnet- case of CrSb

Krishnendu Patra and Priya Mahadevan

Department of Condensed Matter and Material Physics

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

Altermagnets are collinear antiferromagnets which have a net spin polarization along certain symmetry directions[1] .This unique feature has attracted attention for potential uses in spintronics. In altermagnets, the arrangement of non-magnetic atoms around the magnetic ones plays a key role in determining this unusual spin symmetry. This sets them apart from conventional antiferromagnets. Unlike traditional antiferromagnets, where opposite spin sublattices are connected by simple lattice translation or inversion, altermagnets are linked by crystal rotation or mirror operations in real space. This breaks certain symmetries, like time reversal, lattice translation, and space inversion, and allows for momentum-dependent spin splitting of energy bands in an antiferromagnet, even without spin-orbit coupling. CrSb has recently gained attention as a potential altermagnetic material. It has a hyperboloid Fermi surface, which is important for various transport properties. We have examined the Fermi surface of CrSb in different planes to understand its role in transport behavior. This is further supplemented by microscopic analysis to understand how the spin splitting originates.

1.Libor et al Phys. Rev. X 12 ,031042(2022)

Many body correlation effects in electron-electron quantum bi-wire systems

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

The many-body correlation effects in electron-electron quantum wires affect the electronic properties of emergent quantum systems. We study the inter- and intrawire correlation effects on the ground state properties of electron-electron quantum bi-wire systems for various electron densities and interwire separations by using the quantum Monte Carlo method. Particularly, we have calculated the ground-state energy, the correlation energy, the interaction energy, the pair-correlation function (PCF), the static structure factor (SSF), and the momentum distribution (MD) function. The Tomonaga -Luttinger liquid (TLL) exponent is extracted by fitting the MD data near the wave vector $k \sim k_F$, from which the TLL liquid interaction parameter is calculated. The finite wire widths effects on TLL parameter is studied in this work, it shows that as the wire width decreases the electron correlation increases. Furthermore, the onset of a quasi-Wigner crystal phase is observed in the quantum bi-wire system as a function of low electron densities and finite wire widths. In this work, the finite wire widths effects on TLL parameter and electron correlation energy is found to be very significant.

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Dynamics of Moiré Excitons and Quantifying Interfaces in 2D Heterostructures

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Abstract: In this talk I will first give a broad overview of Moiré excitons in twisted 2D material heterostructures [1]. I will then present our group's recent work on localized excitations in near 0-degree twisted $MoSe_2/WSe_2$ heterostructures, where we observe several sub-meV moiré-interlayer exciton emission peaks in photoluminescence (PL) spectra [2]. Remarkably, the time-resolved PL measurements from two closely spaced peaks (separated by < 4 meV) indicate possible optical cascade nature between these states, as well as excited state absorption. We will speculate on the origin of these peaks, possibly arising from domain reconstruction in the samples. I will then discuss how we go beyond simple optical images to quantify heterostructure interfaces using optical microscopy [3,4].

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Title: Signatures of non-trivial doublon formation using a quantum computer

Abstract: Doublons are onsite repulsively bound pairs of particles formed due to the inter-particle interactions on a periodic lattice. Formation of such doublons from particles initially located on two non-local sites is forbidden if the onsite inter-particle interaction is very strong. However, we propose a route to the formation of such non-trivial doublons on a one dimensional lattice through suitable manipulation of the interactions among the particles. In this talk we will discuss the mechanism of such non-trivial doublon formation and show how their signatures can be captured using a noisy intermediate-scale quantum (NISQ) device.

Chiral spin textures in Epitaxial Acentric Quantum materials

Malleswararao Tangi
Department of Physics, IIT Guwahati

Abstract: Magnetic two-dimensional layers and thin films have garnered significant interest within the spintronics community. In this talk, I will discuss the molecular beam epitaxy (MBE) growth of wafer-scale, high-quality, single-crystalline 2D ferromagnetic metallic thin films. Detailed X-ray diffraction analysis reveals that their crystal structure closely mirrors that of bulk crystals, characterized by the space group P3m1. This particular space group supports Néel-type skyrmions, which we have directly observed in these thin films using Lorentz transmission electron microscopy. The MBE deposition technique offers precise control over composition, structure, and thickness, enabling the fabrication of complex heterostructures designed to manipulate spin textures effectively.

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Valley polarized malleable bands near half filling in twisted bilayer graphene

Saisab Bhowmik,[1,*] Bhaskar Ghawri,[2] Youngju Park,[3] Dongkyu Lee,[3,4] Suvronil Datta,[1] Radhika Soni,[1] K. Watanabe,[5] T. Taniguchi,[6] Arindam Ghosh,[2,7] Jeil Jung,[3,4,†] and U. Chandni[1,‡]

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When two layers of graphene are rotated at the magic angle, the low-energy electronic bands become exceptionally narrow due to strong interlayer hybridization. Flat bands provide an ideal platform for exploring strongly correlated physics that cannot be explained by single-particle calculations. In recent years, magic angle twisted bilayer graphene (MATBG) has demonstrated its potential to host a diverse range of correlated phases, including correlated insulators, superconductivity, orbital ferromagnetism, strange metal behavior, Chern insulators, density waves, and nematicity. Interestingly, these phases are highly tunable through external perturbations such as electromagnetic fields, temperature, pressure, and dielectric environments. In this study, we have performed magnetotransport measurements in MATBG proximitized by a layer of tungsten diselenide (WSe_2), inducing a finite spin-orbit coupling in the system. We find anomalous Hall effect near the half filling ($\nu = 2$) with an abrupt switching of magnetization, which can be controlled by the carrier density in the system. A series of Lifshitz transitions accompany the hysteresis near $\nu = 2$ in the zero magnetic field limit. As the magnetic field is increased, we observe the emergence of a perfectly quantized Chern insulator state at $\nu = 2$. The main findings of our work point towards the existence of valley-polarized ground states in the vicinity of $\nu = 2$, which are stabilized by the presence of spin-orbit coupling.

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Title: Signatures of non-trivial doublon formation using a quantum computer

Abstract: Doublons are onsite repulsively bound pairs of particles formed due to the inter-particle interactions on a periodic lattice. Formation of such doublons from particles initially located on two non-local sites is forbidden if the onsite inter-particle interaction is very strong. However, we propose a route to the formation of such non-trivial doublons on a one dimensional lattice through suitable manipulation of the interactions among the particles. In this talk we will discuss the mechanism of such non-trivial doublon formation and show how their signatures can be captured using a noisy intermediate-scale quantum (NISQ) device.

Structure and dynamics of spin-orbit coupled ultra-dilute quantum droplet

Pankaj Kumar Mishra
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Abstract: In recent years, quantum droplets (QDs) have emerged as one of the novel matter forms of ultracold atoms, and the research is still at an infant stage. In general self-bound QDs are formed due to the interplay between attractive mean-field (MF) interactions and repulsive beyond mean-field (BMF) interactions caused by the quantum fluctuations. In one-dimensional systems, QDs in binary mixtures are predicted to arise from a different mechanism. Here, the formation of QDs takes place as a result of the balance between attractive BMF and repulsive MF interaction. The study of droplets in one dimension is particularly interesting because of the significant and nontrivial role of quantum fluctuations.

In this talk we will present our numerical simulation results of the ground state structure and dynamics of quantum droplets in one-dimensional spin-orbit (SO) coupled binary Bose-Einstein condensates. We will discuss the effect of vanishingly small as well as the finite mean-field interaction on the structure, stability and dynamics of the quantum droplet. Further we will discuss various dynamics that ensued in the quantum droplet either due to small velocity perturbation or due to the quenching of either SO or Rabi coupling parameters.

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Liquid and Solids in Ultracold Atomic Gases

Ayan Khan, Bennett University

In recent years, experimentalists across Europe have reported observations of liquid-like states (droplet) in binary Bose Einstein Condensate (BEC) and dipolar BEC. Theoretically, it has been argued that beyond mean-field interaction plays a pivotal role in droplet formation. In this talk, we have planned to explicate the theoretical models to examine the droplet formation in BEC from quantum and classical perspective [1, 2, 3]. Here, we will also shed light on the role of different competiting interactions. We have plan to extend the discussion further in the direction of solid-like (well defined lattice ordering) phase [4]. The BEC in quasi-one-dimensional geometry along with beyond mean-field contribution leads to a novel type of nonlinear Schrodinger equation (NLSE) which contains an additional quartic nonlinearity. We investigate this rather unusual nonlinear contribution in the light of novel quantum phase formation.

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Interaction-induced spin-dependent localization of spin-1/2 Bose-Einstein condensates in a random disordered potential

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(Dated: September 9, 2024)

Abstract

Since the experimental realization of Anderson localization in Bose-Einstein condensates [1], it has sparked significant interest within the ultracold community owing to the adaptability of diverse trap geometries and atomic interactions. In this work, we explore the influence of spin-orbit and Rabi couplings on the localization properties of BECs in the presence of a random disordered potential. Our findings show that spin-orbit coupling introduces distinct localization regimes and significantly alters the spin characteristics of the condensate. Furthermore, the interactions in same- and cross-spin channel break the spin-rotational symmetry, leading to a scenario where one spin component remains localized while the other becomes delocalized, similar to interaction-induced localization phenomena [2]. The combined impact of spin-orbit and Rabi couplings also plays a crucial role in modulating interaction-induced localization, particularly around a phase transition at $k_L^2 = 2\Omega$. Overall, our results highlight the intricate interplay between interactions and spin-dependent couplings, resulting in complex localization and spin behavior in the ground state of the system.

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Structure and dynamics of imbalanced quantum droplet in spin-orbit coupled Bose-Einstein condensates

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Quantum droplets (QDs) are the self-bound states that emerge as a result of the balance between repulsive mean-field interaction and the attractive beyond mean-field interaction in a one-dimensional weakly interacting binary mixture of Bose-Einstein condensates (BECs) [1]. After the first realization of the droplet in the laboratory experiment [2] the research in this field has seen the unprecedented growth in the numerical and theoretical direction [3]. Most analyses have relied on effective one component formalism that does not account for the effect of interaction between the individual components. Some recent works that explicitly consider the two component interaction and report the structure and dynamics of the QDs in spin-orbit (SO) coupled BECs for vanishingly small [4] and finite mean-field interactions [5]. Previous research has primarily focused on QDs with equal intra-species interactions [5]. However, the effect of the different intra-species interactions among the components on the structure, stability, and dynamics of the QDs has not been explored much. In this work, we present the numerical simulation results of the structure and dynamics of the quantum droplet for the imbalanced interaction in one-dimensional SO coupled binary BECs. Upon increasing the interaction imbalance, we find that there is a change in the structure as well as the population of the individual component of the droplet. Beyond a threshold imbalance between the interaction, we notice a transition from the flat top droplet to the Gaussian-like droplet. We have analyzed it for different sets of particle numbers, interaction strength, SO coupling, and Rabi coupling. The population difference between the components decreases upon increasing the Rabi coupling, and further beyond a threshold Rabi coupling, the population difference reaches a minimum value. We analyze the nature of the breathing modes in imbalanced droplet by performing a small quench on the weak trap. Finally, we discuss various dynamics that ensued in the imbalanced droplet due to the quenching of either SO or Rabi coupling parameters in the presence of the weak trap.

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Energy spectra and fluxes of two-dimensional turbulent quantum droplets

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Abstract:

We explore the energy spectra and associated fluxes of turbulent two-dimensional quantum droplets subjected to a rotating paddling potential which is removed after a few oscillation periods. A systematic analysis on the impact of the characteristics (height and velocity) of the rotating potential and the droplet atom number reveals the emergence of different dynamical response regimes. These are classified by utilizing the second-order sign correlation function and the ratio of incompressible versus compressible kinetic energies. They involve vortex configurations ranging from vortex dipoles to vortex clusters and randomly distributed vortex-antivortex pairs. The incompressible kinetic energy spectrum features Kolmogorov ($k^{-5/3}$) and Vinen like (k^{-1}) scaling in the infrared regime, while a k^{-3} decay in the ultraviolet regime captures the presence of vortices. The compressible spectrum shows $k^{-3/2}$ scaling within the infrared regime and k^{1} power law in the case of enhanced sound-wave emission suggesting thermalization. Significant distortions are observed in the droplet periphery in the presence of a harmonic trap. A direct energy cascade (from large to small length scales) is identified in all cases through the flux. Our findings offer insights into the turbulent response of exotic phases-of-matter featuring quantum fluctuations and may inspire investigations aiming to unravel self-similar nonequilibrium dynamics.

Superconductivity in tungsten

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Abstract

Bulk Tungsten does not exhibit superconductivity unless cooled to a very low temperature of 0.011 K, but two other forms of tungsten, the metastable crystalline beta-tungsten and amorphous tungsten, both of which can only be synthesized in thin film form, exhibit superconductivity with Tc in the range of 3-4 K. b-tungsten (beta-tungsten) has attracted considerable attention, since the A15 crystal structure combined with the large spin-orbit coupling, makes it a potential candidate for unconventional superconductivity. We have now shown that b-tungsten might not be a superconductor by itself. Investigating many tungsten films grown under different conditions using a combination of structural, magnetic, transport and scanning tunnelling spectroscopy measurements, they conclude that while amorphous tungsten is a conventional superconductor, superconductivity in the putative b-tungsten films originates from an amorphous tungsten layer that form beneath the b-tungsten phase and induces weak superconductivity by proximity effect in beta-tungsten layer. This finding is likely to change the discourse on investigation of superconductivity in tungsten films.

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Exploring Rashba parameter and superconductivity in anisotropic $KTaO_3$ based two-dimensional electron gases

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The oxide two-dimensional electron gases (2DEGs) based on $SrTiO_3$ (STO) and/or $KTaO_3$ (KTO) offer a wide range of functionalities, including high electronic mobility, gate-tunable Rashba spin-orbit coupling (SOC), and low-temperature superconductivity [1-3]. While superconductivity in STO-based 2DEGs was observed shortly after their discovery, it was only recently detected in KTO-based 2DEGs, with a critical temperature (Tc) of 2 K—an order of magnitude higher than that of STO 2DEGs—in (111)-oriented KTO 2DEGs [4]. Notably, the Tc varies depending on the crystalline orientation of KTO. This finding opens up a vast platform for exploring the superconducting properties of KTO-based 2DEGs and combining them with their intrinsic strong Rashba SOC, advancing the potential for realizing topological superconducting qubits.

In this presentation, we will demonstrate the gate-tunable transport properties of superconducting KTO - based 2DEGs in (111), (110), and (100) orientations, generated by sputtering a thin layer of aluminum. Rashba parameters determined in microdevices based on these systems reveal anisotropy with non-reciprocal responses. We will correlate the magnetotransport data with their band structures, as observed through angle-resolved photoemission spectroscopy (ARPES) measurements [5, 6]. Additionally, microwave transport experiments show that KTO (111) 2DEGs exhibit a nodal-less superconducting order parameter, with a gap value significantly larger than expected from a simple BCS weak-coupling limit model [7]. Furthermore, we have fabricated vertical tunnel junctions using AlO_X//KTO (111) 2DEGs and conducted tunneling spectroscopy studies. These experiments revealed a clear s-wave-like superconducting gap of approximately 245 meV, which aligns well with a T_c of ~1.8 K. Complex in-gap features were also observed, which evolve with both temperature and magnetic field. Finally, we will discuss how these findings provide new perspectives for fundamental research and potential applications in fields such as spin-orbitronics and topological electronics.

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Magneto-transport in 2D van Der Waals Ferromagnets; the case studies on Fe_3GeTe_2 and $Co_8Zn_8Mn_4$

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Two-dimensional (2D) materials have garnered considerable attention in the field of electronic devices due to their remarkable physical properties and the ability to fabricate complex structures from them. Fe_3GeTe_2 (FGT) is a layered, van der Waals-bonded 2D compound that exhibits high-temperature itinerant ferromagnetism. It has attracted significant interest for its properties, such as uniaxial magneto-crystalline anisotropy, Kondo lattice behavior, a large anomalous Hall current, and tunable room-temperature ferromagnetism through ionic gating. Additionally, several studies have shown that this material has an antiferromagnetic ground state below 152K, attributed to the opposing spin alignments of Fe atoms in adjacent layers [1,2]. As an itinerant ferromagnet with a high Curie temperature and a potential nodal line semimetal, FGT provides an excellent platform to explore the relationship between ferromagnetism and topology. In this work, we investigate the scattering mechanisms in a single crystal of high-T_c Fe_3GeTe_2 through resistivity, magneto-transport, and Hall effect measurements. Our findings offer a clear understanding of the impact of electron-magnon scattering on the temperature-dependent evolution of the anomalous Hall effect, excluding a topological band structure as its origin [2].

Cubic Co-Zn-Mn alloys with the β-Mn structure have also attracted significant attention recently due to their ability to stabilize skyrmions at room temperature [3]. Recent magneto-transport studies on different compositions of Co-Zn-Mn alloys have led to contradicting results, with the dominance of the extrinsic mechanism in $Co_7Zn_8Mn_5$ [4] and intrinsic mechanism in $Co_9Zn_9Mn_2$ [5]. Our work focuses on exploring the magneto-transport properties of $Co_8Zn_8Mn_4$, and aims to understand the influence of different scattering mechanisms in the presence of topological invariance and spin fluctuations [6]. Negative magnetoresistance is observed over a broad temperature range from 55K to 300K. A shift from linear to nonlinear behavior in isothermal magnetoresistance curves, as temperatures rise from well below T_c (55K) to around T_c (271K), suggests a transition from magnon dominance to spin fluctuations effect. The scaling between anomalous Hall effect and longitudinal resistivity demonstrates that skew scattering is the prevailing mechanism, which cannot be fully accounted for by existing semiclassical magneto-transport theories. Our experiments identify spin fluctuations as the source of skew scattering in $Co_8Zn_8Mn_4$. While skew scattering is typically dominant in materials with high conductivity, our findings indicate that skyrmionic alloys can be an exception.

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Data-driven discovery of unconventional heat flow regimes in common semiconductors

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Abstract

Lattice vibrations called phonons conduct heat in crystalline semiconductors. Under many commonly encountered situations, phonon transport in these materials is broadly compliant with the Fourier's law, which states that the heat conduction is a diffusion process in which the generated heat flux is directly proportional to the applied temperature gradient, and the constant of proportionality is a material property called the thermal conductivity. In this talk, I will show that, under certain stringent experimental conditions, the phonon-driven heat flow can strongly deviate from the predictions of the Fourier's law, even in common semiconductors. For example, I will show that, within a narrow window of heating lengthscales, heat can flow like a damped wave, in stark contradiction to the prediction from the parabolic Fourier diffusion equation for heat flow. Identification of such exciting "needle-in-ahaystack" heat flow regimes was made possible by my research group's recent effort in developing data-driven approaches, motivated by physical insights, to accelerate the solution of the governing equation for phonon transport in semiconductors - the Peierls-Boltzmann equation, which is computationally intractable for such situations otherwise.

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Ultrafast Laser-inscribed Photonic Topological Materials

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Topological photonics is an emerging field focused on discovering new fundamental science and utilizing *topological protection* to enhance device performance against defects, disorder, and manufacturing imperfections. Recent experimental advancements have generated significant interest in developing photonic topological materials [RMP **91**, 015006, (2019)], opening up new possibilities for studying the interplay of topology, periodic driving, disorder, and nonlinear interactions.

In this presentation, the fabrication and characterization of photonic topological materials consisting of femtosecond laser-written waveguide networks will be discussed. Considering the photonic Su-Schrieffer-Heeger model [arXiv:2402.18340 (2024)], we will show how its non-trivial topology can be experimentally probed in clean and disordered lattices. The emergence of novel nonlinear states within these structures will also be discussed. Additionally, the implementation of two-dimensional Floquet topological materials and synthetic magnetic flux in photonic square lattices will be briefly addressed.

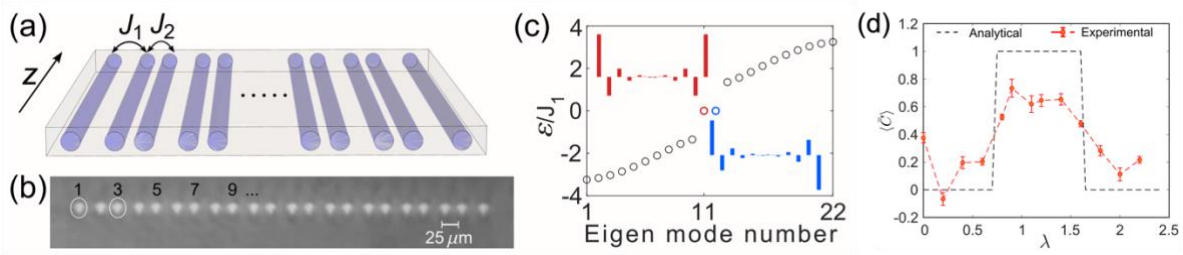

Fig. 1. (a) Sketch of a photonic Su-Schrieffer-Heeger (SSH) lattice terminated with weak couplings $J_1 < J_2$. (b) Micrograph of the cross-section of a fs laser-written SSH lattice. (c) Spectrum of the SSH lattice (open circles). Notice the appearance of the edge modes in the band gap. The inset shows the real-space amplitude profiles of the edge modes. Topological phase transition caused by quasiperiodic disorder in coupling. Mean chiral displacement as a function of quasiperiodic strength λ.

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

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Magneto-optical spectroscopy on 2D materials is traditionally performed by magneto-photoluminescence and magneto-reflectance spectroscopy methods. These techniques provide vital information on various aspects of 2D semiconductors and magnets such as spin-valley-layer-resolved band structure, circularly-polarized excitons and trions, magneto-valley polarization, valley coherence, and single-photon emission. However, one normally needs large magnetic fields such as B>5 T for a reasonable signal-to-noise ratio. For measurements under low magnetic fields (B<1 T), differential magneto-optical spectroscopy such as Faraday and Kerr effect spectroscopy is highly desirable. In this talk, I will discuss our recent developments on establishing some of these techniques (Faraday rotation, Faraday ellipticity, and spectroscopic ellipsometry). We overcome the bottleneck of long measurement times in these methods, and enhance the speed of data acquisition by two-to-three orders of magnitude using our innovations. I will describe our first results of Zeeman spectroscopy of intra- and interlayer excitons, and trions in 2D materials such as MoS2, MoSe2, WS2 and WSe2. For the first time, we are able to extract the complete dielectric tensor of these 2D materials. Many challenges are faced in the development of Kerr spectroscopy on micron scales, which will be discussed. Our work opens new paradigms to explore new spin-valley physics in 2D semiconductors and magnets using sensitive magneto-optical spectroscopy.

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The interplay between magnetism and chemical binding

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Single molecule spintronics aim to identify new spin transport effects near the limit of electronic component's miniaturization. While the focus in this field is on magneto-transport properties, not much is known about the effect of magnetism on the structure of molecular conductors. Here, we reveal a new phenomenon: the direction of applied magnetic field can affect the properties of a metal-molecule chemical bond. Specifically, we show that magnetic field direction affects the formation of metal-single molecule-metal junctions and the stability of the metal-molecule bond. Our findings reveal the interplay between magnetism and chemical binding at the level of a single chemical bond.

Title: Determining entanglement in spatial photonic qutrit pair generated via pump beam modulation technique

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Abstract: We present a novel method for generating photonic qutrits by modulating the pump beam in a spontaneous parametric down conversion (SPDC) process with a three-slit aperture. We derive analytical relationships between statistical correlation measures—mutual predictability (MP), mutual information (MI), Pearson correlation coefficient (PCC)—and entanglement measures—negativity (N) and entanglement of formation (EOF), and experimentally measure MP, MI, and PCC for two-qutrit pure states as a proof of principle to determine N and EOF. This single-measurement approach allows direct determination of multiple entanglement measures, aiding their experimental comparison.

Visualizing isospin magnetic texture in rhombohedral tetralayer graphene

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In recent years, rhombohedral multilayer graphene (RMG) has been considered an alternating platform to study the effect of strong electronic interactions and topology without a moiré superlattice. The annular band of RMG uniquely distributes the Berry curvature and gets modified in the presence of a large out-plane magnetic field. On the other hand, interplay between strong intra and intervalley electronic interaction lifts the native electronic degeneracies (*N*). It creates various symmetry-broken states, providing ground states for intriguing correlated electronic phases. Although several versatile global thermodynamic measurements illustrate the degeneracies of the symmetry-broken states, finding their local isospin textures and underlying determining energy scales are still lacking. Utilizing a nanoscale scanning superconducting quantum interference device in a feeble vector magnetic field, we find the microscopic isospin texture close to zero magnetic fields by detecting the local magnetic stray field in the symmetry broken phases of crystalline ABCA tetralayer rhombohedral graphene. Sharp magnetic transitions have been observed, marking spontaneous time reversal symmetry breaking at the onset of isospin symmetry broken phases. The half metal phase (*N* = 2) is shown to possess isotropic isospin magnetization with the spin orientation dictated by the field direction, providing the first experimental determination of the intervalley Hund's exchange interaction energy U_H. Upon entering the quarter metal phase (*N* = 1), the spin and orbital moments align closely, allowing the determination of the spin-orbit coupling energy λ_{soc} . By contrasting magneto-transport measurements, we trace the enhancement of the quarter metal with a magnetic field and show that high-field electronic states are governed by inimitable topological magnetic band reconstruction. The ability to resolve the local isospin texture and the different interaction energy scales paves the way to a better understanding of the hierarchy of the phase transitions and the numerous correlated electronic states arising from spontaneous and induced isospin symmetry breaking in crystalline graphene.

Absence of Wannier-Stark localization and skin effect in driven non-Hermitian systems

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(Dated: August 31, 2024)

Since long, it is theorized that the electronic eigenstates become completely localized in the presence of an external electric field, manifesting equally spaced energies, known as the Wannier-Stark (WS) localization. The localization behavior also persists in non-Hermitian Hamiltonians, and when the system is governed by a quasiperiodic potential. In this work, we have explored different phases by identifying the delocalization-localization (DL) phase transition in such non-Hermitian quasicrystals in the presence of a time-periodic external electric field. In stark contrast to the static counterparts where the states can either be completely delocalized or localized, we demonstrate that under the time-periodic drive there exists multiple mobility edges separating the metallic and insulating states when the electric field is driven slowly. We find that a time-periodicity introduced in the electric field significantly amplifies the regime of delocalized eigenstates upto an enhanced strength of the quasiperiodic potential, which is analytically verified in the regime of a large driving frequency. We find that the well-known WS energy ladders inherent in the systems with an uniform electric field no longer prevail in the periodically driven framework, and the energy levels exhibit the Poissonian statistics when the eigenstates are localized. Finally, we stress that the extended unitarity leads to the destruction of skin effect, which prevails only beyond some critical value of the non-Hermiticity in the Hamiltonian and is dependent upon the strength of the time-modulated electric field.

Emerging *triferroicity* and *polar metallic* state in two dimensional rare-earth halide based monolayers

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There is a huge surge in research activities, of late, to achieve multiferroicity in two-dimensional materials due to their enormous potential for applications in nanoelectronic and spintronic devices. 2D polar metals with simultaneous presence of polarity and conductivity are also equally rare. I will discuss our recent work [1, 2] on Eu-substituted GdX_2 (X = Cl, I) monolayers. In $GdCl_2$ we predict, based on our first-principle calculations, a triferroic phase with three ferroic orders—ferromagnetism, ferroelectricity, and ferroelasticity— coexisting simultaneously whereas in GdI_2 we observe a polar metallic phase which is ferromagnetic as well as ferroelastic. This is achieved in the GdX_2 monolayers (ferromagnetic semiconductor) by hole doping via substitution of $1/3^{rd}$ of the Gd^{2+} ions with Eu^{2+}. The emerging metallic state in $GdCl_2$ undergoes a bond-centered charge ordering which makes it semiconducting again as well as ferroelastic. Further, the associated lattice distortions break the lattice centrosymmetry leading to a noncentrosymmetric charge distribution, which makes the monolayer ferroelectric, at the same time. The two ferroic orders, ferroelectricity and ferroelasticity, present in the Eu-substituted $GdCl_2$ monolayer are found to be strongly coupled, making it a promising candidate for device applications whereas simultaneous coexistence and coupling of the ferroic orders in a metallic 2D material makes the Eu substituted GdI_2 monolayer an incredibly rare material for nano-electronics and spintronics applications.

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Effect of Defects and Strain on the Optoelectronic Properties of Monolayer TMDs

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The remarkable capacity of two-dimensional (2D) materials to endure substantial strains and their ability to tune optoelectronic properties under strain positions them as highly promising contenders for flexible device applications requiring exceptional performance. The impact of defects within 2D materials on their optoelectronic response to strain is a significant factor to consider. In this context, we present an experimental study that sheds light on the role of intrinsic defects in monolayer MoS2 regarding the properties of strain-induced photoresponse. We observed an enhancement in photocurrent, electron mobility and the emergence of persistent photoconductivity in the presence of strain. Our findings suggest that the activation of defects at distinct strain values plays a pivotal role in augmenting the photoresponse of the material. We will also demonstrate how one can brighten the momentum-forbidden dark exciton by placing monolayer WS2 on top of nanotextured substrates, which imparts tensile strain. The strain modifies its electronic band structure and enables phonon-assisted exciton scattering between momentum valleys, thereby brightening momentum-forbidden dark excitons. Our study unveils the significant role of strain and defects in shaping the optoelectronic properties of 2D materials. These findings not only deepen our understanding of the material but also open up exciting new possibilities for developing multifunctional ultra-thin flexible devices in the next generation of applications.

Using crystallographic motifs to search for new quantum materials

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Search for new quantum materials typically involves meticulous scanning of the material databases and performing density functional theory-based calculations to obtain their electronic band structure. Though effective, this method is relatively computationally expensive. We will show that basic chemical reasoning, especially using crystallographic motifs, can vastly streamline this process. We will discuss a particular material group called the square-net family in the context of topological materials. At the same time, similar chemical reasoning can also be used to find new quantum materials with unique functionalities.

Machine learning-aided study of surface reconstructions of Cu_2O (111) plane

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The recent developments in machine learning have greatly increased its demand in the field of material science because of its ability to address a myriad of challenging problems with exceptional accuracy and minimum human intervention. However, accurate force field generation needs proper training data. Recently developed "on-the-fly learning" technique in VASP, has provided a simplified and efficient approach to address this issue [1, 2]. In this talk, we will address the long-standing problem of the most stable reconstruction of Cuprous Oxide (Cu_2O) (111) surface. Our approach begins with both $(\sqrt{3}\times\sqrt{3})R30^\circ$ and (2×2) supercell under stoichiometric as well as O- and Cu-deficient or rich conditions. Using parallel tempering simulations assisted by Machine Learned Force Fields (MLFFs), we identified two promising nanopyramidal reconstructions along with a Cu-cluster arrangement and several surface topologies consistent with prior density functional theory (DFT) and experimental studies. To identify the most stable reconstruction, we calculated the phase diagram using spin-polarized PBE and HSE06 functionals, revealing an interplay between nanopyramidal and Cu-deficient configurations that provides new insights into the stability characteristics of the Cu_2O (111) surface. Importantly, the study underscores on-the-fly learning to be a fast and efficient way to find the most stable reconstructed surfaces commonly encountered in experiments.

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Quantum Hall Phase Diagram of Bilayer Graphene

Udit Khanna, Ke Huang, Ganpathy Murthy, H. A. Fertig, Jun Zhu and Efrat Shimshoni

Abstract: Bilayer graphene exhibits a rich phase diagram in the quantum Hall (QH) regime, arising from a multitude of internal degrees of freedom, including spin, valley, and orbital indices. The variety of fractional QH states between filling factors 1 and 2 suggests, among other things, a quantum phase transition between valley-polarized and unpolarized states at a perpendicular electric-field D*. We find that the behavior of D* with filling factor changes markedly as the magnetic field B is reduced. We present a theoretical model for lattice-scale interactions, which explains these observations; contrary to earlier studies, it involves finite-ranged terms which may arise from Landau level mixing. Within this model, we analyze the nature of the phase at filling factor 2, and predict that valley-coherence may emerge at high B fields. This suggests that the system may support bond-ordered phases which may be amenable to experimental verification.

Chaos and Eigenstate Multifractality in Disordered Quantum Spin Systems and some Special Random Matrix Models

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

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½-quanta Thermal Conductance of an Isolated Quantum Hall Channel

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The quantum Hall (QH) states, one of the earliest known examples of a topological insulator, are predicted to host exotic quasiparticles that make them one of the most sought-after for application in topological quantum computations. A proposed host of such quasiparticles is the ν=5/2 QH state. However, since the 5/2 state hosts several counter-propagating edge channels (integers, fractional, neutral), in order to exploit the exotic quasiparticles in topological braiding, the exotic edge channel needs to be isolated while retaining its original exotic nature. In this talk, I will present our recent experiment, where we exploited a novel technique to separate-out the integer channels of the ν=5/2 state by interfacing it with the integer states ν=2 and ν=3 [1], and measured the thermal conductance of the *isolated* ν=1/2 channel. The measured thermal conductance $\frac{1}{2}\kappa_0 T$ (with $\kappa_0=\pi^2 k_B^2/3h$, the quantum of thermal conductance), assures the non-abelian nature of the *isolated* ν=1/2 channel and its topological order[2]. Our result opens a new avenue to manipulate and test other QH states and braid via interference of the isolated exotic channels.

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Interface Engineering of Ag@Au Nanohybrid for Ultra-strong Electron-phonon Coupling and Non-classical Electron Transport

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Ultrasmall nanoparticles of noble metals, in particular silver (Ag) or gold (Au), have been extensively investigated for their optical, magnetic, chemical, and physical properties, but assembling such structures in an electrically conducting metallic matrix, where the physical dimension of individual nanoparticles plays a decisive role, has remained elusive. Nanostructuring strategies in noble metals offer unique opportunities to modulate electron-phonon interactions, enabling breakthroughs in material functionality. Here, we report the design and synthesis of an advanced Ag–Au nanohybrid system comprising ultrasmall silver nanoparticles (AgNPs, radius ~1–3 nm) embedded within a crystalline gold (Au) matrix. This architecture overcomes traditional challenges in metallic nanoparticle assemblies, such as tunnel barriers induced by surface ligands, achieving true metallic conduction across nanostructured interfaces whose resistivity can be directly manipulated by the Ag/Au interface of individual nanoparticles. Remarkably, the hybrid exhibits an extraordinary enhancement in electron-phonon coupling ($\lambda \approx 20$), a value unprecedented in metals and over 100 times higher than in pristine Au or Ag. This enhancement leads to deviations from conventional metallic transport, including saturation of electrical resistivity near the Mott-Ioffe-Regel limit and resistance scaling with the net surface area of embedded AgNPs. The interplay of localized phonon modes at the Ag-Au hetero-interfaces with conduction electrons is proposed as the origin of these phenomena. The study highlights a novel architype for engineering nanostructured metals with tailored transport properties, unlocking potential applications in quantum materials, superconductivity, and nanoscale device engineering.

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Investigation of magnetism in 2D material MoS_2

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Two dimensional (2D) materials are being extensively studied for their electronic and optoelectronic properties. Magnetism is a relatively less studied property in 2D materials. 2D magnetism has recently emerged as an interesting topic in materials science. MoS_2 is a well-studied 2D material consisting of covalently bonded three hexagonal atomic layers (S–Mo–S). However, the usual 2H phase of MoS_2 is diamagnetic but becomes magnetic in the 1T-phase. Here we discuss room temperature ferromagnetism observed in the 1T phase MoS_2 samples grown by hydrothermal method. We observe a high coercivity in the sample and discuss the results in the light of enhanced interlayer spacing and the 1T phase content in sample.

$$\Delta S_{kJKg^{-1}K^{-1}}) \text{ and adiabat}$$

Unraveling the Magnetoelectric Coupling in CaMn7O12

Jhuma Sannigrahi*, Jhuma Sannigrahi, Md Salman Khan, Mohamad Numan, Manjil Das, Anupam Banerjee, Manh Duc Le, Giannantonio Cibin, Devashibhai Adroja, Subham Majumdar

Indian Institute of Technology Goa

We investigate magnetoelectric coupling in CaMn7O12 (CMO) through an in-depth spectroscopic study, utilizing inelastic neutron scattering (INS), x-ray absorption spectroscopy (XAS), and synchrotron-based powder x-ray diffraction (PXRD). By exploring the intricate interaction between magnetism and ferroelectricity in CMO, we aim to uncover the underlying mechanisms driving its magnetoelectric behavior. XAS reveals the mixed valency of Mn ions, confirming the presence of both MnÂ³â º and Mnâ ´â º, which plays a crucial role in the compounds magnetoelectric properties. The Mn-K near-edge absorption spectra show a double-peak structure, further emphasizing the multiple Mn sites and their mixed valency. Temperature-dependent synchrotron PXRD highlights structural distortions near CMOs magnetic transition temperatures, coinciding with anomalies in lattice parameters and bond lengths, suggesting a strong link between these structural modulations and the observed magnetoelectric effect. Additionally, INS identifies specific energy bands (Eâ, , Eâ,,, and Eâ,*f*) corresponding to distinct exchange interactions between Mn ions. This study enhances our understanding of magnetoelectric coupling mechanisms, demonstrating the potential of CMO as a multifunctional material for spintronics and other advanced applications.

Metal halide perovskite nanocrystals for various applications

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ABSTRACT

Metal halide perovskite nanomaterials have drawn the attention of commercial and fundamental researchers due to their excellent optical properties and potential applications in the fields of solar cells, LEDs, photodetectors, etc. $CsPbX_3$ (X= I, Br, Cl) perovskite nanocrystals (NCs) have shown remarkable progress in their favorable color tunability, superior emission intensity, narrow emission spectra, and better color purity. However, due to their low formation energy, perovskite nanomaterials are sensitive to high humidity, intense heat, ion migration, the halide exchange process during the mixing of different halide composite NCs, and so on. In addition, it's very challenging to synthesize stable red-emitting perovskite NCs, which are significant components for generating WLEDs. Various strategies have been implemented to improve stability and dispersity. Proper encapsulation of perovskite NCs with various long-chain bulky polymers or high bandgap inorganic shells can successfully transfer them to hydrophilic media, proving to be a potential candidate for different toxic ion detection and bio-imaging applications. Color-tunable LEDs are also proven to have very high luminescence intensity and competitive device efficiency.

Keywords: Perovskite nanocrystals; photoluminescence; stability; LEDs; ion-detection, bio-imaging.

Investigation of Structural, Magnetic, and Dielectric Behavior in Nd-Doped $Gd_3Fe_5O_{12}$ multiferroic samples

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Abstract

In this work, the substitution of Nd in Gadolinium iron garnet ($Gd_3Fe_5O_{12}$, GdIG) i.e., $(Gd_{1-x}Nd_x)_3Fe_5O_{12}$ $(x = 0.0 - 0.2)$ has been investigated for which the material was prepared by solid-state reaction approach. The purity of the garnet phase of the synthesized specimen was examined by XRD patterns and their Rietveld refinement. The lattice constant of the parent sample was obtained as 12.4961 Å that has been enhanced to 12.5189 Å for $x = 0.2$ sample. The larger ionic radii of Nd^{3+} (1.12 Å) ions as compared to Gd^{3+}(1.07 Å) ions is responsible for this increment in lattice constant. Further, the temperature-dependent magnetic data show two transitions: a magnetic compensation transition (T_{comp}) which is only noticed up to $x = 0.2$ samples. Moreover, a spin-reorientation transition (T_{SR}) is also present that can be ascribed to the exchange interactions between rare earth ions and Fe^{3+} moments. Furthermore, the dielectric constant value increases with the temperature rise which can be attributed to the thermal activation of charge carriers that triggers the polarization of the material. Interestingly, the dielectric constant and loss plots show some anomaly around both the magnetic transitions that indicate a multiferroic nature of these Nd-GdIG samples. This multiferroicity makes these compounds highly valuable for applications in telecommunications, capacitors, energy storage devices, magneto-electric sensors, tunable microwave devices, advanced logic devices, electromechanical actuators, spintronic devices, and many other technologies.

Keywords: Rare earth iron garnet, magnetic compensation, spin reorientation, multiferroic

Investigating temperature-induced structural phase transition in Double Perovskite oxides

Akriti Singh, Shalini Badola, and Surajit Saha

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Abstract

Double perovskite oxides (DPOs), with chemical formula $A_2BB'O_6$, have emerged as a versatile class of compounds that is of rich interest due to their vast chemical and structural flexibility applications in photovoltaics, memory devices, sensors, electronic and spintronic devices, etc. [1, 2]. The B-site ordering as well as BO_6 octahedral tilts can lead to rock-salt or layered structures in the double perovskites with a reduction in the crystal symmetry (to tetragonal, rhombohedral or monoclinic), or even allow the formation of 2D and 1D perovskite derivatives [3]. Here, we have explored the structural phase transition in a member of the tungstate family, Ba_2CaWO_6 (prepared by the conventional solid-state reaction), which is a favorable host for luminescence [4], through temperature-dependent Raman scattering measurements. Our findings indicate that as the temperature increases above 220 K, the system undergoes a transition from a tetragonal to a cubic structure driven by a soft mode. This structural phase transition is further corroborated by temperature-dependent X-ray diffraction patterns, which reveal a decrease in tetragonality.

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Abstract

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Canonical spin-glass dynamics in distorted Kagomé and Triangular lattices

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The Kagomè (K) and Triangular (T) lattice compounds are considered as model systems in probing the molecular spin-orbit excitations in the spin-1/2 geometrically frustrated compounds. spinel having corner sharing tetrahedral. The network of corner-sharing tetrahedral ($X_{4\text{-}O}$) in spinel (XY_2O_4) oxides causes inherent geometrical frustration in realizing a complex pyrochlore-like lattice having alternate layers of K and T (…+K-T+K-…) [1,2]. In the current work we report the magnetic properties of one such spinel pyrochlore-spinel $GeCo_2O_4$ diluted with Mn which consists of alternating layered network of (…+K-T+K-…) [3]. In general, the pristine system undergoes a structural distortion at 16 K and shows antiferromagnetic ordering below the Nèel temperature, T_N = 20 K. Below, T_N, this system exhibits three field-induced transitions at critical fields: $H_d \sim 11$ kOe (domain orientation), $H_{C1} \sim 44$ kOe (spin flip-1), and $H_{C2} \sim 97$ kOe (spin flip-1), all of which vanishes while approaching T_N. However, with the substation of 20 atomic percent of Mn at Ge sites in GeCo2O4 leads to reentrant canonical semi spin-glass characteristics as noticed through the dispersion in temperature dependence of dynamical susceptibility, $\chi_{ac}(\omega,T)$ (Fig. 1a,b) without altering the Kagomé symmetry. Complicated magnetic characteristics like longitudinal ferrimagnetic (FiM) order below the Néel temperature $T_{FN} \sim 77$ K due to uneven moments of divalent Co (↑ 5.33 μ_B) and tetravalent Mn (↓ 3.87 μ_B) which coexists with transverse spin-glass state below 72.85 K. Such intricate magnetic behaviour is expected to result from the competing anisotropic superexchange interactions ($J_{AB}/k_B \sim 4.3$ K, $J_{AA}/k_B \sim -6.2$ K and $J_{BB}/k_B \sim -3.3$ K) between the cations, which were evaluated from the Néel's expression for the two-sublattice model of FiM [2]. Empirical scaling-laws such as Vogel-Fulcher law and Power law of critical slowing down have been employed (Fig. 1*c,d*) to study the dispersive nature of frequency dependence of χ_{ac} that reveal the reentrant spin-glass like character which evolves through a number of intermediate metastable states. The magnitude of Mydosh parameter ($\Omega \sim 0.002$), critical exponent $z\upsilon = (6.7 \pm 0.07)$, spin relaxation time $\tau_0 = (2.33 \pm 0.1) \times 10^{-18}$ s, activation energy $E_a/k_B = (69.8 \pm 0.95)$ K and interparticle interaction strength ($T_0 = 71.6$ K) provide the further experimental evidences for canonical re-entrant spin-glass state below the spin freezing temperature $T_F = 72.85$ K.

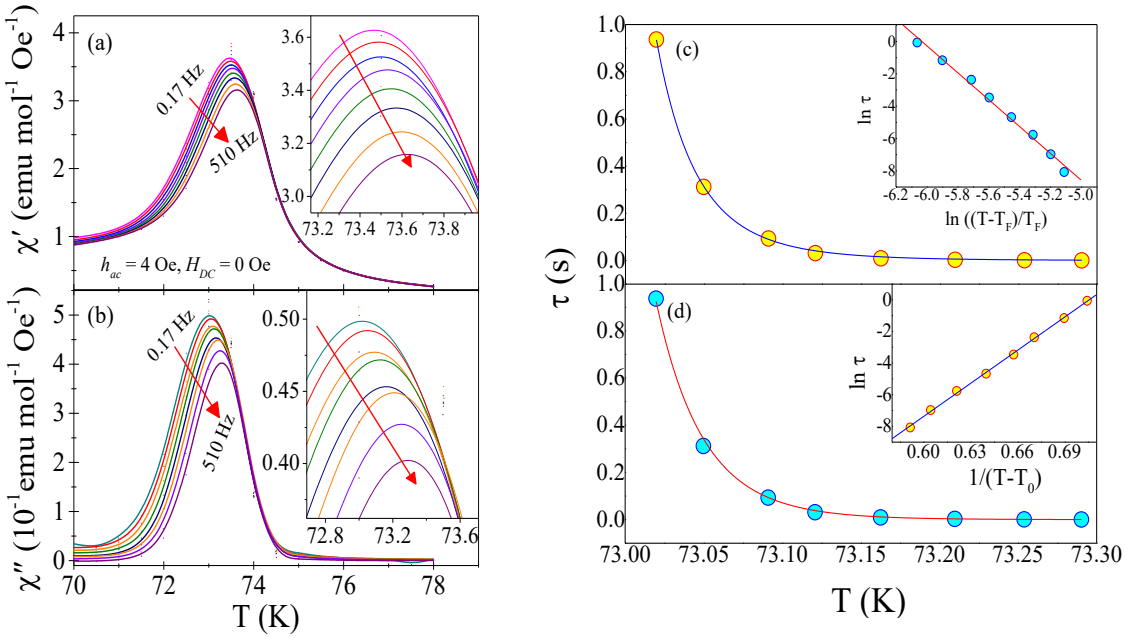

Fig. 1: Temperature dependent ac-magnetic susceptibility, $\chi_{ac}(\omega,T)$ consists of (a) real component, χ' and (b) imaginary components, χ'' recorded for various frequencies from ω = 0.17 Hz to 510 Hz with ac driving field h_{ac} = 4 Oe and H_{DC} = 0 Oe. The inset of (a) and (b) represents the zoomed view of the cusp showing frequency dispersion. Temperature variation of the relaxation time $\tau(T)$ is shown in figures (c) and (d) which are according to the empirical scaling laws Power law and Vogel-Fulcher laws, respectively. The solid lines are the best fits to the experimental data points pertaining to both the scaling laws. While the figures (c,d) shown in the inset represent the logarithmic variation of relaxation time according to both the scaling laws: (c) ln τ vs. ln $(T\text{-}T_F)/T_F$ and (d) ln τ vs. $1/(T\text{-}T_0)$ described in the equations (1) and (2).

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About IIT Guwahati

Indian Institute of Technology Guwahati, the sixth member of the IIT fraternity, was established in 1994. The academic programme of IIT Guwahati commenced in 1995. At present the Institute has eleven departments, seven inter-disciplinary academic centres and five schools covering all the major engineering , science, healthcare, management and humanities disciplines, offering B.Tech., B.Des., M.A., M.Des., M.Tech., M.Sc., MBA and Ph.D. programmes. Within a short period of time, IIT Guwahati has been able to build up world class infrastructure for carrying out advanced research and has been equipped with state-of-the-art scientific and engineering instruments. Besides its laurels in teaching and research, IIT Guwahati has been able to fulfil the aspirations of people of the North East region to a great extent since its inception in 1994.

Indian Institute of Technology Guwahati's campus is on a sprawling 285 hectares plot of land on the north bank of the river Brahmaputra around 20 kms from the heart of the city. With the majestic Brahmaputra on one side, and with hills and vast open spaces on others, the campus provides an ideal setting for learning.

IIT Guwahati is the only academic institution in India that occupied a place among the top 100 world universities – under 50 years of age – ranked by the London-based Times Higher Education (THE) in the year 2014 and continues to maintain its superior position even today in various International Rankings. IIT Guwahati gained rank 32 globally in the 'Research Citations per Faculty' category and overall 364 rank in the QS World University Rankings 2024 released recently. IIT Guwahati has retained the 7th position among the best engineering institutions of the country in the 'India Rankings 2023' declared by the National Institutional Ranking Framework (NIRF) of the Union Ministry of Education. IIT Guwahati has been also ranked 2nd in the 'Swachhata Ranking' conducted by the Govt. of India. Also, IIT Guwahati ranks 6th globally in Sustainable Development Goal 7 (Affordable and clean energy) of the Times Higher Education Impact Rankings 2023.

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