
BOSE FEST
2022
27-29 April 2022
Abstract
e-book

BOSE FEST 2022

Department of Astrophysics and Cosmology

Department of Chemical Biological and Macromolecular Sciences

Department of Condensed Matter Physics and Material Sciences

Department of Theoretical Sciences

SCHEDULE

DAY 1: 27.04.2022

Venue: Silver Jubilee Hall	
Time	**Programme**
9:00 A.M to 10:00 A.M	Registration
10:15 A.M to 10:30 A.M	Inauguration, welcome address by the Director and the Dean (AP)

Oral Presentation Session		
Time	**Speaker**	**Title of the talk**
10:30 A.M to 10:45 A.M	Aayatti Mallick Gupta	Effect on the conformations of spike protein of SARS-CoV-2 due to mutation
10:45 A.M to 11:00 A.M	Aishwaryo Ghosh	Understanding the Trend in Core−Shell Preferences for Bimetallic Nanoclusters: A Machine Learning Approach
11:00 A.M to 11:15 A.M	Amrita Mondal	Composition and Temperature Dependent Dielectric Relaxation Study in PVA/water Hydrogel: Impact of Chain Length and Possible Origin of Relaxation Timescales
11:15 A.M to 11:30 A.M	Animesh Hazra	Hydrodynamics of the Manna sandpile
11:30 A.M to 12:00 noon (Tea Break)		
12:00 noon to 12:15 P.M	Anirban Roy Chowdhury	Entanglement wedge cross-section for noncommutative Yang-Mills theory
12:15 P.M to 12:30 P.M	Ankur Srivastav	Vortices in a Rotating Holographic Superfluid
12:30 P.M to 12:45 P.M	Ardhendu Pal	Study of *l*-type doubling in N_2O isotopologue using cavity ring-down spectroscopy
12.45 P.M to 1:00 P.M	Biswajit Panda	Direct and 2f-wavelength modulation spectroscopy of NO and OCS using an astigmatic multipass cell coupled with a mid-IR 5.2 µm cw-QCL
1:00 P.M to 2:30 P.M (Lunch Break)		
2:30 P.M to 2:45 P.M	Buddhadeb Pal	Quasi-one-dimensional superconductivity in single crystal of $(TaSe_4)3I$
2:45 P.M to 3:00 P.M	Debashis Saha	The inconsistency in quantum theory

3:00 P.M to 3:15 P.M	Debayan Mondal	Jump to Molecular Contact in A Single Molecular Junction and Post Rupture Evolution
3:15 P.M to 3:30 P.M	Edwine Tendong	Viscoelastic response of fluid trapped between two dissimilar van der Waals surfaces
3:30 P.M to 4:00 P.M (Tea Break)		
4:00 P.M to 4:15 P.M	Ipsita Basu	Rational Design Principle Towards Allosteric Inhibitor for PCSK9-LDLR Interaction
4:15 P.M to 4:30 P.M	Jyotirmoy Sau	Anomalous transport driven by topological Nodal line in ferromagnetic compound Fe_3GeTe_2
4:30 P.M to 4:45 P.M	Kanchan Meena	A Mechanism to Attract Electrons
4:45 P.M to 5:00 P.M	Monalisa Chatterjee	Ferromagnetically coupled Shastry-Sutherland lattice: Ground state properties and quantum phase diagram
5:00 P.M to 5:15 P.M	Narayan Chandra Maity	Spatio-temporal heterogeneity in octanol rich region: time resolved fluorescence measurements
5:15 P.M to 5:30 P.M	Parushottam Majhi	Observation of supercooled metallic phases below metal-insulator transition temperature (T_{MI}) in $NdNiO_3$ film and understanding the phenomena with a Monte-Carlo simulative approach
5:30 P.M to 5:45 P:M	Piyali Saha	Investigation of the Radiation Driven Implosion in L1616
5:45 P.M to 6:00 P.M	Prasanta Kundu	A Revisit to Turnover Kinetics of Individual *Escherichia coli* β-Galactosidase Molecules
6:00 P.M onwards: Photo-Fest (Radhachura Dining Hall)		

DAY 2: 28.04.2022

Venue: Silver Jubilee Hall		
Oral Presentation Session		
Time	**Speaker**	**Title of the talk**
10:30 A.M to 10:45 A.M	Prasun Boyal	Robust antiferromagnetism in $NaOsO_3$ under pressure
10:45 A.M to 11:00 A.M	Premashis Kumar	Control of energy, dissipation, and error in kinetic proofreading through chemostatted concentration
11:00 A.M to 11:15 A.M	Rafiqul Alam	Investigation of non-trivial electronic band in layered Lanthanum based Silver Antimonide ($LaAgSb_2$)
11:15 A.M to 11:30 A.M	Rajib Kumbhakar	Optical Photometric Variability in Young Brown Dwarfs and Very Low Mass Stars in the Taurus Star-Forming Region
11:30 A.M to 12:00 noon (Tea Break)		
12:00 noon to 12:15 P.M	Ria Saha	Multivalent cation induced phase separation in proteins: ion specific THz hydration studies
12:15 P.M to 12:30 P.M	Ruchi Pandey	Study of 2021 outburst of the recurrent nova RS Ophiuchi: Photoionization and morpho-kinematic modeling
12:30 P.M to 12:45 P.M	Saheli Samanta	Observation of giant exchange bias effect in Ni-Mn-Ti all-*d*-metalHeusler alloy
12.45 P.M to 1:00 P.M	Snehamoyee Hazra	High performance piezoelectric nanogenerator based on BTO-PVDF nanocomposites
1:00 P.M to 2:30 P.M (Lunch Break)		
2:30 P.M to 2:45 P.M	Shiladitya Karmakar	High-performance thermoelectric properties of strained two-dimensional tellurium
2:45 P.M to 3:00 P.M	Shobhan Dev Mandal	Effect of receptor clustering on E.coli chemotaxis: Sensingversus adaptation
3:00 P.M to 3:15 P.M	Shubham Purwar	Coexistence of superconductivity and ferromagnetism in magnetically anisotropicSn intercalated Cr_3Te_4
3:15 P.M to 3:30 P.M	Siddhartha Biswas	Studies of the pre-main sequence stars in the H II region Sh2-87
3:30 P.M to 4:00 P.M (Tea Break)		

4:00 P.M to 4:15 P.M	Soumya Chakrabarti	Scalar-Fermion Interaction as the Driver of Cosmic Acceleration
4:15 P.M to 4:30 P.M	Sreya Pal	Direct measurement of interfacial Dzyaloshinskii–Moriya interactionand atomic layer thickness dependence in a ferromagnet-WS_2 heterostructure
4:30 P.M to 4:45 P.M	Suchetana Mukhopadhyay	Femtosecond laser-induced ultrafast spin dynamics in ferromagnetic thin films: comparative study using two theoretical models
4:45 P.M to 5:00 P.M	Sudipta Chatterjee	Slow relaxation and decoupling of electrons from the phonon bathas a precursor of Mott metal-insulator transition
5:00 P.M to 5:15 P.M	Sumana Pyne	Addition of cholesterol alters the hydration at the surface of model lipids: a spectroscopic investigation
5:15 P.M to 5:30 P.M	Sumit Nandi	Monogamy of entanglement
5:30 P.M to 5:45 P:M	Susanta Ghosh	Anomalous Hall Effect Studies of Stoichiometric Mn_3Ge
5:45 P.M to 6:00 P.M	Tanmoy Chakraborty	Bulk-diffusion and anomalous transport of self-propelled particles
6:00 P.M onwards: Photo-Fest (Radhachura Dining Hall)		

DAY 3: 29.04.2022

10:30 AM to 12:30 PM: Poster presentation

Venue: Basundhara

Serial No.	Poster Presenter	Poster title
P1	Abhik Ghosh Moulick	Conformational fluctuations and binding in molten globule state of α-lactalbumin
P2	Ariful Hoque	Variations in CO−to−H_2 Column Density Ratio in Star-forming Filaments
P3	Arun Kumar Das	Resource theoretic efficacy of the single copy of a two-qubit entangled state in a sequential network
P4	Dhrubajyoti Majhi	Solubility enhancement of paracetamol in choline chloride-based deep eutectic solvents: Atomic insights using molecular dynamics simulation
P5	Dibyendu Maity	Effect of additives on the growth of methane hydrate
P6	Didhiti Bhattacharya	Two-dimensional $Mo_xW_{1-x}S_2$ alloys for nanogenerators producing record piezo-output and coupled photodetectors for self-powered UV Sensor
P7	Diya Ram	Magnetic Activity of M-dwarfs: Optical and NIR Spectroscopic Studies
P8	Gesesew H Reta	Photo-ionization and Morpho-kinematic Study of V477 Sct
P9	Ishita Jana	Improvement of magnetic and electric properties of Co doped $GaFeO_3$ ceramics
P10	Jayanta Mondal	Temperature dependent dielectric relaxation measurement of an amino acid derivative based deep eutectic solvent: origin of timescales via experiment and molecular dynamics simulation
P11	Koushik Pradhan	Exploration of the Origin of Magnetism in Potassium Manganese Tellurides
P12	Krishnendu Patra	Perturbing the bond disproportionated state in $NdNiO_3$
P13	Manjari Dutta	Investigation of a harmonic oscillator in a magnetic field with damping and time dependent noncommutativity

P14	Monodip	Spin Peierls transition of $J_1 - J_2$ and extended models with ferromagnetic J_1.Sublattice dimerization and thermodynamics of zigzag chains in β-$TeVO_4$
P15	Nishant Garg	Relation between filaments and clumps in a few Galactic star-forming regions
P16	Pratap Kumar Pal	Variation of Magnon–Magnon Coupling Strength with Microwave Power and Bias-Field Angle in $Ni_{80}Fe_{20}$ Nanocross Array
P17	Rahul Karmakar	Tracer motion through an entangled polymeric network within a confined asymmetric geometry in presence of a driving force
P18	Riju Pal	Anomalous Hall Effect in a Two-dimensional van der Waals Ferromagnet Fe_4GeTe_2
P19	Ritwick Sarkar	Boundary resetting driven transport in harmonic chain
P20	Saikat Mitra	Theoretical and Experimental study of Universal Ammonia Gas Sensing by Family of Lead Halide Perovskites ABX_3 (A= CH_3NH_3, $CH(NH_2)_2$, B=Pb, X=Br, I)
P21	Samir Rom	Designing oxide heterostructure with improved physical properties: A case study of the SIO/LCO ($SrIrO_3$/$LaCoO_3$) heterostructure
P22	Shivam Mishra	Nanoplatelets of CdSe - Why do they form?
P23	Shubhrasish Mukherjee	High Responsivity UV-Visible Broadband Phototransistor Based on Graphene – WS_2 Heterostructure
P24	Sk Saniur Rahaman	Machine Learning approach to study quantum phases of a frustrated one dimensional spin-1/2 system
P25	Soham Saha	p-$ZnCo_2O_4$/n-ZnO Nano-heterojunction Photoanode for Photoelectrochemical Water Splitting
P26	Soham Sen	Equivalence principle and HBAR entropy of an atom falling into a quantum corrected black hole
P27	Soma Dutta	Role of Spin Transport on Ultrafast Demagnetization in β-Ta/$Co_{20}Fe_{60}B_{20}$ Bilayers
P28	Soumen Mondal	Observation of Imbert–Fedorov shift in monolayer MoS_2 via quantum weak measurement

P29	Soumyadipta Chakraborty	High-resolution ro-vibrational spectral analysis of dideutero-methane isotopomer ($^{12}CH_2D_2$) in the $\nu_9(B_2)$ fundamental band
P30	Subhajit Kar	Spectroscopic study of [KSF2015] 1381-19L: A high temperature WC9-type star
P31	Subhankar Bera	Nonclassical temporal correlation powers quantum random access codes

Time	Program	Venue
4:00 P.M to 8:00 P.M	Cultural Event	EZCC
8:00 P.M onwards	Family Dinner	EZCC

ORAL PRESENTATIONS

Effect on the conformations of spike protein of SARS-CoV-2 due to mutation

Aayatti Mallick Gupta[1*] and Jaydeb Chakrabarti[1]

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The spike protein of SARS CoV-2 mediates receptor binding and cell entry and is the key immunogenic target for virus neutralization and the present attention of many vaccine layouts. It exhibits significant conformational flexibility. We study the structural fluctuation from closed to open conformations of spike protein among the most common mutations appeared in variant of concerns (VoC). We report the thermodynamics of conformational changes in mutant spike protein with respect to the wildtype from the distributions of the dihedral angles obtained from the equilibrium configurations generated via all-atom molecular dynamics simulations. We find that the mutation causes the increase in distance between N-terminal domain and receptor binding domain leading to an obtuse angle cosine θ distribution in the trimeric structure in spike protein. Thus, increase in open-state is conferred to the more infectious variants of SARS-CoV-2. The thermodynamically destabilized and disordered residues of receptor binding motif among the mutant variants of spike protein are proposed to serve as better binding sites for host factor. We identify a short stretch of region connecting the N-terminal domain and receptor binding domain forming linker loop to play vital role in the overall dynamics of spike protein due to mutation. This linker loop may generate target related objectives of mutant strains of SARS-CoV-2.

Keywords: SARS-CoV-2, spike protein, mutant strains, structural dynamics, dihedrals, thermodynamics

Understanding the Trend in Core−Shell Preferences for Bimetallic Nanoclusters: A Machine Learning Approach

Aishwaryo Ghosh, Soumendu Datta, and Tanusri Saha-Dasgupta

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Bimetallic nanoclusters find ample applications in diverse fields, starting from catalysis to biomedicine. For the efficient designing of these binary nanoalloys, it is pertinent to know the driving factors behind their core-shell preference. We calculate the segregation energies of binary-alloyed metallic nanoparticles encompassing a vast range of alkali, alkaline, basic, 3d, 4d, and 5d transition metals, and p-block metals to determine their core-shell preference. A machine learning workflow developed with this database is then employed to identify the key factors guiding the core-to-shell segregation. We also comment on the cases where instead of core−shell structure, mixed and Janus structures are stabilized.

References

Understanding the Trend in Core−Shell Preferences for Bimetallic Nanoclusters: A Machine Learning Approach; Aishwaryo Ghosh, Soumendu Datta, and Tanusri Saha-Dasgupta; The Journal of Physical Chemistry C (2022); 10.1021/acs.jpcc.2c01096.

Composition and Temperature Dependent Dielectric Relaxation Study in PVA/water Hydrogel: Impact of Chain Length and Possible Origin of Relaxation Timescales

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Hydrogels are three-dimensional structure of water-swollen network produced by physically or chemically cross-linked hydrophilic homopolymers or, co-polymers.[1] PVA based hydrogels are used in advanced medical & pharmaceutical fields,[2] cell & drug delivery[3] and tissue engineering science,[4] in particular due to its remarkable properties such as non-toxicity, high degree of swelling in water (or, biological fluid), elastic nature and the ability to mimic natural tisssue into the body. A molecular weight dependent (M_W~ 10 &~85 kDa) structural and dynamical changes is investigated in PVA hydrogel *via* dielectric relaxation spectroscopy in the frequency window 0.2 ≤ ν/GHz ≤ 50 and temperature range 298 ≤ T/K ≤ 328. DR measurement reports two different time constants, τ_1 ~30-50 ps and τ_2 ~8 ps in PVA gel of M_W~10000 Da whereas another sub-nanosecond time component is observed for polymer of M_W ~85000 Da. Substantial amount of slow water is recognized along with bulk-water molecules and the amplitude of slow time component regarding bound water is strongly dependent upon molecular weight (i.e, chain length) of the polymer. The impact of temperature on static dielectric constant and the time components is very less for both the PVA-water solutions. Dynamic light scattering (DLS) experiment reveals different structure formation in two different aqueous PVA solution. Large size particle (~1000 nm) is developed as the concentration of polymer increased upto 20 wt% in solution, on the other hand small aggregation is found in high molecular weight hydrogel which is consistent upon varying temperature. Structural changes in PVA gel is further supported by DSC experiments.

References

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4. A. Kumar, S. S. Han, *Int. J. Polym. Mater. Polym. Biomater.* **2017**, 66(4), 159-182.

Hydrodynamics of the Manna sandpile

Animesh Hazra, Punyabrata Pradhan

We derive hydrodynamics of the conserved-mass continuous-time Manna Sandpile having muti-toppling. An active site topples with unit rate, where all particles at the site are transferred randomly, and independently, to one of its nearest neighbors. Upon tuning the global density below a critical density, the model goes to an absorbing phase devoid of any dynamical activity. For this model, we calculate two transport coefficients - the bulk- diffusion coefficient and the conductivity, which govern density relaxation in the system. We find that the two transport coefficients are connected to particle number fluctuation through an Einstein's relation. We also demonstrate that, away from criticality and on large spatio-temporal scales, the system exhibits diffusive relaxation of an initial density perturbation.

Entanglement wedge cross-section for noncommutative Yang-Mills theory

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The signature of noncommutativity on various measures of entanglement has been observed by considering the holographic dual of noncommutative super Yang-Mills theory. We have followed a systematic analytical approach in order to compute the holographic entanglement entropy corresponding to a strip-like subsystem of length l. The relationship between the subsystem size (in dimensionless form) (l/a) and the turning point (in dimensionless form) introduces a critical length scale (lc/a) which leads to three domains in the theory, namely, the deep UV domain (l< lc; aut>> 1, aut ~ aub), deep noncommutative domain (l> lc , aub>aut>>1) and deep IR domain (l> lc, aut <<1). This in turn means that the length scale lc distinctly points out the UV/IR mixing property of the non-local theory under consideration. We have carried out the holographic study of entanglement entropy for each of these domains by employing both analytical and numerical techniques. We have also looked at the behavior of this quantity over all the domains of the theory. We then move on to compute the minimal cross-section area of the entanglement wedge by considering two disjoint subsystems A and B. On the basis of EP = EW duality, this leads to the holographic computation of the entanglement of purification. The correlation between two subsystems, namely, the holographic mutual information I(A:B) has also been computed. Moreover, the computations of EW and I(A:B) has been done for each of the domains in the theory. We have then briefly discussed the effect of the UV cut-off on the IR behaviors of these quantities.

References

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Vortices in a Rotating Holographic Superfluid

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In this talk, I shall be talking about novel vortex solutions in a rotating superfluid using gauge/gravity duality. The models of superfluid built using this duality are known as holographic superfluids. We have found that these holographic vortices follow a Feynman like linear relation between winding number and the rotation velocity of the superfluid. We have also observed the dissipative role of imaginary chemical potential in this system.

References

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2. Chuan-Yin Xia et.al., Phys. Rev. D 100, 061901(R) (2019)

Study of *l*-type doubling in N_2O isotopologue using cavity ring-down spectroscopy

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[†]Presenting author

N_2O is a linear non-symmetrical molecule (N-N-O) composed of few site-specific isotopologues. We have investigated the *l*-type doublets [1] of the β-site isotopomer of N_2O, i.e. $^{15}N^{14}N^{16}O$ (or $^{15}N^{\beta}$) [2] in the $(11^10)\leftarrow(01^10)$ transition for *l*=1 (i.e. Π state) vibrational state in the mid-IR region. High-resolution spectroscopic measurements of *l*-type doublet splittings of β-N_2O were carried out using cavity ring-down spectroscopy (CRDS) technique employing a continuous-wave (cw) external-cavity quantum cascade laser (EC-QCL) operating at ~7.8 μm. The rotationally resolved spectra of *l*-type doublet splittings between the parity doublet e and f sub-states of β-N_2O were recorded by probing the rotational lines corresponding to the $(11^10)\leftarrow(01^10)$ transition in P- and R- branches. Further, from this recorded spectra we have obtained several spectroscopic parameters such as *l*-type doubling constants, band centres, rotational constants and centrifugal distortion constants. We also investigated the effects of temperature and pressure on the *l*-type doublets along with the dependency of pressure broadening coefficients on the rotational quantum number J. These experimental data will improve our understanding of the molecular properties of the site-specific ^{15}N-isotopomers of N_2O.

References

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Direct and 2f-wavelength modulation spectroscopy of NO and OCS using an astigmatic multipass cell coupled with a mid-IR 5.2 μm cw-QCL

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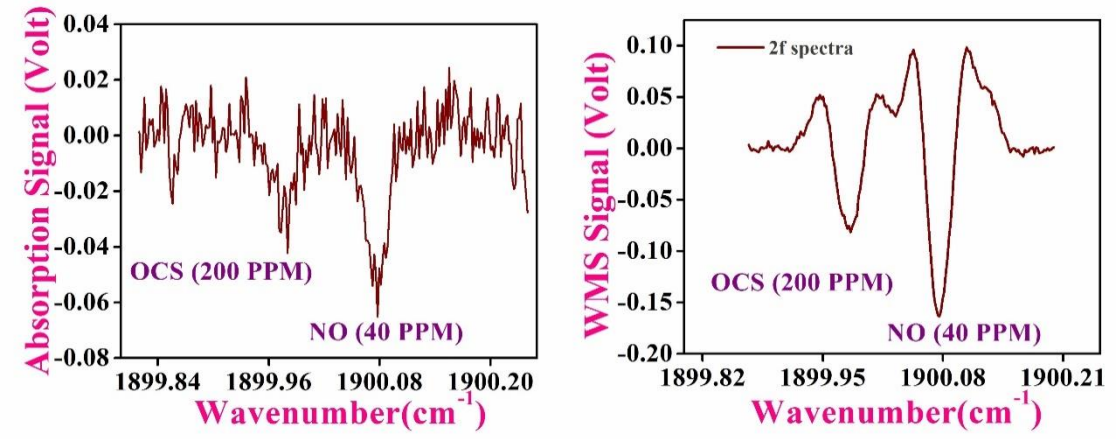
We developed a mid-IR 2*f*-wavelength modulation spectroscopy (WMS) detection system combining a continuous wave (cw) external-cavity quantum cascade laser (EC-QCL) at 5.2 μm and an astigmatic multipass cell. The high-sensitivity performance of the 2*f*-WMS system was validated by simultaneously probing the strongest interference-free absorption lines of Λ-doublet components of R (6.5) rotational line in $^2\Pi_{1/2}$ magnetic electronic sub-state of nitric oxide (NO) centred at 1900.0706 cm^{-1} and the R (18) rotational line of carbonyl sulfide (OCS) in the (v_1+2v_2) combination band centred at 1899.9756 cm^{-1}. We compared the results with the direct absorption spectroscopy and have shown that a detection limit of 300 ppb for NO and 3 ppm for OCS could easily be achieved by the 2*f*-WMS method with an optical pathlength of 76 m. Hence, we believe that in the future the present QCL based 2*f*-WMS detection method with high sensitivity and specificity could be deployed for real-time monitoring of NO and OCS in a harsh environment.



References

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Quasi-one-dimensional superconductivity in single crystal of $(TaSe_4)3I$

Buddhadeb Pal[1], Riju Pal[1], Arnab Bera[2], Prabhat Mandal[1], Mintu Mondal[2] and Atindra Nath Pal[1]

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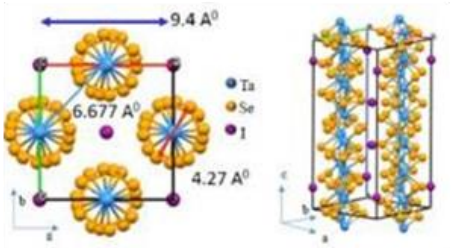
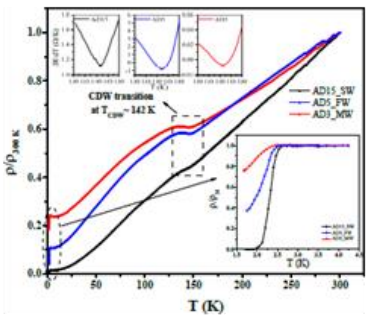
We observe charge density wave (CDW) at TCDW ~ 142 K and the superconducting phase transition at Tc ~ 2.6 K in the quasi-one-dimensional crystals of a new compound (TaSe4)3I. The Single crystals of (TaSe4)3I were grown by chemical vapor transport method and the crystals formed in ribbon-like fibers [1]. The CDW is a well-known phenomenon in the one- dimensional system and it is observed as a metal-insulator transition in the temperature dependent resistivity [2]. The Fermi surface of a metal may become unstable below a transition temperature and then the Fermi surface instability leads to redistributions of the charge density to form a periodic spatial modulation [3]. Our magneto-transport measurements show an anisotropic nature of superconductivity. The positive curvature of the upper critical field has been observed in our samples and we try to fit various model to find out the nature of superconductivity. The critical field Hc2(0) was found in the range of 0.5 T to 1 T. We estimated the London penetration depth (l) from the I-V characteristics and the temperature dependent l fits well with the BCS s-wave symmetry. The calculated value of superconducting energy gap from s-wave fitting is close to BCS value. The multiple voltage steps in I-V characteristics [4] and the angle dependent critical field are also representing the strong signatures of a typical quasi-1D superconductivity in (TaSe4)3I.





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The inconsistency in quantum theory

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As Mermin said, ".. quantum theory is the most useful and powerful theory physicists have ever devised. Yet today, nearly 90 years after its formulation, disagreement about the meaning of the theory is stronger than ever. New interpretations appear every day. None ever disappear .. " [Phys. Today 65, No. 7, 8–10 (2012)]. This disagreement about the underlying reality of quantum theory (QT) is rooted in two conflicting dynamics (unitary evolution and post-measurement evolution) of quantum theory, which is also referred to as the measurement problem. Wigner had nicely illustrated this fundamental issue in his famous thought experiment [1] in which one observer, namely, Friend performs a quantum measurement and one super-observer, namely, Wigner describes the whole measurement process including Friend. Wigner pointed out that, in universal quantum theory, where any macroscopic system or any observer has a quantum mechanical description, the state of a system with respect to these two observers differ in certain situation. Although argued byWigner that such a discrepancy can be avoided if we do not associate quantum state with any underlying reality of physical systems and take the standpoint that quantum state only represents some knowledge about physical systems.

In our work [2], we first propose an extension of Wigner's Friend thought experiment, named as" Wigner's Friend and Student", that gives rise to inconsistent predictions at the empirical level between two super-observers Wigner and his Student. To resolve this inconsistency, we hypothesize two distinct solutions inspired by the perspectives of Student and Wigner: (1) "Absoluteness of Measurement (AoM)", that the measurement is an absolute event (irrespective of other observers) and yields a single outcome, (2) "Non-absoluteness of measurement (NoM)", that physical systems always evolve via time-evolution with respect to an observer unless the observer observers an outcome. We provide a criteria in terms of empirical probabilities to falsify the hypothesize AoM, without assuming the details of the thought experiment. In general, we show that set of probabilities obtainable for AoM is a proper subset of the set of probabilities obtained for NoM. We also analyze whether different interpretations of QT are compatible with these two perceptions and provide consistent predictions or not.

References

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Jump to Molecular Contact in A Single Molecular Junction and Post Rupture Evolution

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Understanding the formation of metal-molecule contact at the microscopic level is the key to controlling and manipulating atomic-scale devices. A route towards exploring atomic-scale transport has involved forming mechanical break junctions. Various metals like Au, Pt, Cu, and Ag exhibit a jump to contact, while there are others like Ir, Ni, and W in which a jump to contact can be absent. The formation of a metal-molecule bond is rather complex and highly dependent on the nature of binding groups and the geometry of the electrodes. In this work, we investigate the formation of a metal-molecule bond by studying charge transport through single molecular junctions and we establish that contact formation is strongly connected with the molecular structure of the electrodes as well as how the junction is broken during the breaking process [1].

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Viscoelastic response of fluid trapped between two dissimilar van der Waals surfaces

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Employing grand canonical Monte-Carlo and molecular dynamics simulations, the viscoelastic response of trapped fluid under molecularly thin confinement by walls having different wall–fluid interaction strengths, is investigated. With increase in slit asymmetry, given by the ratio of interaction strengths of the wall having strong wall–fluid interaction to that of the wall with weak wall–fluid interaction, a crossover in effective density of the fluid film, from rarer (R) to denser (D) than the bulk density is observed. Upon increasing asymmetry further, the dense fluid (F) layers undergo bond-orientational (S) ordering. The variation of viscoelastic relaxation time with scaled asymmetry shows a universal behavior, independent of slit width, with two distinct regimes. Below a critical value of asymmetry, the viscoelastic relaxation time is a slowly varying function of asymmetry, comparable with the structural relaxation time. Beyond the critical asymmetry, on the other hand, viscoelastic response time shows a sharp increase upon increasing asymmetry, deviating markedly from the structural relaxation time. Interestingly the critical asymmetry value is found to correlate with R to D crossover. The microscopic origin of the two-regime universal behavior of viscoelastic response time is found to stem from the fact that below critical asymmetry, the overall viscoelastic behaviour of the slit is dominated by that of the fast relaxing layer close to the weakly attracting surface, while above the critical asymmetry, the relaxation behaviour is guided by the dense fluid layer adjacent to the strongly attracting wall. In vicinity of fluid to ordering transition, the loss and storage moduli merge for low frequencies as in gel-like mechanical behaviour. The storage modulus takes over the loss modulus in the phase co-existence region even before the long ranged order sets in. Our findings bear important implications for fluid transport in hetero structured geometry in nanotechnology.

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Rational Design Principle Towards Allosteric Inhibitor for PCSK9-LDLR Interaction

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PCSK9 is the proprotein convertase (PC) subtilisin/Kexin type 91, which is known to be responsible for heart disease, associated with the raised level of the low-density lipoprotein (LDL)-cholesterol (LDL-C). LDL receptors, i.e., LDLRs, capture LDL particles at the hepatocyte surface to form LDLR•LDL complexes, then undergo rearrangement of the LDLR extracellular domain by the acidic environment in the endosome, releasing bound LDLs, and LDLR is recycled back to the plasma membrane2. PCSK9 interacts with LDLR, and the rearrangement of LDLR in LDLR•LDL complexes is hindered in the presence of PCSK9. The complex and PCSK9 then enter lysosomes, where LDL, LDLR, and PCSK9 are degraded instead of recycling LDLR3. Thus, inhibition of PCSK9-LDLR interaction is crucial to reduce the plasma lipoprotein level as it would release free LDLRs at hepatocyte to capture LDLs. Statin therapy is a well-known treatment for reducing LDL-C levels by inhibiting cholesterol synthesis, but like other drugs, it also adversely affects the body. The other way is to block the PCSK9-LDLR interaction site. Thus, in medicinal research, PCSK9-LDLR is an authentic target. Despite the existence of few FDA-approved antibody drugs4 without serious side effects, there is still a desire for small molecule drugs, based on the mode of administration, cost, etc. The most common approach was to mimic the PCSK9-LDLR interaction surface, though there are limited reports of such compounds as finding a specific molecule for the broad area of the PCSK9-LDLR interface is crucial.

Here we come up with an effective new method to inhibit PCSK9-LDLR interaction. We hypothesize that the flexible and inflexible areas of the protein are in a dynamic equilibrium, and restriction of degrees of freedom in the flexible regions of the protein might lead to an increase of degrees of freedom in the inflexible regions, thus creating a new thermodynamic state. We have found such flexible areas in PCSK9 and observed the change in the dynamics in one loop region is modulated to PCSK9/LDLR interaction via another loop. Thus, exploiting the idea of dynamic allostery in controlling the loop dynamics in PCSK9 seems to be a promising strategy towards controlling binding efficacy with LDLR.

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Anomalous transport driven by topological Nodal line in ferromagnetic compound Fe_3GeTe_2

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Topological ferromagnetic (FM) semimetals have attracted tremendous attention. Topological semimetals shows several band-crossing points or lines are generally expected to evince topological properties. Most of the work has been done for non-magnetic materials and the correlation between topology and magnetism in this class of quantum materials has not been largely investigated. On the theoretical front, the adoption of Berry-phase concepts has established a link between the Anomalous Hall Effect (AHE), Anomalous Nernst Effect (ANE) and the topological nature of the hall currents which originate from spin-orbit coupling. Utilizing the first-principle calculations together with group theory analysis we investigate intrinsic berry phase related anomalous transport properties (anomalous Hall, Nernst).In these ferromagnetic semimetal we observe topological nodal line in first brillouin zone (BZ). By breaking time reversible symmetry we produce a large berry curvature which leads to large anomalous hall and Nernst conductivity.we observed that AHC 150 S/cm for Fe3GeTe2.The anomalous Nernst conductivity are observed -1 A/Km for Fe3GeTe2 near the Fermi energy at room temperature.

A Mechanism to Attract Electrons

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In a startling discovery it has been recently found that certain density of states (DOS) can become negative in mesoscopic systems wherein electrons can travel back in time. We give a brief introduction to the hierarchy of density of states in mesoscopic systems as we want to point out some robust phenomenon that can be experimentally observed with our present day technologies. They can have direct consequences on thermodynamic effects and also can provide indirect evidence of time travel. Essentially certain members of the hierarchy of DOS become negative in these regimes and that can attract other electrons.

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Ferromagnetically coupled Shastry-Sutherland lattice: Ground state properties and quantum phase diagram

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The ground state properties of ferromagnetically coupled dimers on Shastry-Sutherland lattice (SSL) have been studied here. In this model, exchange couplings J_x and J_y along X- and Y-axis are of ferromagnetic type and diagonal exchange coupling (J) is antiferromagnetic. We have noticed the existence of six different phases in the system using density matrix renormalization group (DMRG) method. Depending on different values of interaction strength, the model shows dimer stripe (0,π), dimer stripe (π,0), perfect dimer, dimer spiral along X-direction, dimer spiral along Y-direction and ferromagnetic alignments of the spins. Phase boundaries of these phases are determined using the correlation functions and gs energies. We have noticed that the bond order along diagonal direction is very strong even at very large value of J_x or J_y. We have also calculated correlation length at different parameter regimes and we have also divided our phase diagram depending on correlation length (<1 and >1). We confirm the existence of spiral phase in which the pitch angle between two consecutive spins lie between 0 and π. Our singlet-triplet gap calculations show that there is always a finite gap existed in the system even at stripe region for large values of interaction strength.

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Spatio-temporal heterogeneity in octanol rich region: time resolved fluorescence measurements

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Neat 1-octanol and wet-octanol has been the subject of numerous studies due to their property of membrane mimics.1-3 Interaction and dynamics as well as solution heterogeneity aspect pure octanol and water/octanol mixtures have been investigated via dielectric relaxation spectroscopy (DRS), steady state and time-resolved fluorescence (TRF) measurements in the temperature range of 283≤T/K≤323 with various mole fraction of water in the octanol rich region. Coumarin 153 (C153)4, Coumarin 343 (C343)5, trans-2-[4'-(dimethylamino)styryl]benzothiazole (DMASBT)6 fluorophores have been employed as local reporters to investigate relaxation dynamics in this aqueous mixture in presence of reactive and non-reactive fluorophores. Excitation wavelength dependence of fluorescence emissions7,8 suggest that the neat and aqueous binary mixtures, within the lifetime DMASBT (~ 0.5 ns), are spatially heterogeneous.9 Solute-medium frictional coupling in neat and wet-octanol have been further explored *via* time-resolved fluorescence anisotropy studies of the two non-reactive fluorophores, C153 and C343. Inspite of nearly similar size, rotational diffusion of C153 exhibits fractional viscosity dependence while C343 nearly follows the Stoke-Einstein-Debye model.10 Dynamic fluorescence Stokes's shift registered by C153 and C343 report bimodal relaxation processes in these media. The inter and intra relationship between rotation and solvation process associated with solvation and rotation of the hydrophobic C153 differ from hydrophilic C343 which reflects their qualitatively different local environments scene these two probes due to their chemical nature.

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Observation of supercooled metallic phases below metal-insulator transition temperature (T_{MI}) in $NdNiO_3$ film and understanding the phenomena with a Monte-Carlo simulative approach

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In this work we have observed the existence of metastable supercooled metallic phases within the insulating phase matrix below T_{MI} in $NdNiO_3$ film which shows temperature driven metal-insulator transition. The investigation has been carried out in $NdNiO_3/LaAlO_3$ (NNO/LAO) thin film grown by Pulse Laser Deposition technique (PLD). We have used the resistance relaxation method [1] which is a viable method to study relaxation kinetics of co-existing phases with different resistivities. A model based on Monte Carlo simulation has been taken to understand the metal to insulating phase conversion phenomena in the supercooling regime.

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Investigation of the Radiation Driven Implosion in L1616

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In understanding the formation and evolution of our own solar system, we would like to know: How does star formation happen? Theoretical and observational analyses reveal the importance of various factors in star formation, such as turbulence and magnetic field. Also, massive OB stars have a profound impact on the star formation in their surroundings. Their strong UV flux ionizes the surface of the nearby molecular cloud, causes it to collapse, and thus triggers subsequent star formation, which is known as Radiation Driven Implosion (RDI). The best way to understand what drives the star formation in a cloud is to investigate its various properties. Our study focuses on LDN 1615/1616 and CB 28 (hereafter, L1616), which together form a cometary globule, located at about 8 degrees west of the Orion OB1 association. The presence of massive stars in the Orion belt, especially epsilon Ori, is considered to be responsible for the RDI mode of star formation in L1616. We carried out optical polarimetry towards L1616 to map the plane-of-sky component of the ambient magnetic field and found it to follow the cloud structure. This could be the effect of dragging of the magnetic field lines by the impact of the ionizing radiation from epsilon Ori. Based on the Gaia Early Data Release 3 measurements of the identified young stellar objects (YSOs) associated with L1616, we investigated their plane-of-sky motion with respect to epsilon Ori and found them to move away from the ionizing star. The results will be discussed in detail at the conference.

A Revisit to Turnover Kinetics of Individual *Escherichia coli* *β*-Galactosidase Molecules

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Competing stochastic approaches centred on the kinetic framework and the dynamics of flexible polymers are suggested to elucidate the outcomes of the turnover kinetics of the individual *β*-galactosidase molecules.[1] The original multistate theory for the dynamically disordered single-molecule reaction, although seems realistic, remained unable to distinguish the extent of disorder at different substrate concentrations.[2] Detailed two-state kinetic analysis of the present study clearly established that an account of larger conformational states of the active species is indeed essential to satisfy the quantified randomness at growing substrate concentrations.[3] Consequently, the further investigation focused on the particularity of the dynamics of structural transitions which was modelled with the temporal fluctuations of the spatial distance between the different locations along a coarse-grained polymer chain. Combining Zwanzig's idea of dynamic disorder[4] and the simplest possible Rouse-dynamics of a flexible polymer[5], our theoretical results successfully recovered the findings of the experiment quantitatively and thereby removed the limitations posed by the routine state-based sketch of the reaction system.

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Robust antiferromagnetism in $NaOsO_3$ under pressure

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$NaOsO_3$ is known to be an insulator with a small band gap of 0.2 eV, favoring a G-type antiferromagnetic state below 410 K. It is believed to be an example of a Slater insulator [1], with spin-orbit interactions playing a significant role here in modifying the electronic structure[2]. The unusually high antiferromagnetic temperature has been explained as emerging from the half-filling of the t_{2g} state [3]. We have examined the pressure dependence of the electronic structure, as well its evolution under pressure both in the presence and absence of spin-orbit interactions within ab-initio electronic structure calculations. Mapping the Hamiltonian to a tight-binding model, we use pressure as a parameter to tune the interaction strengths and bring it to the point where magnetic order just sets in. This allows us to throw light on the mechanism of magnetism.

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Control of energy, dissipation, and error in kinetic proofreading through chemostatted concentration

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Extraordinary accuracy in central biological events can be rationalized through a mechanism known as kinetic proofreading [1, 2]. Here, dynamic and thermodynamic features of this mechanism are investigated systematically at the level of nonequilibrium steady states by implementing a chemical thermodynamic framework [3, 4, 5]. Quantifying the dissipation and energy cost through concentration control of the chemical fuel, we have unveiled the association of thermodynamic entities with the optimal operating region of this error-correcting mechanism. We have also introduced a performance measuring entity of the proofreading network corresponding to different energetic discrimination magnitudes for the whole range of chemical fuel.

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Investigation of non-trivial electronic band in layered Lanthanum based Silver Antimonide ($LaAgSb_2$)

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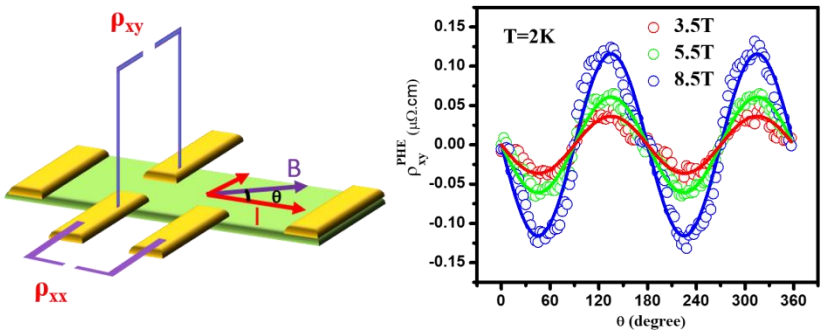
Here, we demonstrate the low-temperature magnetoresistance (MR) study of charge density waves system LaAgSb 2 with linear dispersive electronic band 1 and successfully observe the planar Hall effect (PHE) which is often ascribed to the non-trivial band or chiral anomaly 2 , 3 . The observed planar hall signal shows a period of with a variation of angle between current and magnetic field, which is in accordance with the theoretical description. To further shed light on the origin of PHE, we investigate the in-plane anisotropic magnetoresistance, and observe no negative longitudinal magnetoresistance. The in-plane angular magnetoresistance (In-AMR) shows higher order oscillation. We measured the ordinary hall effect which showed a non-linear behaviour with the change of magnetic field which indicates that carriers from the multiple bands are taking part in the electronic transport. Analysis of the experimental data suggests that the observed PHE in LaAgSb 2 is caused by anisotropic orbital magnetoresistance rather than a non-trivial band.



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Optical Photometric Variability in Young Brown Dwarfs and Very Low Mass Stars in the Taurus Star-Forming Region

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Photometric variability studies of very low-mass stars (VLMs) and Brown Dwarfs (BDs) are an important tool to probe the physical nature of their atmospheres. Photometric variability in these dwarf is due to the presence of surface features like magnetic spots (strong magnetic fields) or dust clouds, which cause optical modulation as it rotates, and it is possible to measure the period of rotation of an object from its light curve. The time-series photometric variability is a key probe of atmospheric inhomogeneities in VLMs and BDs. BDs are known to be rapid rotators (priod~ hours to days), so the rotation modulation of their lightcurves gives information about surface features such as magnetic spots or dust clouds, which provides an opportunity to measure the period of rotation in these dwarfs. However, it is very challenging to detect their variability amplitude, which is the order of a few tens milli-magnitudes. We have taken optical I-band time-series photometric observations on a few BDs and VLMs in the Taurus star-forming region. From our preliminary analysis of the observed data in the I-band on CFHT Tau 6 and CFHT Tau 8, we found that CFHT Tau 8 shows significant periodic variability, and we estimate a rotation period of 6.6 hours. While CFHT Tau 6 shows no significant variability with a given accuracy with the observed ground based time-series I-band data. Some of the BDs are also observed using Transisting Exoplanet Satellite Survey (TESS) and CFHT Tau 6 and CFHT Tau 8 both are shows sinusoidal variability.

Multivalent cation induced phase separation in proteins: ion specific THz hydration studies

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Multivalent (specifically trivalent) metal ions are known to induce microscopic phase separation (commonly termed as *liquid-liquid phase separation* (LLPS)) in negatively charged globular proteins even at ambient temperatures, the process being mostly driven by protein charge neutralization followed by aggregation.[1] Such self-aggregation of protein is entropy driven,[2] however, associated with a solvation effect which could as well be different from the usual notion of *hydrophobic hydration*. Here we have experimentally probed the explicit change in the hydration associated with ion-induced LLPS formation of a globular protein bovine serum albumin (BSA) at ambient temperature using FIR-THz FTIR spectroscopy (50-750 cm^{-1}; 1.5-22.5 THz). We have used ions of different charges: Na^{+}, K^{+}, Ca^{2+}, Mg^{2+}, La^{3+}, Y^{3+}, Ho^{3+} and Al^{3+}. In the THz frequency domain we estimate the various stretching/vibrational modes of water and we found that ions forming LLPS produce definite perturbation in the overall hydration, the extent of which is ion specific, invoking the definite role of hydrophilic (electrostatic) hydration of ions in the observed LLPS process.

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Study of 2021 outburst of the recurrent nova RS Ophiuchi: Photoionization and morpho-kinematic modeling

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We present the evolution of the optical spectra of the 2021 outburst of RS Ophiuchi (RS Oph) over about a month after the outburst. The spectral evolution is similar to the previous outbursts. Early spectra show prominent P Cygni profiles of hydrogen Balmer, Fe II, and He I lines. The emission lines were very broad during the initial days, which later become narrower and sharper as the nova evolves. This is interpreted as the expanding shocked material into the winds of the red giant companion. We find that the nova ejecta expanded freely for ~ 5 days, and afterward, the shock velocity decreases monotonically with time as $v \propto t^{-0.61}$. The physical and chemical parameters associated with the system are derived using the photoionization code CLOUDY. The best-fit CLOUDY model shows the presence of a hot central white dwarf source with a roughly constant luminosity of ~ 1.00×10^{37} erg s^{-1} . The best-fit photoionization models yield absolute abundance values by number, relative to solar of He/H ~ 2.1 − 2.5, N/H = 70-95, O/H = 1.05 - 1.80, and Fe/H ~ 3.1 for the ejecta during the first month after the outburst. Nitrogen is found to be heavily overabundant in the ejecta. The ejected mass is estimated to be in range 1.41 − 8.36 × 10^{-6} $M_{\odot}$. The 3D morpho-kinematic modeling shows a bipolar morphology and an inclination angle of i = 30° for the RS Oph binary system.

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Observation of giant exchange bias effect in Ni-Mn-Ti all-*d*-metal Heusler alloy

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Large exchange bias (EB) has always been an attractive research topic owing to its high potential impact on many technological applications such as magnetoresistive random access memory (MRRAM), magnetic recording media, and spin-valve devices. The essential characteristics which determine the properties of EB systems are; asymmetry of the hysteresis loop, the magnitude of loop shift and its sign, training effect, and time dependence of thermoremanent magnetization [1,2]. EB is usually observed to arise due to ferromagnetic (FM) unidirectional anisotropy coupling formedat the distinct type of interfaces between FM-antiferromagnetic (AFM), FM- ferrimagnetic (FI), FM spin glass (SG) phases. Here, we report a giant EB field of about 3.68 KOe during field-cooled process in all d-metal Ni40(FeCo)4Mn36Ti20 Heusler alloy. The study of magnetic memory effect andisothermal magnetic relaxation processes suggest that the giant EB field arises due tothe strong exchange coupling between FM and AFM phases in the studied system attemperatures below 35 K. Furthermore, the temperature and cooling field dependenceof EB effect are analyzed which are related to the change in unidirectional anisotropyat FM/AFM interfaces. The study of a well-established training effect confirms the intrinsic nature of the observed EB behavior.

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High performance piezoelectric nanogenerator based on BTO-PVDF nanocomposites

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Barium titanate ($BaTiO_3$) nanowires of high aspect ratios are synthesized by the cost effective hydrothermal route. The electromechanical response was measured by using the PFM, which shows the as synthesized BTO NWs are highly ferroelectric and have a piezoelectric coefficient (d_{33}) of 308 pm/V. We have fabricated a flexible, environment friendly piezoelectric nanogenerator (PENG) based on the ferroelectric Polyvinylidene fluoride (PVDF) composite incorporated with Barium titanate ($BaTiO_3$) nanowires. It is demonstrated that the single-layered piezoelectric nanogenerator can deliver output power density of 10 μW/cm^2 and an output voltage of 2 V with a nominal mechanical load of 1 kPa. We show that there exists a critical value of BTO NWs loading, beyond which the piezoelectric energy harvesting characteristics of the PVDF nanocomposites decrease. It is observed that the intrinsic defects of BTO NWs favor the molecular interaction for promoting strongly polar β phase. The origin of the high power output from the BTO-PVDF based nanogenerator is attributed to the combined effect of enhanced polar phase content, interfacial polarization and low internal resistance. The present work provides a systematic pathway for the development of BTO nanostructures based nanogenerators with high energy output.

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High-performance thermoelectric properties of strained two-dimensional tellurium

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Elemental two-dimensional (2D) materials in monolayer form are attractive due to their simplicity and indigenous properties [1]. In the present study [2], we investigate the influence of biaxial strain on group VI elemental 2D material of tellurium, which has been discussed for its potential in various applications. Considering realistic estimates of strain that may be imposed to monolayer Te through van der Waals heterostructing with other known 2D materials, we demonstrate that the structural, electrical, and thermal transport properties can get strongly influenced by strain. Importantly, through strain engineering, the thermoelectric performance of elemental 2D Te in p-type doping can be made comparable to that of the known binary or ternary layered compound at room temperature, and can outperform the known binary or ternary layered compounds at high to moderate temperature. The *ZT* of monolayer Te is found to reach a value of 6.07 at 800 K under tensile strain, being larger than 2 for temperature greater than 400 K. Our study provides a way to tune the thermoelectric properties of 2D Te for future applications.

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Effect of receptor clustering on E.coli chemotaxis: Sensing versus adaptation

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The cooperative behaviour of receptor dimers forming densely packed clusters is recently found to be a significant source of fluctuation in E. coli chemotaxis pathway. It influences the adaptation module of the pathway to respond strongly and increase the methylation level of chemoreceptors. Again, highly dense large clusters can sense the nutrient concentration more efficiently. Therefore, a competition develops between sens-ing and adaptation. At very large cluster size adaptation wins the competition resulting decrease in the sensitivity of chemoreceptors hence chemotactic efficiency deteriorates re- sulting in a performance peak[1]. To explore the sensing versus adaptation competition further we have observed the methylation dynamics of chemoreceptors during a run[2]. Change of the methylation level in a run depends sensitively on strength of concentra- tion gradient and direction of cell movement. In weak gradient, for both uphill and downhill runs, after initial demethylation we see late time methylation and range of this methylation-demethylation gets amplified as cluster size increases. In strong gradient also, uphill runs show similar behaviour in methylation dynamics. But the downhill runs in strong gradient show highly non-trivial dependence on cluster size due to sensing and adaptation interplay[2]. Switching rate of receptor activity determines how fast chemotac- tic cell shifts between run and tumble states. We find chemotactic performance to increase with switching rate and reach a saturation[3]. In probing further we see that downhill run duration falls at a faster rate than the same of uphill ones. The activity variation during downhill runs for small and large switching rate actually shows qualitatively different be- haviour but similar behaviour in case of uphill runs. This causes downhill run duration to fall faster and enhance the performance as switching rate increases.

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Coexistence of superconductivity and ferromagnetism in magnetically anisotropic Sn intercalated Cr_3Te_4

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The recent discovery of 2D magnets such as CrI_3, $CrGeTe_3$, $CrSiTe_3$, Fe_3GeTe_2 and Cr_xTe_y have stimulated significant interest due to remarkable physical properties [1]. Superconductivity (SC) and ferromagnetism (FM), these two are antagonistic phenomena. Experimentally, a coexistence of SC and FM was discovered in the compounds UGe_2, $ZrZn_2$, and $RuSr_2GdCu_2O_8$ [2,3,4]. In Cr-Te phase diagram, there are many crystals structure such as hexagonal, monoclinic, and trigonal [5]. Here, we have successfully grown high quality single crystals of Sn intercalated Cr_3Te_4 by flux-free melt growth process. Structural and elemental analysis have been performed using X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDXS), respectively. The single crystal XRD patterns confirm monoclinic crystal structure with a C12/m1 space group. We have performed electrical resistance and magnetization measurements of $Sn_xCr_3Te_4$ within the temperature range of 2-300 K. We found the occurrence of superconductivity in $Sn_xCr_3Te_4$ single crystal at below 3.53 K. Magnetic measurements confirm the coexistence of SC and FM in this material. Various other superconductivity parameters viz. kappa parameter, coherence length and penetration depth are also calculated to probe the as-grown sample's characteristics.

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Studies of the pre-main sequence stars in the H II region Sh2-87

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H II regions are the low-density clouds of ionized gas excited by massive stars (O, early B). The molecular clouds, associated with H II regions and young embedded clusters, serve as the ideal targets to probe the formation of stars as well as star clusters. Here, we identify and characterize thepre-main-sequence stars associated with the H II regions Sh2-87, which is located at a distance of ~2.3 kpc and is a member of the Vulpecula OB association. We have utilized both the new spectroscopic observational data as well as several archival catalogues, e.g., IPHAS, WISE, UKIDSS. Low-resolution spectroscopic observations revealed the presence of few massive (early- B) sources. Using the near-infrared colour excess, several young populations are identified, that suggest active star-formation activity toward this region. Additionally, the presence of a significant number of Hα emitters indicates strong ionization activity. Thus using multi-wavelength datasets, anoverall star formation activity will be presented here.

Scalar-Fermion Interaction as the Driver of Cosmic Acceleration

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We argue that an interacting scalar-fermion distribution can be used to demonstrate the cosmic acceleration in General Relativity. The interaction is of Yukawa nature andit drives the fermion density to decay with cosmic time. The consistency of the model isestablished through, (a) a generalization of the Om(z) parameter, the present matter density contrast of the universe and (b) a comparison of theoretical results with reasonable sets of observational data, using a Markov Chain Monte Carlo code. A simple model of unified cosmic expansion history is also discussed. There are more than one instance where the universe goes through a transition between subsequent epochs of cosmic expansion. This pattern of evolution imposes a few constraints on the scalar-fermion interaction and on the overall cosmological dynamics.

Direct measurement of interfacial Dzyaloshinskii–Moriya interactionand atomic layer thickness dependence in a ferromagnet-WS2 heterostructure

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Two-dimensional transition metal dichalcogenides (TMDs), exhibiting rich physics including high spin orbit coupling [1], have immense potential for spintronics applications. Here, atomic layer thickness dependence in WS2/Co3FeB heterostructures is predicted theoretically by density functional theory and demonstrated experimentally by the layer dependence of the interfacial Dzyaloshinskii-Moriya interaction (iDMI). Notably, we have observed the iDMI in WS2 to be larger than that for heavy metals such as W [2]and Ta, which is important to stabilize chiral structures. Inversion symmetry is not preserved with an oddnumber of layers, while it exists with an even number of layers. This symmetry rule is reflected in the temperature dependence of the effective damping parameter of the heterostructure in a way that the damping parameter decreases (increases) in odd (even) layers can be resolved at low temperature. Thissuggests that the layer dependence has its origin at the WS2 interface, where the spin-valley coupling and spin-orbit coupling activate these features. Being an experimental observation of odd-even layer dependence from two different experiments like Brillouin light scattering and ferromagnetic resonance technique, further low temperature experiments on different types of TMDs are considered to be important for designing 2D materials-based quantum devices.

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Femtosecond laser-induced ultrafast spin dynamics in ferromagnetic thin films: comparative study using two theoretical models

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Beaurepaire's pioneering work demonstrating laser-induced ultrafast magnetization loss in ferromagnetic nickel [1] opened up a vista of exciting research for the decades to comeThe phenomenon is of special interest in the field of spintronics as it implies that magnetization switching in spin-based memory devices could be achieved at these ultrashort timescales. Several theoretical and phenomenological models have been proposed to explain this phenomenon, among which Beaurepaire's three temperature model and Koopmans' microscopic three temperature model [2] are two of the most prominent. We revisit these two models to perform a comparative analysis of ultrafast demagnetization measured in electron-beam evaporation deposited 20 nm-thick nickel, cobalt and permalloy thin films. Measurements were carried out using a two-color pump-probe time-resolved magneto-optical Kerr effect (TR-MOKE) setup with a 400 nm pump beam (repetition rate = 1 kHz, pulse width > 40 fs) and 800 nm probe beam (repetition rate = 1 kHz, pulse width ~ 40 fs) [3] with a pump-probe cross-correlation width ~100 fs. To study the modulation of the demagnetization response with the fluence of the exciting laser pulse, TR-MOKE measurements were performed while varying the pump fluence in the range 0.87-8.7 mJ/cm^2 keeping the probe fluence unchanged around 0.4 mJ/cm^2. The experimentally obtained demagnetization traces are analyzed by performing a least-squares fitting routine in tandem with numerical integration of the models. The demagnetization times extracted for the largest value of pump fluence used are about 280 fs, 300 fs and 250 fs for Ni, Co and Py respectively. Further, from the results of the fitting routine, we extract the values of relevant microscopic constants that best reproduce the experimental data.

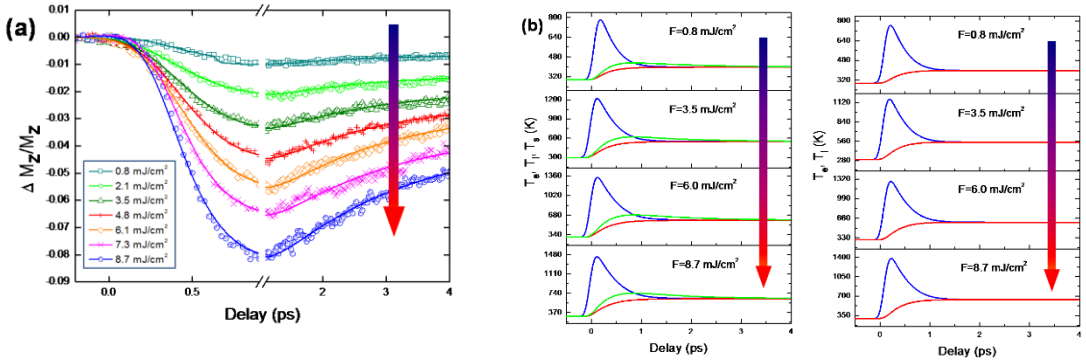

Figure 1: (a) Pump fluence variation of demagnetization response in cobalt and (b) simulated electron temperature profiles using the 3TM (left) and M3TM (right).

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Slow relaxation and decoupling of electrons from the phonon bath as a precursor of Mott metal-insulator transition

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In recent years, the exciting issue of slowing down of charge relaxation close to metal-insulator transition (MIT) have been investigated. Critical slowing down has been observed through Noise measurements as well as in NMR relaxation time measurements in polymeric /organic conductors as well as in oxides like in V_2O_3 undergoing Mott transition [1-3].

In this paper, we report that close to a Mott transition, over a small temperature range,the predominance of slow relaxations leads to decoupling of electrons from the thermalbath. This has been established by observation of large deviation of the thermal noisein the films of Mott system $NdNiO_3$ from the canonical Johnson-Nyquist value of $4K_BTR$close to the transition. It is suggested that such a large noise arise from small pocketsof nanometric metallic phases (estimated size ≈ 15-20 nm) within the insulating phasewith the Coulomb charging energy as the control parameter.

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Addition of cholesterol alters the hydration at the surface of model lipids: a spectroscopic investigation

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Lipids are the building blocks of cell membrane which not only compartmentalize the cell but also do regulate many physico-chemical mechanism (i.e, diffusion, active transport, energy conversion) in the cell.[1] Cholesterol modifies the structure and organization of lipid membrane and modulates the fluidity and rigidity of membrane.[2] Here we investigate the alteration of hydrogen bond network structure of water at the interface of zwitterionic DOPC, anionic DOPG and (1:1) DOPC/DOPG in absence and in presence of cholesterol using ATR-FTIR spectroscopy in the FIR-THz region (1.5-13.5 THz). Our measurements and analysis lead us to probe the collective H-bond network explicitly at the lipid surface and concludes that the water-water H-bond vibration dynamics gets slower at the lipid surface as compared to bulk water, the effect being more prominent in case of the charged phospholipid, DOPG. However, as cholesterol is added and more bulk like water protrude into the lipids surface, the H-bond vibration gets weaker and correspondingly the dynamics gets accelerated.

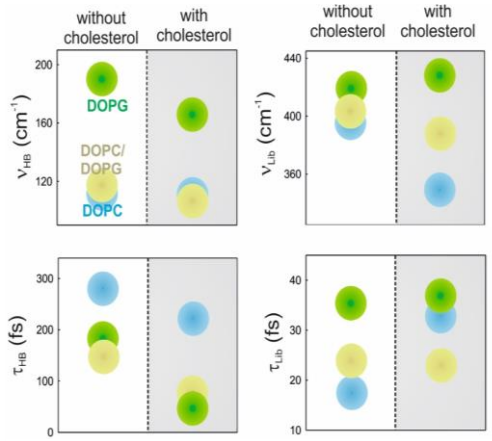

Fig1: Peak frequency and lifetime corresponding to HB-stretch and librational mode of hydration layer of three lipids in absence (clear region) and in presence of cholesterol (shaded region).

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Monogamy of entanglement

Sumit Nandi

Entanglement manifests several counter-intuitive phenomenon of quantum mechanics which is remarkably distinguished from its classical counterpart. Unlike classical correlation, entanglement cannot be shared freely among the parties. Nature imposes severe restriction on sharing entanglement arbitrarily between the subsystems of a given multipartite state and it was referred to monogamy of entanglement. For example, given a tripartite state shared by three parties namely, A, B and C, if A and B are maximally entangled between themselves then there cannot be any entanglement between A (B) and C. We have studied monogamy nature in higher dimension and derived a proper inequality to describe monogamous nature of entanglement.

Anomalous Hall Effect Studies of Stoichiometric Mn_3Ge

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Large Anomalous Hall effect in noncollinear inverse triangular kagome antiferromagnet Mn3X (X= Sn, Ge, Ga) [1,2] is originated from the Berry curvature effect, having enormous potential technological applications. We have synthesized the stoichiometric hexagonal phase of single crystalline Mn3Ge unlike in previous reports [3,4] where it was always with excess Mn. From magnetic measurements, we observed antiferromagnetic ordering below 365K which is in good agreement with earlier reports. In addition, we noticed another magnetic transition below 150K for both orientations of the crystal with applied field, which is not observed in earlier reports on this system. Also, a significant change in the anomalous Hall effect is noticed in both directions below 150K. We suggest that Mn concentration in the system is responsible for suchkind of drastic changes in its properties.

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Bulk-diffusion and anomalous transport of self-propelled particles

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We numerically calculate the bulk-diffusion coefficient in a one dimensional model of interacting Run-and-Tumble particles (RTPs) with hardcore exclusion for arbitrary density ρ and tumbling rate D_r . We find that the bulk-diffusivity is a nonmonotonic function of the tumbling rate, but, as a function of density, it decays as a power law; indeed, in a broad parameter regime, a system of such interacting RTPs is shown to exhibit ballistic (anomalous) density relaxation. Moreover, we propose a model of self-propelled particles, with hardcore exclusion and long-range hopping, which is analogous to the model of RTPs. In this model, we analytically calculate the bulk-diffusivity, which, like in the model of RTPs, is a nonmonotonic function of the typical hopping length-scale (related to inverse of the tumbling rate, or the persistence length, of a RTP) and decays with density as a power law. We find that, upon suitable rescaling of time, these two models are qualitatively quite similar.

POSTER PRESENTATIONS

Conformational fluctuations and binding in molten globule state of α-lactalbumin

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Molten globule (MG) state is an intermediate state of protein observed during folding into native structure. Evidences suggest that MG state of some protein is functionally relevant even if there is no well defined tertiary structure. MG state of protein is induced by various denaturing agent (like Urea), extreme pH, pressure and heat. Earlier experimental and theoretical observations suggests that MG state of the protein is dynamic in nature where conformational states are interconverted in nanosecond time scales. These observations of MG state suggest similarity with intrinsic disorderd protein (IDP) where protein lacks specific secondary structure but can participate in various interactions. Here we explore if the conformational fluctuations of MG state of protein bear any kind of analogy with IDP. We considered α-Lactalbumin(aLA) protein which shows MG state at low pH upon removal of calcium (Ca^{2+}) ion. In MG state aLA binds to fatty acid like oleic acid (OA) to form a complex that shows cytotoxic activity against cancer cell line. We use constant pH molecular dynamics simulation (CpHMD) to maintain low pH during simulation. At first we compare radius of gyration (R_g), root mean square fluctuations (RMSF), native/non-native contact map in support of formation of MG state at low pH. To observe the metastability in MG state, we use dihedral principal component analysis, density based clustering method and machine learning technique to identify the essential coordinates in the MG state. We find that ψ80 (Phenylalanine) dihedral near the calcium binding loop is the most essential coordinate to get the metastable state. The residues containing the essential coordinates belong to stable helix in crystal structure, but most of them prefer unstructured or bend conformation in MG state suggesting lack well-defined secondary structure in MG state. This observation suggest that at MG state protein behaves as intrinsic disorder protein, athough the disorder here is induced by external conditions.This scenario may be helpful to understand the function of a protein in MG state. Next, we check binding of the protein at MG state with OA. At first, we use clustering method to identify representative MG structure of aL protein. We identify destabilized and disordered residues at MG state of the protein w.r.t neutral one using conformational thermodynamics. Therefore, OA is docked near the disordered and destablilized hydrophobic and basic residues of cleft region which is experimentally known to bind with OA acid at MG state. We perform both biased (normal molecular dynamics) and unbiased simulation (umbrella sampling) with the docked structure. The binding energy of OA with the protein is -8.3kcal/mol which is comparable with earlier experimental predicted result.

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Variations in CO−to−H_2 Column Density Ratio in Star-forming Filaments

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Molecular hydrogen is the most abundant molecule in the interstellar medium, but its rotational emission lines are not excitable at the temperatures found in most Galatic molecular clouds. On the contrary, CO, the second most abundant molecule has rotational transitions (in the mm wavelengths) that are easily excitable within typical GMCs, making CO a good tracer of molecular gas. Thus, in absence of molecular hydrogen (H_2) data, CO is often used to infer the H_2 density by using a constant CO-to-H_2 abundance ratio. But several studies found that this abundance ratio is not constant over the molecular clouds. The observed variation in the abundance ratio might be a result of different physical condition (such as density, temperature, magnetic fields) of the molecular clouds. In this study, we constructed CO column density maps for a few Galactic molecular clouds and compare them with the available archival H_2 column density maps constructed from Herschel far-infrared observations. We primarily targeted the filamentary structures of the molecular clouds that are commonly detected in both the column density maps. Our study suggests a broad range of values for CO-to-H_2 abundance ratio, and the abundance ratio show a linear dependancy on the density of the medium. We also find that the abundance ratio decreases linearly as temperature of the cloud increased.

Resource theoretic efficacy of the single copy of a two-qubit entangled state in a sequential network

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How best one can recycle a given quantum resource, mitigating the various difficulties involved in its preparation and preservation, is of considerable importance for ensuring efficient applications in quantum technology. Here we demonstrate quantitatively the resource theoretic advantage of reusing the single copy of a two-qubit entangled state towards information processing. To this end, we consider a scenario of sequential detection of the given entangled state by multiple independent observers on each of the two spatially separated wings. In particular, we consider equal numbers of sequential observers on the two wings. We first determine the upper bound on the number of observers who can detect entanglement employing suitable entanglement witness operators. In terms of the parameters characterizing the entanglement consumed and the robustness of measurements, we then compare the above scenario with the corresponding scenario involving the sharing of multiple copies of identical two-qubit entangled states among the two wings. This reveals a clear resource theoretic advantage of recycling the single copy of a two-qubit entangled state in the sequential network.

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Solubility enhancement of paracetamol in choline chloride-based deep eutectic solvents: Atomic insights using molecular dynamics simulation

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Administration of drugs is one of the most important subjects in pharmaceutics. Oral pharmacotherapy is most convenient for patients having difficulties in swallowing tablets or capsules. Liquid form of drugs is easy to intake for very sick patients, children and elderly persons. Drugs are needed in liquid form for efficient delivery in certain routes like nasal, otic, or ophthalmic. Unfortunately, most of the common drugs are sparingly soluble in water. Therefore, alternate solvents for efficient dissolution of drugs are needed. In this work we have observed solubility of Paracetamol (acetaminophen) in water and two deep eutectic solvents: choline chloride + ethylene glycol, and choline chloride + propylene glycol via molecular dynamics simulation. Our results are well-matched with experimentally observed solubility limits. Moreover, we tried to present molecular level pictures to characterize inherent interactions causing the enhancement of solubility. We have found that hydrogen bonding and hydrophobic interactions are two main origins to solvate paracetamols.

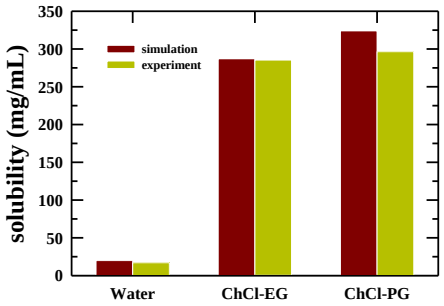

Figure. Solubility of paracetamol in water, and ChCl-DESs. Both simulation and experimental data are shown.

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Effect of additives on the growth of methane hydrate

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Blockage of oil and gas transmission lines by gas hydrates has become a challenging problem in most of the oil and gas industries. Generally, organic alcohols in the aqueous phase affect the gas hydrate formation both thermodynamically and kinetically. Organic alcohols having high concentrations can be coined as “thermodynamic inhibitors” which are capable to inhibit gas hydrate formation effectively. In this work, we try to understand how organic alcohols and common osmolytes when used in small concentrations (~1wt %) alter hydrate growth kinetics and possibly act as either hydrate promoters or inhibitors. We use the all-atom molecular dynamics simulation method to investigate methane hydrate growth kinetics with and without additives. Hydrate formation conditions were similar to that of experiments that were utilized to understand hydrate growth kinetics in presence of without additives and 1 wt % alcohol or 1wt % osmolyte solutions. The studied alcohols are ethanol, ethylene glycol, glycerol, and isopropyl alcohol, and common osmolytes used as additives are urea, DMSO(Dimethyl Sulfoxide), and TMAO(Trimethylamine N-oxide). Our MD study reports that the aforementioned organic alcohols (~1 wt %) reduce the possibility of water molecules forming cage structures. All the osmolytes gradually act as potential hydrate growth inhibitors, whereas urea initially shows growth-promoting ability. A few alcohol molecules have been observed near the hydrate cages. Dynamic behavior of water in presence of alcohol has also been reported.

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Two-dimensional $Mo_xW_{1-x}S_2$ alloys for nanogenerators producing record piezo-output and coupled photodetectors for self-powered UV Sensor

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In this work we propose a novel sustainable, self-driven UV photodetection system using ternary TMDC alloy ($Mo_xW_{1-x}S_2$) by coupling a photodetector as a light intensity sensor and a piezoelectric nanogenerator (PENG) as a power source. We have synthesized crystalline $Mo_xW_{1-x}S_2$ ternary alloy nanosheets via cost effective hydrothermal method to fabricate a UV (365 nm) photodetector with extraordinary high responsivity (~229 A/W). The microstructural, optical properties of different ternary alloy composition, along with their binary counterparts, have been studied. The optimized $Mo_{0.5}W_{0.5}S_2$ ternary alloy nanosheets are used as fillers in PVDF matrix to fabricate flexible self-polled PENGs, exhibiting piezoelectric open-circuit output ~50 V under finger tapping and a record high piezo-voltage ~187 V under impact of 12 kPa. By coupling the two devices, the output voltage of the PENG is tuned by the resistance of the photodetector, exhibiting superior voltage sensitivity (~ 0.75 V $\mu W^{-1}cm^{-2}$) with UV illumination. The impedance matching between the PENG and photodetector has been utilized to demonstrate self-powered UV sensors by monitoring the on/off states of LED directly. This self-powered, portable ternary TMD alloy device is attractive for future real-time monitoring of UV radiation and smart health sensors for IOT applications.

Magnetic Activity of M-dwarfs: Optical and NIR Spectroscopic Studies

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M dwarfs are the most numerous stars in our Galaxy, amounting to about two-thirds in number and about 40 percent in stellar mass. M dwarfs are the lowest-mass hydrogen-burning stars, which are found at the bottom of the main sequence in the H-R diagram. These stars possess masses of 0.08 – 0.6 M and have effective temperatures of 2500 - 4000 K. We have undertaken optical/Near-IR ⊙ spectroscopic studies of a unique sample of M-dwarfs including a few M-dwarfs having strong magnetic fields. Using Himalayan Faint Object spectrograph (HFOSC) and TIFR Near-IR spectrograph (TIRSPEC) back-end instruments on the 2-m Himalayan Chandra Telescope (HCT) telescope and using TIFR-ARIES Near Infrared Spectrometer (TANSPEC) instruument on the 3.6-m Devasthal Optical Telescope (DOT), we have taken optical and near-IR spectra of a sample of M dwarfs to investigate the chromospheric activity and evolution of the atmosphere of M-dwarfs. Several important atomic and molecular lines in the optical and Near-IR wavelengths (e.g.,(H alpha, Ca II IR triplet, He 10833, Na, CO, etc) will be used to characterize these late-type dwarfs. From a preliminary analysis of our observed spectra, we have detected and identified several important atomic and molecular lines to characterize those dwarfs, and data analysis is ongoing. These observations could be used to establish a road map for future target selection of transit search around young and old populations of nearby M dwarfs.

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Photo-ionization and Morpho-kinematic Study of V477 Sct

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In this study, we investigate the photo-ionization process and morpho-kinematics of nova V477 Scuti, in the IR region with the help of CLOUDY 17.02 and SHAPE v5. From the best fit CLOUDY model of the 4th day spectra, we estimated the values of various physical and chemical parameters, like the temperature and luminosity of the central compact object to be 2.5 × 104 K and 7 × 1037 erg s^{-1} respectively, the clump and diffuse density found to be 9 × 10 ∼ 11 cm−3 and 5 × 10 ∼ 9 cm^{-3} respectively, and the absolute abundance values by number, relative to solar value are found to be He/H = 0.2, C/H = 4.0, N/H = 80, O/H = 35, N a/H = 2.0, and Mg/H = 2.5. The 3D modeling which is mainly intended to study the geometry of the ejecta is particularly done for the 10th day from the outburst for three different line profiles (Paschen beta 1.2818 μm, Bracket 10 1.7362 μm, and Bracket gamma 2.1655 μm) using SHAPE. The line profile in most cases has prominent triple and above peak features along with two smaller peaks in both the red and blue sides of the central peak. Several synthetic spectra, as well as data points, are generated with different parameter sets of inclination and velocity. Finally, we obtained the Position velocity (P-V) diagram which shows how the velocity varies with distance and the best fit modeled velocity profile of the selected three lines among the three bands. The best fit line spectra give the inclination i = 250.

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Improvement of magnetic and electric properties of Co doped $GaFeO_3$ ceramics

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In this work, we have synthesized the $GaFe_{1-x}Co_xO_3$ (GFCO, $0 \leq x \leq 0.1$) polycrystalline sample using the sol-gel technique. We have investigated the effect of Cobalt (Co) substitution at Fe-site of $GaFeO_3$ (GFO) on the microstructure, magnetic, electric, and dielectric properties. The phase purity and structural determination were performed using X-Ray Diffraction (XRD) and Energy Dispersive X-Ray Spectroscopy (EDAX), repectfully. Rietveld refinement indicates that all the samples are prepared in orthorhombic phase with space group Pc21n with an additional secondary cubic phase with space group Fd-3m. For 5% of cobalt doping, leakage current density decreases by approximately 4 orders of magnitude as the formation of Fe^{2+} is decreased. Two-phase-like magnetic behavior in magnetic hysteresis and two magnetic transition temperature (TC) are observed in the doped samples. The frequency and temperature-dependent dielectric properties, and complex impedance of GFCO imply an increase in dielectric constant in all doped samples. Therefore, Co substitution improves the magnetic, electric, and dielectric properties of GFO.

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Temperature dependent dielectric relaxation measurement of an amino acid derivative based deep eutectic solvent: origin of timescales via experiment and molecular dynamics simulation

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We report here temperature dependent (303≤T/K≤343) dielectric relaxation (DR) measurement of [Betaine+Urea+Water] 1 deep eutectic solvent (DES) 2 in the frequency window from 20Hz to 50 GHz (with a gap from 10 MHz to 200 MHz). We also performed molecular dynamics simulation of DR in the above-mentioned temperature range employing General Amber Force Field (GAFF) 3 model interaction. Experimental DR measurement of this DES require multi-debye fits and produce well separated DR time scales that are spread over sub-10 picosecond to few nanoseconds (~3ns). A comparison between simulation predictions and the experimental DR data in the KHz-GHz frequency regime describes the well similarities of the dynamics(time-scales). A well correlation between the measured DR and simulated DR activation energies further revels the strong connection between the measured DR and the simulated C M (t) (dipole moment-moment autocorrelation function). The simulated single dipole reorientation dynamics also contributes to the collective polarization relaxation. Average experimental DR times exhibits fractional viscosity dependence. Deviation from hydrodynamic predictions confirms partial decoupling of the solute rotation from the medium frictional resistance exerted by the viscosity. Also, viscosity related activation energy (E a =57 kJ/mol) is ~1.5 times larger than activation energy related to experimental average DR times (E a =39 kJ/mol) which supports the above finding.

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Exploration of the Origin of Magnetism inPotassium Manganese Tellurides

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We have analyzed the origin of magnetism of $KMnX_2$(X=O,S,Se.Te) combining ab initio and model Hamiltonian approaches. Our result indicate that the magnetism is due to two sub lattice double exchange mechanism between Mn and X as first discovered in Sr_2FeMoO_6 double perovskite. Though these chalcogenides are new type of compounds, they are structurally different from double perovskite but the underlying physics remain same. Also these type of compounds are cleavable. We can extract out 2D layer of MnX_2 , which may give a possibility of discovering new type of 2D ferromagets..

Perturbing the bond disproportionated state in $NdNiO_3$

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The rare-earth nickelates with the exceptions of $LaNiO_3$ are found to exhibit a bond disproportionated state. This was shown[1] to emerge in the regime where the effective charge transfer energy between the O p and the Ni d unoccupied states was negative. We perform ab-initio electronic structure calculations and perturb the bond disproportionated state by various routes. Electron and hole doping are both found to tune the effective charge transfer energy,with the latter increasing it and providing a route to tune to a positive value. Our calculations indicate that the doped carriers are localized in the vicinity of the dopant while the bond disproportionation of the rest of the lattice survives.

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Investigation of a harmonic oscillator in a magnetic field with damping and time dependent noncommutativity

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This work is devoted to find the eigenstates of a two dimensional damped harmonic oscillator in the presence of an external magnetic field varying with respect to time with a time dependent spatial noncommutativity. It is observed that there are some specific choices of the damping factor, the time dependent frequency of the oscillator and the time dependent external magnetic field for which one can obtain interesting solutions of the time dependent noncommutative parameters. These solutions follow from the non-linear Ermakov-Pinney equation. We then obtain exact analytic forms for the phase which relates the eigenstates of the Hamiltonian with the eigenstates of the Lewis invariant. An important aspect of this study is to see the relationship between the damping and the applied magnetic field on the energy profile of the system. For this we compute the expectation value of the Hamiltonian. These are found to vary with time for different solutions of the Ermakov-Pinney equation corresponding to different choices of the damping factor, the time dependent frequency of the oscillator and the time dependent applied magnetic field. Finally, we compare our results with those in the absence of the magnetic field to determine the effect of the applied field on our system.

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Spin Peierls transition of $J_1 - J_2$ and extended models with ferromagnetic J_1.Sublattice dimerization and thermodynamics of zigzag chains in β-$TeVO_4$

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The spin−1/2 chain with ferromagnetic exchange $J_1 < 0$ between first neighbors and antiferromagnetic $J_2 > 0$ between second neighbors supports two spin-Peierls (SP) instabilities depending on the frustration $\alpha = J_2/|J_1|$. Instead of chain dimerization with two spins per unit cell, $J_1 - J_2$ models with $\alpha > 0.65$ and linear spin-phonon coupling are unconditionally unstable to sublattice dimerization with four spins per unit cell. Unequal J_1 to neighbors to the right and left extends the model to gapped ($\gamma > 0$) chains with conditional SP transitions at TSP to dimerized sublattices and a weaker specific heat C(T) anomaly. The spin susceptibility χ(T) and C(T) are obtained in the thermodynamic limit by a combination of exact diagonalization of small systems with $\alpha > 0.65$ and density matrix renormalization (DMRG) calculations of systems up to $N \sim 100$ spins. Both $J_1 - J_2$ and $\gamma > 0$ models account quantitatively for χ(T) and C(T) in the paramagnetic phase of β-TeVO4 for $T > 8$ K, but lower T indicates a gapped chain instead of a $J_1 - J_2$ model as previously thought. The same parameters and TSP = 4.6 K generate a C(T)/T anomaly that reproduces the anomaly at the 4.6 K transition of β-TeVO4, but not the weak χ(T) signature.

Relation between filaments and clumps in a few Galactic star-forming regions

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Even though filamentary structure of Galactic molecular clouds were known for decades, Herschel far-infrared observations revealed the universality of the filamentary structure in Giant Molecular Clouds (GMC's). These filamentary structures are believed to play an important role in star formation by regulating gas flow to clumps along their axes. It is believed that star-forming clumps are predominantly associated with such filamentary structures of the molecular clouds. Here, we investigate whether clumps are indeed predominantly associated with filaments or they are isolated structures of the molecular clouds. Further, we also examine if filaments have a tendency to host more gravitationally unstable clumps as compared to the isolated ones. Note that these unstable clumps are the sites of future star formation. For this case study we analyzed the mm-band archival CO line data of a 12 sq-degree patch of the sky towards the inner Galactic plane. Our study suggests that clumps have a tendency to be associated with filaments. Also, the ratio of unstable clumps is slightly higher in filaments in comparison to their isolated counter parts. We also found a threshold column density of filaments for the formation of unstable clumps. Below that critical value filaments are unable to produce gravitationally unstable clumps.

Variation of Magnon–Magnon Coupling Strength with Microwave Power and Bias-Field Angle in $Ni_{80}Fe_{20}$ Nanocross Array

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Hybrid magnonic systems are becoming rising contenders for coherent information processing, owing to their capability of coherently connecting distinct physical platforms in quantum systems as well as the rich emerging physics for new functionalities [1,2]. Magnons have been demonstrated to efficiently couple to cavity quantum electrodynamics systems including superconducting resonators and qubits. Magnonic systems are therefore well-positioned for the next advances in quantum information. In addition, recent studies also revealed the potential of magnonic systems for microwave-optical transduction, which are promising for combining quantum information, sensing, and communication [3]. Here, we have been employed ferromagnetic nanocross array to investigate the role of spin-density in such kind of structures. We observe magnon-magnon coupling in permalloy (Py: hereafter) nanocross array with the virtue of broadband FMR technique and micromagnetic simulations. The number of spins in the nanocross structure is several orders of magnitude smaller than the smallest value ($N \sim 10^{13}$) reported in the literature. We observe two anticrossing phenomena at two different bias fields entangled with a prominent mode-softening phenomena at very low bias magnetic field strength. The first anti-crossing gap shows strong dependence on microwave power, while the anti-crossing at higher field value does not appear to change much with external sources. The dynamic dipolar interactions between neighboring nanocross structures, driven by the microwave power tend to affect the strong magnon-magnon coupling. The mode-softening field varies systematically with microwave power leading towards control of phase transition in nanostructures system just by externally tuning microwave power. Py nanocross array with arm length (L) of 350 nm, edge-to-edge separation (S) of 150 nm, and thickness of 20 nm were fabricated on self-oxidized Si substrate (001) by a combination of e-beam lithography and e-beam evaporation and a coplanar waveguide (CPW) made by Au of 150 nm thickness, having 30-μm central conductor width (w), 300-μm length, and 50 Ω nominal characteristic impedance (Z_0), was integrated on top of the nanocross array. Excitation power of the microwave input signal is varied in the range of −15 dBm to +6 dBm by a vector network analyzer (VNA). Additionally, an in-plane bias magnetic field *H*, is applied along the x-axis and the output scattering parameter S_{11} for reflection is measured by the VNA connected with the CPW. We have observed anti-crossing or avoided crossing phenomenon at two bias field strengths entangled with a mode-softening phenomena at lower bias field value. The anti-crossing strength is tunable over a wide range with variation of microwave power. The simulated magneto-static field distribution plays a significant role in enhancing the magnon-magnon coupling strength. Whereas, the mode-softening phenomenon is appearing due to the phase transition from onion to S-magnetic state, which is widely tunable with bias field angle. Micromagnetic simulations have also reproduced the power-dependent FMR frequency shift. Overall, the observed tunability of magnon-magnon coupling over a wide range in ferromagnetic nanocross array is promising for applications in microwave-assisted fast magnetic storage, logic, and communication devices.

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Tracer motion through an entangled polymeric network within a confined asymmetric geometry in presence of a driving force

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Here, we study tracer particle motion through an entangled network of identical polymeric strands, each strand composed of two kinds of beads in a given ratio with different characteristic interaction parameters. The beads with stronger mutual interaction is called H-beads and the other set is designated as P-beads. The entangled mass is taken within an asymmetric confinement where a wall favorably interacts with one type of bead, H-wall favoring the H-beads and P-wall favoring the P-beads. The tracer particles are taken to interact more favorably with P-beads and the P-wall than the H-beads and H-wall, respectively . We study the permeation of the tracer particles from the H-wall end to reach the P-wall end through the network in presence of a driving force using the Langevin dynamics simulations. The efficiency of the network to stop the tracer particles is given by 100%-P where P is integrated density of the tracer density profile near the P-wall. We find that the efficiency decreases linearly with driving force for tracer particles below a critical size, given by the mean pore size of the network. We also observe that the permeability of tracer particles follows an Arrhenius dependence on temperature, suggesting an activated process. Our finding may help to understand the factors to control efficiency of a mask to stop respiratory droplets.

Anomalous Hall Effect in a Two-dimensional van der Waals Ferromagnet Fe_4GeTe_2

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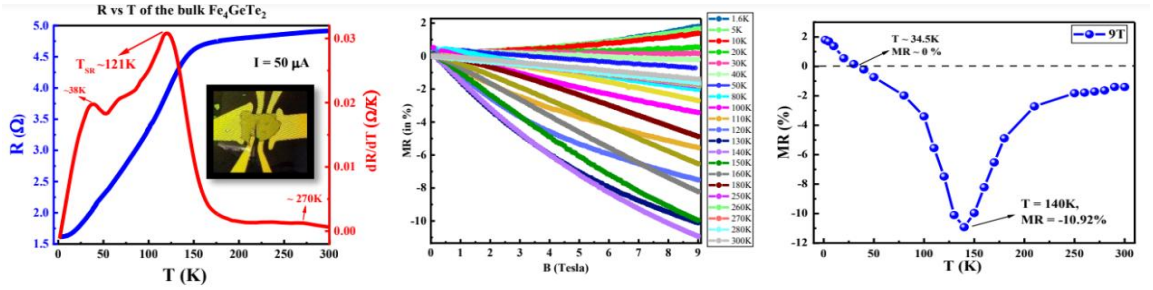
The discovery of two-dimensional (2D) van der Waals ferromagnet has opened up a new vista for investigating low dimensional magnetism as well as for the development of potential 2D spintronic devices. Here, we investigated the AHE mechanisms in a multi-layer Hall bar device of Fe_4GeTe_2 (F4GT) sample, which is discovered recently[1]. The temperature-dependent four-terminal resistance of the exfoliated bulk F4GT sample exhibits metallic behaviour and from the derivative curve (dR/dT), we obtain three transitions, a ferromagnetic transition: TC ~ 270K, spin re-orientation transition: TSR ~ 121K and a new anomaly: T ~ 38K, not reported earlier. We have also obtained positive magnetoresistance (MR) upto temperature 33K (MR = 0) and then negative MR with increasing of temperature and a maximum large negative MR at around 140K, which is near to the spin re-orientation transition temperature (TSR). Additionally, we observed that, the types of the majority charge carriers are changing at 5K, 73K and 133K, associated with the spin-reorientation transition. The anomalous Hall effect (AHE) mechanisms in these 2D ferromagnets have not been yet investigated systematically. The analysis indicates that this AHE is mainly dominated by intrinsic Karplus–Luttinger (K-L) mechanism2 or the extrinsic side-jump mechanisms[3]. We also observed that in the anomalous Hall effect (AHE) curve, the hysteresis is maximum close to the TSR. Above TC, Hall resistivity increases linearly with field. These finding suggests that, the F4GT can be an excellent candidate for future spintronic applications.



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Boundary resetting driven transport in harmonic chain

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We study energy transport in ordered harmonic chain of N oscillators connected to two walls which undergo diffusive dynamics with stochastic resetting. Intermittent resetting of the wall positions effectively emulates non-equilibrium reservoirs which exert temporally correlated forces on the boundary oscillators. These reservoirs are characterized by the diffusion constant and resetting rates of the walls. We compute the average energy current and the kinetic temperature profile exactly. Despite the uniform nature of the latter in the bulk, the system remains different from a harmonic chain driven by thermal reservoirs at the two ends. This is illustrated by numerically measuring the local velocity and current distributions.For any finite chain, the velocity distribution remains non-gaussian, as evidenced by a non-zero bulk kurtosis which decays ~ 1/N. Moreover, the current distribution also remains quantitatively different than the thermally driven case.

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Theoretical and Experimental study of Universal Ammonia Gas Sensing by Family of Lead Halide Perovskites ABX_3 (A= CH_3NH_3, $CH(NH_2)_2$, B=Pb, X=Br, I)

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In this poster presentation I will show gas sensing mechianism of ammonia by ABX 3 (A=CH 3 NH 3 (MA)/CH(NH 2) 2 (FA) ,B=Pb ,X=Br/I) lead halide perovskite with the aid of Molecular dynamics simulation results. It is experimentally observed that lead halide perovskite decomposes to corresponding lead halide with the presence of ammonia gas. It is also observed that for a fixed ammonia gas concentration, sensitivity of lead halide perovskite is MAPI>MAPB>FAPI respectively and sensitivity decreases with increasing temperature. These observations are corroborated by theory.

Designing oxide heterostructure with improved physical properties: A case study of the SIO/LCO ($SrIrO_3$/$LaCoO_3$) heterostructure

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Developing new heterostructures with improved physical properties is always a challenging task for both the experimentalist and theorist. Still, people are interested because of the emerging phases like two-dimensional free electron gas (2DEG), superconductivity, etc., that occur at the interface between two perovskite oxides. By experimenting with the charge, spin, orbital, and structural degrees of freedom, it creates the possibility of tunable physical properties. Recently, there has been a growing interest in 5d transition metal oxide, which shows new and exciting quantum phenomena due to its strong spin orbit coupling and weak electron-electron correlation effect. As a result, in general, ferromagnetic order is not possible in this type of 5d perovskite oxide. For example, $SrIrO_3$ (SIO) belongs to this category, and it is a paramagnetic semi-metal in its bulk orthorhombic (Pbnm) structure. We investigated a number of pseudo-tetragonal [$(SIO)_{m.5}$/$(LCO)_{n.5}$] (m=5, n= 4,5, 6) heterostructures in superlattice geometry using $SrTiO_3$ (STO) as a substrate in this study. And we have shown that structural modifications and the exchange interaction with the 3d transition metal Cobalt (Co) from the LCO block can stabilise ferromagnetic order in SIO. And as we know, SIO is a well-known topolgical semimetal in its orthorhombic structure. So we focused on its topological behavior, specifically whether proximity-induced ferromagnetism retains its topological behaviour or not.

Nanoplatelets of CdSe - Why do they form?

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CdS, CdSe are semiconductors which favour three-dimensional structures and occur in either the zinc-blende or the wurtzite phase. Recent advances have allowed for the formation of nanoplatelets of these materials which are just a few monolayers thick [1]. Although these are grown by colloidal chemistry methods, one finds an extremely narrow full width at half maximum associated with their photoluminescence spectra. The thickness are also found to range from 4 to 11 layers. This level of precision in the growth allows one to examine quantum well physics in the absence of a substrate. The reasons allowing for nanoplatelet formation as well as the evolution of the electronic structure would be presented.

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High Responsivity UV-Visible Broadband Phototransistor Based on Graphene – WS_2 Heterostructure

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Recent progress in the synthesis of highly stable, eco-friendly, cost-effective transition metal-dichalcogenides (TMDC) quantum dots[1] (QDs) with their broadband absorption spectrum and wavelength selectivity features have led to their increasing use in broadband photodetectors. With the solution-based processing, we demonstrate a super large (~0.75 mm^2), UV-Vis broadband (365-633 nm), phototransistor made of WS 2 QDs decorated CVD graphene as active channel with extraordinary stability and durability in ambient condition (without any degradation of photocurrent till 4 months after fabrication). Here, colloidal 0D WS 2 -QDs are used as the photo absorbing material and graphene acts as the conducting channel. A high photoresponsivity (3.1 × 10 2 A/W), higher detectivity (2.2×10 12 Jones) and low noise equivalent power (4×10 -14 W/Hz 0.5) are obtained at a low bias voltage (V ds = 1V) at an illumination of 365 nm with an optical power as low as 0.8 µW/cm 2 , which can further be tuned by modulating the gate bias. While comparing the photocurrent between two different morphologies of WS 2 (QDs and 2D nanosheets), a significant enhancement of photocurrent is observed in case of QDs based device. Our work reveals a strategy towards making a scalable, cost-effective, highly performing hybrid two-dimensional (2D/0D) photo detector with graphene-WS 2 QDs, paving the way towards the next generation optoelectronic applications [2] .

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Machine Learning approach to study quantum phases of a frustrated one dimensional spin-1/2 system

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Frustration driven quantum fluctuation leads to many exotic phases in the ground state and studyof these quantum phase transitions is one of the most challenging areas of research in condensed matter physics. Here, a frustrated Heisenberg J_1-J_2model of spin-1/2 chain with nearest exchange interaction J_1 and next nearest exchange interaction J_2 is studied using the principal componentanalysis (PCA) which is an unsupervised machine learning technique. In this method most probable spin configurations (MPSC) of ground-state (GS) and first excited state (FES) for different J_2/J_1 are used as the input in PCA to construct the co-variance matrix. The 'quantified principal component' of the largest eigenvalue of co-variance matrix $p_1(J_2/J_1)$ is calculated and it is shown that the nature and variation of $p_1(J_2/J_1)$ can accurately predict the phase transitions and degeneracies in the GS. The $p_1(J_2/J_1)$ calculated from the MPSC of GS can only exhibit the signature of degeneracies inthe GS, whereas,$p_1(J_2/J_1)$ calculated from MPSC of FES captures the gapless spin liquid (GSL)-dimer phase transition as well as all the degeneracies of the model system. We show that jump in $p_1(J_2/J_1)$ of FES at $J_2/J_1\approx0.241$, indicates the GSL-dimer phase transition, whereas its kinks give the signature of the GS degeneracies. The scatter plot of first two principal components of FES shows distinct band formation for different phases.

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p-$ZnCo_2O_4$/n-ZnO Nano-heterojunction Photoanode for Photoelectrochemical Water Splitting

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In this work, p-$ZnCo_2O_4$/n-ZnO nano-heterojunction photoanode was synthesized via simple growth techniques such as chemical bath deposition and electrodeposition. The so prepared photoanode displayed superior solar light absorption. The type-II analogous band alignment between p-$ZnCo_2O_4$ and n-ZnO resulted in decreased photo-generated charge carrier recombination hence better charge separation and transport. p-$ZnCo_2O_4$ was also observed to act as Oxygen Evolution Reaction (OER) catalyst, boosting charge transfer at the electrode/electrolyte interface. Hence we report an overall better performing photoanode due to increased light harvesting capabilities, better charge separation and improved OER kinetics, as compared to pristine ZnO nanorods.

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Equivalence principle and HBAR entropy of an atom falling into a quantum corrected black hole

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In this work, we have investigated the phenomenon of acceleration radiation exhibited by an atom falling into a quantum corrected Schwarzschild black hole. We observe that the excitation probability of an atom with the simultaneous emission of a photon satisfies the equivalence principle when we compare it to the excitation probability of a mirror accelerating with respect to an atom. We also demonstrate the validity of the equivalence principle for a generic black hole geometry. Then we calculate the horizon brightened acceleration radiation entropy for this quantum corrected black hole geometry. We observe that the horizon brightened acceleration radiation entropy has a form identical to that of Bekenstein-Hawking black hole entropy along with universal quantum gravity corrections.

References

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Role of Spin Transport on Ultrafast Demagnetization in β-Ta/$Co_{20}Fe_{60}B_{20}$ Bilayers

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Femtosecond laser pulse has been widely used for the manipulation of magnetization dynamics in an extremely fast and energy-efficient manner. Interaction of such laser pulse with magnetic material in saturated magnetization conditions leads to an instantaneous magnetization quenching within sub to few hundred femtoseconds, named ultrafast demagnetization. However, its underlying microscopic mechanism in nonmagnet (NM)/ferromagnet (FM) heterostructure involving strong spin-orbit coupling is still in its morning. We have investigated ultrafast magnetization dynamics in β-Ta/CoFeB/SiO_2 heterostructure using all-optical time-resolved magneto-optical Kerr effect magnetometry. We have established a linear relationship between the ultrafast demagnetization rate and Gilbert damping unfolding the dominant mechanism of spin pumping behind both the demagnetization and the damping. For the higher thickness regime (≥ 7 nm) of β-Ta, we have found that the spin accumulation coefficient is approximately 0.24 which is 1.8 times smaller than its value in the lower thickness regime (< 7 nm). This systematic investigation of magnetization dynamics in technologically pertinent heterostructures as a function of both the NM and FM thickness will add important knowledge to the development of ultrafast spin orbitronic devices having a wide range of functionalities.

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Observation of Imbert–Fedorov shift in monolayer MoS_2 via quantum weak measurement

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The basic optical phenomena of reflection and refraction of light at a plane dielectric interface are generally governed by Fresnel formulas and Snell's laws following the geometrical optics picture of light evolution. Unlike plane waves, a real optical beam with a finite transverse extent can undergo longitudinal (in the plane of incidence) as well as transverse (out of the plane of incidence) shifts which are known as Goos Hänchen (GH) and Imbert Fedorov (IF) shifts, respectively [1, 2, 3].Here, we are focusing only the Imbert Fedorov (IF) shifts which originates due to conservation of total angular momentum of light beam, including its intrinsic spin part along with the orbital angular momentum [3]. As these optical beam shifts are exceedingly small, the measurement of shifts is a massive challenge [4]. Quantum weak measurement technique [5, 6] is a precise and promising method among the available techniques of measuring optical beam shifts due to its simplicity and large amplification of the shift values. Though weak measurement method has been invented in the context of quantum mechanics, it is widely applicable in the framework of classical optics as well. In the optical analog of the quantum weak measurement theory [1], we need to consider two basic things. Firstly, in addition to preparation of a given system in a definite quantum state(pre-selection), we have to post-select the final state. Secondly, the interaction should be weak enough. By suitably post-selecting the final state nearly orthogonal to the initial state, amplification of the beam shift can be achieved. There has been a burgeoning research interest on two dimensional (2D) materials (graphene, TMDCs etc.) due to their unique optical, electrical, and chemical properties. MoS_2 is one of the widely studied TMDCs. Hence, We report the experimental evidence of the Imbert–Fedorov (IF) shift in monolayer MoS_2 for a fundamental Gaussian beam. Using Jones vector formalism, we have shown a novel, to the best of our knowledge, pathway to apply the quantum weak measurement technique for easy and accurate determination of the IF shift. We have revealed the dependence of IF shift over a large range of angles of incidence along with the mode of polarization of the incident light.Our experimental findings via the weak value amplification scheme are in good agreement with the theoretical analysis. The present method is a general one and can also be implemented for other materials to observe such tiny transverse shifts.

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High-resolution ro-vibrational spectral analysis of dideutero-methane isotopomer ($^{12}CH_2D_2$) in the $\nu_9(B_2)$ fundamental band

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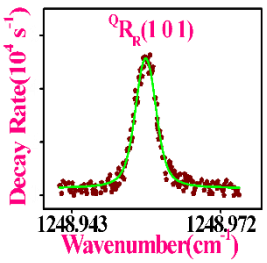
Dideutero-methane ($^{12}CH_2D_2$) is the only asymmetric-top isotopomer among all the methane isotopomers. In this work, the fine ro-vibrational gas-phase spectra of $^{12}CH_2D_2$ isotopomer in the a-type ν_9 (B_2-symmetry) fundamental band was reported, near 7.8 µm using an ultra-sensitive cavity ring-down spectroscopy (CRDS) instrument coupled a high-resolution external-cavity quantum cascade laser (EC-QCL) in the mid-infrared spectral region. Gaussian 16 and PGOPHER were used to calculate the relevant spectroscopic parameters of $^{12}CH_2D_2$ and subsequently done simulation for precise assignments of the fine ro-vibrational lines of $^{12}CH_2D_2$. Further, the pressure broadening dynamics of $^{12}CH_2D_2$ isotopomer were performed with various foreign gases and the pressure broadening coefficients, γi in cm-1 atm-1 [i = He, Ar, N_2, Hydrogen mixture(H_2+N_2) and zero air] of various transition lines of $^{12}CH_2D_2$ were accurately determined with respect to each perturbing gas. The new spectroscopic data are a significant advance over the earlier works and will provide a new window for better understanding of the doubly-deuterated methane structure and its vibrational dynamics.



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Spectroscopic study of [KSF2015] 1381-19L: A high temperature WC9-type star

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TWolf Rayet (WR) stars are a class of Population I-type massive stars known for their high temperatures and luminosities. WR stars are predicted to have evolved from the O-type Main sequence stars (M>25M⊙) due to a combined effect of extreme mass loss and rotational mixing. Although being about 1% of the total galactic population, these stars are considered to be one of the major sources for chemical and mechanical feedback to its surroundings and thus have a huge impact towards galactic evolution and also provide necessary habitat for young star formations. Spectroscopically WR stars are identified from the presence of strong & broad emission lines of dominant heavier alpha elements: WN (He & N), WC (He & C) & WO (C & O). These subtypes are further classified on the basis of line strength ratios of various ionization states of the most abundant heavier element. It is considered that the WC-type stars generate from the WN-type when the surface carbon composition exceeds 20 percent and He-burning starts at the core. WC9 (a WC-Late type) stars are generally claimed to have the least luminosity and temperature and also have much slower stellar winds in comparison to the earlier subtypes of the WC sequence. From our long term ground based observations using the 2m-Himalayan Chandra Telescope, we have obtained Optical/Near-IR spectra of several objects. From the line profile analysis using SPECTOOL of the reduced and calibrated optical spectra of these objects we have obtained significant evidence of fast stellar winds in case of [KSF2015] 1381-19L (WC9-type). Using the PoWR stellar atmospheric model grids, we have further obtained the best fitting model spectrum and consequently derived the physical and chemical properties of this object. From our study, we have found the object to be much hotter (70,800K) and luminous (105.578L⊙); and with high wind terminal velocities (2000kms-1) in comparison to the other stars belonging to the WC9 subtype. Also, from the Geneva 1D stellar evolutionary models database, we have retrieved the best fitting evolutionary track for the object. The estimated physical parameters from the derived evolutionary model were found to be very well comparable with the same that were obtained from the spectroscopic data modelling of the object.

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Nonclassical temporal correlation powers quantum random access codes

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We explore the fundamental origin of the quantum advantage behind random access code. We propose new temporal inequalities compatible with noninvasive-realist models and show that any non-zero quantum advantage of n bits encoded to 1-bit random access code in presence of shared randomness is equivalent to the violation of the corresponding temporal inequality. As an immediate consequence of this connection we also prove that maximal success probability of n bits encoded to 1-bit random access code can be obtained when the maximal violation of the corresponding inequality is achieved. We then show that any non-zero quantum advantage of n bits encoded to 1-bit random access code, or in other words, any non-zero violation of the corresponding temporal inequality can certify genuine randomness.

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