BOSE FEST 2021

(An Annual Celebration of Science)

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Abstracts e-Book

Programme Schedule

Sl. No.	Name	Department	Title	Date	Time
DAY 1 : 03/08/2021				
	Inauguration				10:15
1	Abhinandan Das	CBMS	An insilico approach to validate anti-diabetic drugs for Alzheimer's disease	03/08/2021	10.30
2	Achintya Low	CMPMS	Effect on Magnetic and Electronic transport properties of a Correlated Kagome Magnet Mn 3 Sn with Fe doping	03/08/2021	10.45
3	Aishwaryo Ghosh	CMPMS	Machine Learning in Material Sciences	03/08/2021	11.00
4	Akash Das	CBMS	Experimental Observation of Optical Beam Shifts for Gaussian Beams	03/08/2021	11.15
	BREAK 15 Minutes				
5	Amrit Kumar Mondal	CMPMS	Investigation of interfacial Dzyaloshinskii-Moriya interaction in monolayer graphene/CoFeB heterostructures	03/08/2021	11.45
6	Ankur Srivastav	TS	Holographic Superconductors	03/08/2021	12.00
7	Anupam Gorai	CMPMS	Multi-layered nano-hollow spheres : An efficient electromagnetic wave absorber	03/08/2021	12.15
8	Anwesha Chakraborty	TS	Forced Harmonic Oscillator in Non-commutative Space-time and Emergence of Geometrical Phase	03/08/2021	12.30
9	Bihalan Bhattacharya	A&C	Generating and detecting bound entanglement in two-qutrits using a family of indecomposable positive maps	03/08/2021	12.45
	LUNCH BREAK				
10	Biswajit Pabi	CMPMS	Probing Metal-Molecule Contact in molecular junction via transport measurements	03/08/2021	2.30
11	Biswajit Panda	CBMS	Ro-vibrational spectral features and pressure broadening dynamics of dideutero-methane (12CH2D2) in the v9(B2) fundamental band	03/08/2021	2.45
12	Debashish Paul	CBMS	Biomarker Hyaluronan on Colon Cancer Extracellular Vesicles: Biophysical Dissections	03/08/2021	3.00
13	Debayan Mondal	CMPMS	Shape Control of Emissive Properties of Mn-Doped CsPbBr3 Nanocrystals	03/08/2021	3.15
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14	Dhiraj Tapader	TS	Density relaxation in conserved Manna sandpiles	03/08/2021	3.45
15	Dhrubajyoti Maji	CBMS	Structure and Dynamics of Glucose/Ethylene Glycol Cryoprotectant System: A Molecular Dynamics Study	03/08/2021	4.00
16	Didhiti Bhattacharya	CMPMS	Flexible bio-mechanical energy harvesters with colossal piezoelectric output (~ 2.07 V/kPa) based on transition metal dichalcogenides-PVDF nanocomposites	03/08/2021	4.15
17	Dipanjan Mukherjee	CBMS	Host assisted molecular recognition by human serum albumin: Study of molecular recognition-controlled protein/drug mimic binding in a microfluidic channel	03/08/2021	4.30

			DAY 2 : 4/8/2021		
18	Dusmanta Patra	A&C	Galactic plane survey at 325 MHz using Giant Meterwave Radio Telescope	04/08/2021	10.30
19	Ipsita Basu	CBMS	A Computational study of electrostatics and dynamics of PCSK9 protein towards controlling interactions with LDLR	04/08/2021	10.45
20	Jayanta Mondal	CBMS	Dielectric relaxation of a fully biodegradable glucose containing naturally abundant deep eutectic solvent: origin of timescales via experiment and molecular dynamics simulation.	04/08/2021	11.00
21	Kanchan Meena	CMPMS	Propagation Under the Barrier	04/08/2021	11.15
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22	Krishnendu Sinha	CBMS	Regulation of RhoA GTPase by Phosphorylation of RhoGDI	04/08/2021	11.45
23	Monalisa Chatterjee	CMPMS	Quantum phase diagram of ferromagnetically coupled Shustry-Sutherland Model	04/08/2021	12.00
24	Partha Nandi	TS	Evidence of a non-trivial Berry phase in lowest Landau levels	04/08/2021	12.15
25	Partha Pyne	CBMS	Alteration of water absorption in THz region traces the onset of fibrillation in proteins.	04/08/2021	12.30
26	Parushottam Majhi	CMPMS	Diffused metal-insulator transition in $NdNiO_3$ film grown on $BaTiO_3$: Likely evidence of electronic Griffiths phase	04/08/2021	12.45
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27	Prantik Nandi	AC	A physical explanation of soft-excess emission of Seyfert 1 AGNs	04/08/2021	2.30
28	Prasun Boyal	CMPMS	Topological insulators in the 1T' phase of MX_2 (M=Mo,W; X=S,Se,Te) revisited	04/08/2021	2.45
29	Premashis Kumar	CBMS	Thermodynamics of Chimera	04/08/2021	3.00
30	Rahul Karmakar	CBMS	Long ranged order in ligand capped nanoparticles in presenceof temperature difference	04/08/2021	3.15
31	Rituparna Mandal	TS	Cosmology in asymptotically safe quantum gravity	04/08/2021	3.30
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32	Samir Rom	CMPMS	A First-Principle Study of $SrIrO_3$/$LaCoO_3$ Perovskite Oxide n-type Interface	04/08/2021	4.00
33	Sasthi Charan Mandal	CBMS	Quantum chemical studies on chelation in nano-bio conjugate between ZnO nanoparticle and cellular energy carrier molecules, ATP, ADP and AMP	04/08/2021	4.15
34	Sayan Routh	CMPMS	Experimental Observation of Exchange Bias in Antiferromagnetic $Cr_{0.79}Se$ due to Itinerant Weak Ferromagnetism at Low-temperature	04/08/2021	4.30
35	Shantonu Mukherjee	TS	Flux attachment and fractional statistics from electron-vortex interaction	04/08/2021	4.45

			DAY 3 : 05/08/2021		
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37	Shiladitya Karmakar	CMPMS	Enhanced thermoelectric properties of double transition metal MXenes	05/08/2021	10.45
38	Shobhan Dev Mandal	TS	Effect of receptor clustering on E.coli chemotaxis: Sensing versus adaptation	05/08/2021	11.00
39	Shubhadip Moulick	CMPMS	Flicker noise in large area Graphene FET on lightly doped substrate	05/08/2021	11.15
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40	Shubhrasish Mukherjee	CMPMS	Gate tunable strong photoresponse from a few layered MoS_2 transistor	05/08/2021	11.45
41	Siddhartha Biswas	A&C	Studies of Pre-main sequence stars in Galactic star-forming regions	05/08/2021	12.00
42	Sk Imadul Islam	CBMS	Excited-state Proton Transfer in Reverse Micelles: Effect of Temperature and a Possible Interplay with Solvation	05/08/2021	12.15
43	Sk Saniur Rahaman	CMPMS	Quantum phases and thermodynamics of afrustrated spin- 1/2 ladder with alternateIsing–Heisenberg rung interactions	05/08/2021	12.30
44	Snehamoyee Hazra	CMPMS	Effect of Schottky barrier height and morphology of nanostructured PZT on the output power density of piezoelectric nanogenerators	05/08/2021	12.45
			LUNCH BREAK		
45	Soumya Chakrabarti	TS	Cosmic acceleration in an extended Brans-Dicke-Higgs theory	05/08/2021	2.30
46	Subhajit Kar	A&C	Physical characteristics of Wolf Rayet Stars	05/08/2021	2.45
47	Sudip Majumder	CMPMS	Strong Magnon-Magnon Coupling in Two-Dimensional Diamond Shaped Ferromagnetic Nanodots Array	05/08/2021	3.00
48	Surya Narayan Panda	CMPMS	Crystal Structure Dependent Interfacial Spin Transparency in W/CoFeB Thin Films	05/08/2021	3.15
			BREAK 15 Minutes		
49	Susmita Mondal	CBMS	Synthesis and spectroscopic characterization of a target specific nano-hybrid for redox- buffering in cellular milieu	05/08/2021	3.45
50	Swarnali Hait	CMPMS	Magnetoelectric properties of Ba and Y co-doped Bismuth Ferrite Nanoparticles	05/08/2021	4.00
51	Tanmoy Chakraborty	TS	Transport and fluctuations in mass aggregation processes: mobility- driven clustering	05/08/2021	4.15

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An insilico approach to validate anti-diabetic drugs for Alzheimer's disease

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Alzheimer's disease continues to be a potent matter of concern amidst our respected senior clan. It is a major cause of dementia that affects normal lifestyle of the patient. Novel methods to alleviate the pain associated with the disease is still an area of active research. One such method involves targeting the enzyme Acetyl cholinesterase that is majorly responsible for the symptoms associated with the disease. There has been a plethora of attempts made to block the activity of the enzyme by different inhibitor molecules that helped patients see the light of relief. Recently, a very interesting link has been highlighted that happens to draw a relation between another potent disease of concern, Type II Diabetes Mellitus and Alzheimer's disease that further unleashes an interesting scope for the scientific community to uncover whether repurposing of already anti-diabetic drugs can open new horizons for treatment of Alzheimer's disease.

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Effect on Magnetic and Electronic transport properties of a Correlated Kagome Magnet Mn$_3$Sn with Fe doping

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Mn$_3$Sn is a well-known topological Weyl semi-metal which has a non-collinear magnetic structure. In this system, Mn atoms are arranged in a Kagome or a star lattice and with the introduction of antiferromagnetic interactions among the Mn atoms make the system magnetically frustrated. Such a frustrated magnetic system stages many interesting phenomena such as Quantum Spin Liquid and/or Magnetic Topological properties. In this presentation, we discuss our research work on the effect of Fe atom doping at the Mn site. We have seen dramatic changes in the electrical and magnetic properties of Mn$_3$Sn with Fe doping as small as 0.7%. Further increase of Fe doping concentration in Mn3Sn, the anisotropic magnetic behaviour is enhanced. Moreover with Fe doping, we witnessed a metal to semiconductor transition.

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Machine Learning in Material Sciences

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In recent times the screening of materials with definite properties of choice and discovery of new materials has become a topic of interest to the community. Machine learning (ML) has widely been employed in such problems of this field to enhance the pace and efficiency of the process by making statistical estimations and bringing the focus to the useful region of the configurational space. A high throughput machine learning model can detect patterns (linear or non-linear) by mining data retrieved from literature and the ever-expanding repositories of materials properties. In this talk, I try to present briefly the idea of Machine learning in general, and its necessity in the field of present materials science research through the discussion of two examples. The first work employs Machine learning to classify binary semiconductor heterostructures[1] built on features characterizing the constituent semiconductors. In the second example, rare earth lean novel permanent magnet candidates are suggested using a combined ML and ab-initio approach[2].

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Experimental Observation of Optical Beam Shifts for Gaussian Beams

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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]. Over the years, the phenomena of GH & IF shifts have found enormous applications in the area of plasmonics, photonics, metamaterials, chiral materials [3, 5], etc. As these optical beam shifts are exceedingly small, the measurement of shifts is a massive challenge [3]. Quantum weak measurement technique [4, 5] 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 can be achieved comfortably.

In the present work, we have developed a quantum weak measurement setup for the measurement of the optical beam shifts. Lately, there has also been a burgeoning research interest on two dimensional (2D) materials (graphene, TMDCs etc.) due to their unique optical, electrical, and chemical properties. MoS2 is one of the widely studied TMDCs. Hence, we have studied the reflection of a Gaussian light beam (He-Ne laser, 632.8nm) reflected from a prism both in the presence and in the absence of MoS2. We have presented the behavior of the spatial shifts with a change in the post-selection states gradually from the orthogonal position. The nature of the horizontal and vertical shift of the beam with the angular deviation from the orthogonal position has been discussed and the validity of the AAV approximations has been verified in case of the optical weak measurement setup. Furthermore, we have also examined the variation of GH & IF shifts with different angle of incidences in presence of monolayer MoS2 as well as in its absence. Subsequently, we have discussed the special features of the shifts for monolayer MoS2 signifying differences from other 2D materials. The results have also been compared with the previous theoretical results to infer about the region of the applicability of the AAV approximations. We believe the present work to be of fundamental significance and may provide a new avenue toward plenty of interesting applications in the optical sensor and device industry.

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Investigation of interfacial Dzyaloshinskii-Moriya interaction in monolayer graphene/CoFeB heterostructures

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The quest for advanced spin-based computational technology began a few decades ago as the present charge based technology would cease to fufill the ever-increasing demands from mankind in terms of miniaturization, speed and energy consumption. In field of graphene spintronics [1], promises to use graphene instead of high atomic number heavy metal because of its unique characterization. The interefacial Dzyaloshinskii-Moriya(iDMI) is one of essential quantity to stabilized chiral spin textures and magnetic skyrmion is one of them. In this work, we have studied the defect induced iDMI and gilbert damping parameter on chemical vapour deposited monolayer graphene-ferromagnetic (MLG/CoFeB) heterostructure using Brillouin Light Scattering spectroscopy. We systematically vary CoFeB thinkness from 1.5nm to 6nm. We find, a remarkable enhancement of iDMI and extrinsic gilbert damping in case of CoFeB(1.5nm)/MLG sample. From the variation of iDMI and gilbert damping parameter with CoFeB thickness, we extracted two purely interfacial coefficient such as surface DMI and spin mixing conductance parameter originated from the spin-orbit couping (SOC) at the interface of MLG and CoFeB. Additional observation of raman spectroscopy indicates that the defect peak intensity is increases with decrease of CoFeB thickness. The correlation of iDMI and defect peak intersity with CoFeB thickness suggested that extrinsic SOC in graphene layer is controlled by defect [2,3]. This work pave the way for control SOC in two-dimensional system based spin-orbitronics.

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Holographic Superconductors

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Holography, popularly known as Gauge/Gravity duality, is the statement of an equivalence between theories of gravity in (d+1)-dimensional space-time and strongly interacting quantum field theories at its d-dimensional boundary. Utilizing holographic principle, a gravity dual model was proposed which mimicked some key properties of high-T_c superconductors [1]. Such models are known as Holographic Superconductors. In this talk, I shall present our work related to such a holographic model. We have investigated, in the probe limit, s-wave holographic superconductors in rotating AdS_{3+1} space-time using the matching method as well as the Stürm- Liouville eigenvalue approach. We have calculated the critical temperature and the condensation operator. The results obtained share the same features as found numerically [2]. We observe that the rotation parameter of the black hole affects the critical temperature and the condensation operator in a non-trivial way [3]. We have also worked on p-wave holographic superconductor model [4]. In this model, we have calculated the conductivity following a self- consistent approach and have explicitly shown that the DC conductivity indeed diverges.

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Multi-layered nano-hollow spheres: An efficient electromagnetic wave absorber

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Ferrite nano-hollow spheres (NHS) have great significance to improve electromagnetic (EM) wave absorption performance. Herein, the deposition of dielectric SiO_2 and ferrimagnetic $CoFe_2O_4$ (CFO) layers on $MnFe_2O_4$ (MnFO) NHS are found as an effective strategy to enhance EM wave attenuation. EM wave absorption properties of as-synthesized bare and bi-layered samples are investigated within a widely-used frequency range of 1–17 GHz. MnFO@CFO bi-layered NHSs exhibit an excellent reflection loss (RL) of −47.0 dB at only 20 wt% filler content with an effective broad bandwidth (BW) of ~2.2 GHz (frequency region for RL < −10 dB). The attenuation constant is observed to increase from 191.6 Np m^{-1} to 457.8 Np m^{-1} for bare MnFO and MnFO@CFO NHSs respectively. Larger interfacial area, additional pairs of dipole, higher magnetic anisotropy, internal reflections and scattering from NHSs are responsible for superior absorption properties of MnFO@CFO NHSs. Moreover, the best impedance matching, $|Z_{in}/Z_0|$ ~ 1, promotes the optimum RL in MnFO@CFO at 5.96 GHz. MnFO@SiO_2 bi-layered NHSs result in a sufficiently high RL ~ −30.0 dB with a composite absorber of a thickness of only 3 mm. Analysis from the $\lambda/4$ model for best matching thickness (t_m) displays a good agreement between experimental and simulated tm values. This study demonstrates optimized MnFO@CFO NHS as a highly promising low-cost and lightweight EM wave absorber suitable for practical high-frequency applications.

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BOSE FEST 2021

Forced Harmonic Oscillator in Non-commutative Space-time and Emergence of Geometrical Phase

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We show the emergence of Berry phase in a forced harmonic oscillator system placed in a quantum space-time. An effective commutative description of the system gives a time dependent generalized harmonic oscillator system with perturbation linear in position and momentum. The system is then diagonalised to get a generalized harmonic oscillator and then its adiabatic evolution over time-period T is studied in Heisenberg picture to compute the expression of geometrical phase-shift.

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Generating and detecting bound entanglement in two-qutrits using a family of indecomposable positive maps

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The problem of bound entanglement detection is a challenging aspect of quantum informa- tion theory for higher dimensional systems. Here, we propose an indecomposable positive map for two-qutrit systems, which is shown to detect a class of positive partial transposed (PPT) states. A corresponding witness operator is constructed and shown to be weakly op- timal and locally implementable. Further, we perform a structural physical approximation of the indecomposable map to make it a completely positive one, and find a new PPT- entangled state which is not detectable by certain other well-known entanglement detection criteria.

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Probing Metal-Molecule Contact in molecular junction via transport measurements

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Understanding the formation of metal-molecule contact at the microscopic level is the key towards controlling and manipulating atomic scale devices. The formation of contacts between two metallic surfaces often involves a jump from tunneling to the contact regime. It was shown that the local electrode configuration and material composition before contact primarily determine the presence or absence of a jump [1]. In the case of molecular junctions, however, jump to contact is rarely observed mostly due to the fact that molecules tend to lay flat on the surface after the breaking process [2]. Employing two isomers of bipyridine: 4, 4' bipyridine and 2, 2' bipyridine between gold electrodes, here, we investigate the formation of metal-molecule bond by studying charge transport through single molecular junctions using mechanically controlled break junction technique (MCBJ) at room temperature. In both cases, we observe formation of molecular junction in the breaking traces, consistent with previous reports [3]. A closer look at the closing traces reveals that 4, 4' bipyridine forms molecular junctions via a conductance jump from the tunnelling regime, whereas, 2, 2' bipyridine does not form a clear molecular junction showing molecular assisted tunnelling till the formation of metallic contact. Through statistical analysis of the experimental data, along with, molecular dynamics and first-principles calculations, we establish that contact formation is strongly connected with the molecular structure as well as how the junction is broken during breaking process, providing important insights for using a single-molecule in an electronic device.

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Ro-vibrational spectral features and pressure broadening dynamics of dideutero- methane (^{12}CH2D2) in the ν9(B2) fundamental band

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Dideutero-methane ^{12}CH2D2 is unique among all the methane isotopomers because of its asymmetric-top nature (1). The study of high-resolution rovibrational spectral features and dynamics of ^{12}CH2D2 is therefore specially interesting (2). Here, we first report the fine ro- vibrational gas-phase spectra of ^{12}CH2D2 isotopomer in the *a*-type ν9 (B2-symmetry) fundamental band near 7.8 μm using a high-resolution external-cavity quantum cascade laser (EC-QCL) equipped with an ultra-sensitive cavity ring-down spectroscopy (CRDS) instrument in the mid-infrared spectral region. We utilized Gaussian 16 to calculate the relevant spectroscopic parameters of ^{12}CH2D2 and subsequently performed the PGOPHER simulation for precise assignments of the fine ro-vibrational lines of ^{12}CH2D2. Further, we conducted the pressure broadening dynamics of ^{12}CH2D2 isotopomer with various foreign gases and accurately determined the pressure broadening coefficients, $\square_i$ in cm^{-1} atm^{-1} [i = He, Ar, N2, Hydrogen mixture(H2+N2) and zero air] of various transition lines of ^{12}CH2D2 with respect to each perturbing gas. Finally, the absolute line intensities, transition dipole moments of ^{12}CH2D2 spectral lines and the *J*-dependence of spectral features are also reported. 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.
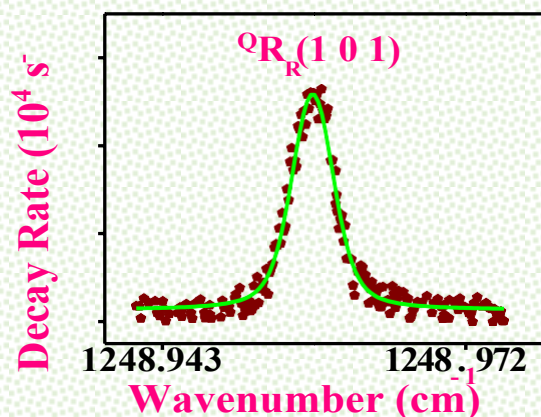
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Biomarker Hyaluronan on Colon Cancer Extracellular Vesicles: Biophysical Dissections

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Extracellular vesicles (EVs), naturally occurring nanosized vesicles secreted from cells, are essential for intercellular communication. They carry unique biomolecules on the surface or interior that are of great interest as biomarkers for various pathological conditions such as cancer. In this work, we use high-resolution atomic force microscopy (AFM) and spectroscopy (AFS) techniques to demonstrate differences between EVs derived from colon cancer cells and colon epithelial cells at the single vesicle level. We show that both EVs display an EV marker, CD9, while EVs derived from the cancer cells are slightly higher in density. Hyaluronan (HA) is a nonsulfated glycosaminoglycan linked to malignant tumor growth according to recent reports (1). Interestingly, at the single-vesicle level, colon cancer EVs exhibit significantly increased HA surface densities compared to the normal EVs. Spectroscopic measurements such as Fourier transform infrared (FTIR), circular dichroism (CD), and Raman spectroscopy unequivocally support the AFM and AFS measurements (2). Next, we show that, colon cancer EVs display intrinsic mechanical characteristics unlike the normal colon epithelial EVs. We measure the contour length of HA polymers at single vesicle level which corresponds to low molecular weight HA (<200 KDa) exploiting HA interactions with Hyaluronan Binding Protein (HABP) by AFM based Single Molecule Force Spectroscopy (SMFS). Our data reveal that colon cancer cell derived HA decorated EVs are significantly elastic in comparison to the normal colon cell EVs which is linked to HA abundance on EV surface (3). We envision this assay could potentially act as a biosensor for early detection of colon cancer.

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BOSE FEST 2021

Shape Control of Emissive Properties of Mn-Doped CsPbBr3 Nanocrystals

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II-VI semiconductor nanocrystals have been extensively studied by soft chemistry method. In addition to a control on the size, one has found modulation of the shape under various experimental conditions. This increases the surface area for similar sized objects and facilitates use in various applications such as catalysis where the increased surface area would imply more active sites. While experiments on hybrid perovskites have found only cubic facets, recently it was shown for $CsPbX_3$ (X= Br,Cl) under certain experimental conditions [1] one found a faceted polyhedron which could be transformed into a hexapod. In this talk I will present our recent work in which we have examined Mn doping into the low energy facets. Doping into different facets is found to lead to emissive facets in some instances, and non-emissive facets in other instances. These studies help us explain how the same dopant atom in different shapes of the same material could have different emissive properties.

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BOSE FEST 2021

Density relaxation in conserved Manna sandpiles

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We study relaxation of long-wavelength density per- turbations in one dimensional conserved Manna sand- pile. Far from criticality where correlation length ξ is finite, relaxation of density profiles having wave num- bers k $\to$ 0 is diffusive, with relaxation time τ_R k-2/D with D being the density-dependent bulk-diffusion coefficient. Near criticality with $k\xi \ll 1$, the bulk diffu- sivity diverges and the transport becomes anomalous; accordingly, the relaxation time varies as $\tau_R \sim k^{-z}$, with the dynamical exponent $z = 2 - (1 - \beta)/\nu_\perp < 2$, where β is the critical order-parameter exponent and and $\nu_\perp$ is the critical correlation-length exponent. Re- laxation of initially localized density profiles on infinite critical background exhibits a self-similar structure.

In this case, the asymptotic scaling form of the time- dependent density profile is analytically calculated: we find that, at long times t, the width σ of the density perturbation grows anomalously, i.e., $\sigma \sim t^w$, with the growth exponent $\omega = 1/(1 + \beta) > 1/2$. In all cases, theoretical predictions are in reasonably good agree- ment with simulations.

BOSE FEST 2021

Structure and Dynamics of Glucose/Ethylene Glycol Cryoprotectant System: A Molecular Dynamics Study

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Cryoprotectants are a unique class of compounds, essential for surviving and thriving of living bodies in harsh, cold conditions. The mechanism of interactions between cryoprotectants and biomolecules are an interesting area to explore. The most effective cryoprotectants are often sugars and polyhydroxy alcohols. In line with this we are investigating the structure and dynamics of a mixture of potential cryoprotectants: glucose and ethylene glycol. We have performed molecular dynamics simulation to get insight of the properties in molecular level. We have taken pure ethylene glycol and three ethylene glycol/glucose mixtures containing glucose weight percentage 20, 30 and 40 at 298 K. With increasing glucose content in mixtures, the interactions among ethylene glycol molecules becomes weak and rather they tend to interact with glucose molecules. Structural changes are monitored via radial distribution function (RDF), radial angular distribution function (RADF) and static structure factor. Both reorientational dipolar dynamics and hydrogen bond dynamics get slower with increasing glucose concentration. Hydrogen bond population study reveals the affinity of interspecies and intraspecies hydrogen bonding. As glucose concentration increases ethylene glycol prefers to bind with more glucose molecules rather than itself. On the other hand, glucose molecules also prefer intraspecies H-bonding. This study is still going on and thorough analysis of obtained properties will help to comprehend the systems better.

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BOSE FEST 2021

Flexible bio-mechanical energy harvesters with colossal piezoelectric output (~ 2.07 V/kPa) based on transition metal dichalcogenides-PVDF nanocomposites

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A simple and scalable technique is reported to demonstrate self-poled, flexible and superior-performance piezoelectric nanogenerators by using chemically exfoliated layered MoS_2 nanosheets embedded in poly (vinylidene fluoride) PVDF polymers. These self-poled nanogenerators can produce an open-circuit voltage up to ~ 22 V, even with an application of a very low mechanical compression (~10.6 kPa) leading to an unprecedented piezoelectric output (2.07 V/kPa) using a two-dimensional material. On the other hand, in bending condition (~0.11% strain), the nanogenerator device generates ~ 2.5 V with a piezoelectric energy conversion efficiency of ~ 17.8%, which is capable to drive multiple commercial light emitting devices. The fabricated flexible self-poled MoS_2-PVDF nanogenerators have been used to harvest biomechanical energy from simple human activities (finger tapping, variation in movements of finger and wrist etc.) which offers an excellent power density of ~88.5 $\mu W/cm^2$ upon finger tapping (~3.1 kPa) and display a significant enhancement of performance over control PVDF devices. Our results open up the feasibility of using chemically exfoliated two-dimensional transition metal di-chalcogenides for the design and development of high-efficiency, portable energy harvesting devices.

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Host assisted molecular recognition by human serum albumin: Study of molecular recognition-controlled protein/drug mimic binding in a microfluidic channel

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Human serum albumin (HSA) plays a pivotal role in drug release from its delivery vehicles such as cyclodextrins (CDs) by binding to the drugs. Here molecular recognition and binding of a drug mimic (CD1) to HSA have been explored in a microfluidic channel when CD1 is encapsulated in β-cyclodextrin (βCD) and heptakis(2,3,6-tri-O-methyl)-β-cyclodextrin (TRIMEB), respectively, to investigate whether change of the host vehicle modulate the rate of drug binding to the serum protein. Molecular recognition of βCD encapsulated CD1 by HSA occurs by the conformational selection fit mechanism leading to rapid binding of CD1 to HSA ($k1 \sim 700$ s-11) when the βCD/CD1complex interacts with HSA. In contrary, HSA recognizes CD1 encapsulated in TRIMEB by an induced fit mechanism leading to a significantly slower binding rate ($k1 \sim 20.8$ s−1) of the drug mimic to the protein. Thus, molecular recognition controls the rate of HSA binding by CD1 which in turn modulates the rate of delivery of the drug mimic from its macrocyclic hosts. The remarkable change in the molecular recognition pathway of CD1 by HSA, upon change of the host from βCD to TRIMEB, originates from significantly different conformational flexibility of the host/drug mimic complexes.

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Galactic plane survey at 325 MHz using Giant Meterwave Radio Telescope

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We report 325 MHz observations of the Galactic plane using the Giant Metrewave Radio Telescope (GMRT) with an angular resolution of 13 arc-sec ×12 arc-sec. The observations were done along the Galactic plane between $53^{\circ} < l < 63^{\circ}$ and $|b| < 3^{\circ}$ with the main goal to catalogue all point and extended sources in the region and identify possible pulsar candidates, H II regions and variable radio sources. We have achieved a median noise of 1 mJy beam^{-1} . Twenty six hundred and twenty five radio sources are detected using 5σ limit where σ is the local RMS noise. We have cross- correlated sources detected in our survey with the NRAO VLA Sky Survey (NVSS) source catalogue at 1.4 GHz and the TIFR GMRT Sky Survey Alternative Data Release 1 (TGSS ADR1) catalogue at 150 MHz and calculated the two-point spectral index for these sources. We study the differential source counts and discuss the source population at different flux-density ranges. We found thirteen possible pulsar candidates. We also identified forty one candidate variable sources, which show more than 20% variation.

A Computational study of electrostatics and dynamics of PCSK9 protein towards controlling interactions with LDLR

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PCSK9 is the proprotein convertase (PC) subtilisin/Kexin type 9, which is known to be responsible for heart disease, associated with the raised level of the low-density lipoprotein (LDL)-cholesterol (LDL-C) (1). 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 membrane (2). 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 LDLR (3). 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 drugs 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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BOSE FEST 2021

Dielectric relaxation of a fully biodegradable glucose containing naturally abundant deep eutectic solvent: origin of timescales via experiment and molecular dynamics simulation

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Deep eutectic solvents (DESs)[1] are multicomponent mixtures having much lower melting temperature than the individual melting temperature of the components. This system is getting considerable attention in the field of research because of its potential to be replaced over conventional organic solvents. If the components of the DES are chosen carefully then it can be made biodegradable and environment friendly green solvent.

A new room temperature biodegradable DES composed of glucose, urea and water has been prepared[2] and its relaxation and dynamics has been explored via broadband dielectric relaxation spectroscopy in the frequency range combining two instruments: i) Impedance analyzer (20 Hz – 10 MHz) and ii) Network analyzer (200 MHz – 50 GHz). Temperature dependent dielectric measurement has been carried out for this DES in the mentioned frequency region. Simultaneous fits to the measured permittivity (ε') and loss (ε'') spectra of this DES in the temperature range $303 < T/K < 343$ requires a sum of five and or four debye processes with relaxation times spread over picosecond to nanosecond regime. In the low temperature region that is at 303K this system gives a five debye relaxation process with a long timescale of ~30 ns. The other temperatures measurements required four debye processes. Upon increasing temperature, the static dielectric constant gradually decreased as in the higher temperature the alignments of the dipoles are affected. The undetected dispersion remains to be $\varepsilon_\infty - n_D^2 \approx 4 - 5$ due to inaccessibility of the frequency window beyond 50 GHz. Fractional viscosity dependence has been observed for the longest dielectric (DR) time scale for this DES with a power value p = 0.7. Also, activation energy estimated from viscosity and average DR time scale support the fractional viscosity dependence. Molecular dynamics simulations of dielectric relaxation have been carried out in this DES in three different temperatures via employing OPLS-AA force field. Intraspecies interaction of glucose in the temperature of 303 K generate a time scale of 30 ns range, which may dictate the experimental finding. The remaining timescales of the experiment have been well understood by the inter and intra species interaction among urea, glucose and water.

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BOSE FEST 2021

Propagation under the Barrier

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Quantum mechanical tunneling of particles for energy less than the barrier is a magical phenomenon with no classical analogue or classical correspondence. It is not explained within the axioms of quantum mechanics. Wave packets cannot be constructed under the barrier and group velocity cannot be defined. Tunneling, though a physical reality, is shrouded in mystery. The tunneling particle can be observed on either side of the barrier but its state under the barrier has never been probed due to several problems related to quantum measurement. We show that there are ways to bypass these problems in mesoscopic systems and one can even derive an expression for the quantum mechanical current under the barrier. One can use mesoscopic phenomenon to subject the expression to several theoretical and experimental cross checks. A general scheme is developed to derive an expression for currents under the barrier for any arbitrary interaction and system.

For this we consider an ideal 1D quantum ring with Aharonov-Bohm flux Φ. The evanescent states are largely stable and robust against phase fluctuations. So we expect that devices operating in the evanescent regime can withstand the limitations of decoherence and dissipation.

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Regulation of RhoA GTPase by Phosphorylation of RhoGDI

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The guanine dissociation inhibitor (RhoGDI) plays a crucial role in the regulation of Rho GTPases. It acts as a negative regulator by blocking the activation of Rho GTPase from an inactive GDP-bound state.[1-4] Activation of Rho GTPase requires release of Rho GTPase from the GDI-bound complex. Experimental studies suggest phosphorylation of RhoGDI as a key post-translational modification for dissociation of the complex. There seems to be a "phosphorylation code" that controls the release of specific Rho GTPase from the complex. For instance phosphorylation at SER-101 and SER-174 by p21-activated kinase 1 leads to the release of Rac1[5] (but not RhoA). On the other hand, phosphorylation of SER-34[6] or SER-96[7] by protein kinase Cα (PKCα) selectively releases RhoA (but not Rac1 or cdc42).

We have performed atomistic molecular dynamics and metadynamics simulations of the wild-type and phosphorylated state of the RhoA-GDI complex and propose a molecular-interaction-based mechanistic model for the dissociation of the complex as an effect of phosphorylation. Due to phosphorylation of SER-34, the RMSD of GDI increases indicating a major structural change. Using residue-wise RMSF we have shown that the major structural changes are occurring in the polybasic region of RhoA and the N-terminal region of GDI. Also, the distance between the CYSG group of RhoA and the hydrophobic cavity of GDI has increased which indicates a weakening of interaction between RhoA and GDI. MM/PBSA calculation shows a significant decrease in binding energy between RhoA and GDI. Due to phosphorylation, the number of contacts between the PBR region of RhoA and N-terminal of GDI decreases leading to the decrease in binding energy between RhoA and GDI. Using hydrogen bond occupancy analysis and energetic perturbation analysis we propose a mechanistic model for the distant signal propagation from the site of phosphorylation to the PBR region and buried geranyl group in the form of rearrangements of hydrogen bonds and charge-charge interactions, which demonstrates the crucial role of electrostatic interactions in the allosteric response.

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Quantum phase diagram of ferromagnetically coupled Shustry Sutherland Model

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We study spin-1/2 distorted Shustry-Sutherland model with antiferromagnetic next- nearest neighbor interaction (J) and ferromagnetic nearest neighbor interactions with different values along the length and along the width, J_2 and J_1 respectively. This type of distorted structure has been observed in $(CuCl)LaNb_2O_7$ in which a noticeable distortion has been occurred in Cu-Cl bonds shown experimentally. We study this model with taking 4-leg geometry and extends this upto 8-leg geometry applying PBC along the width and OBC along the length. Finally, we construct the quantum phase diagram based on the nature of spin-spin correlations and magnetization using DMRG technique. Phase diagram consists of four phases, (i) stripe order along both X- and Y-directions, (ii) spiral order along both X- and Y- directions, (iii) formation of perfect dimer and (iv) ferromagnetic alignments of the spins. The main noticeable fact is that we are able to clearly show the existence of spiral order in the system which was predicted by Mean-field calculations in Furukawa et al. We calculate pitch angle in spiral order which is always between 0 and π. Spin-spin correlations follow exponencial decay which show very short range order exists in the system.

Evidence of a non-trivial Berry phase in lowest Landau levels

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Appearance of the geometric phase (Berry's phase) shift in the context of the generalized Landau system with additional time-dependent non-parabolic external potential is investigated, wherein the system Hamiltonian depends on a set of parameters which are slowly varying periodic functions of time. In Heisenberg picture, an exact expression for the geometric phase shift under adiabatic approximation is found.

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BOSE FEST 2021

Alteration of water absorption in THz region traces the onset of fibrillation in proteins

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Protein aggregation leads to the formation of amyloid fibrils, a key factor for many neurodegenerative diseases[1]. Fibrils are enriched with β sheet and thermodynamically the most stable state. Fibrillation pathway (native→ fibril) consists of three steps: lag phase, elongation phase and asymptotic phase. In spite a lot of studies are being carried out on protein aggregation, there is still illusion that which factor governs most for the transition of native protein to its aggregated (fibrillar) form. Earlier studies have concluded that conformational change of protein and protein-protein interaction is the governing factor for such transition, but whether protein hydration (nearby water of protein molecule) has any impact on protein aggregation is not explored experimentally. In this contribution we aim to explore the effect of protein associated hydration during the fibrillation process of a model protein bovine serum albumin (BSA) using terahertz (THz) frequency domain spectroscopy and correlate the change in protein hydration with the structural conformation (as obtained from the circular dichroism spectroscopy) of protein. We conclude that water dynamics changes systematically with protein conformational change as it experiences a hydrophobic environment during the initial protein unfolding process, followed by a release of bound water during oligomerization and finally the hydrophobic interior of the fibrillation process.
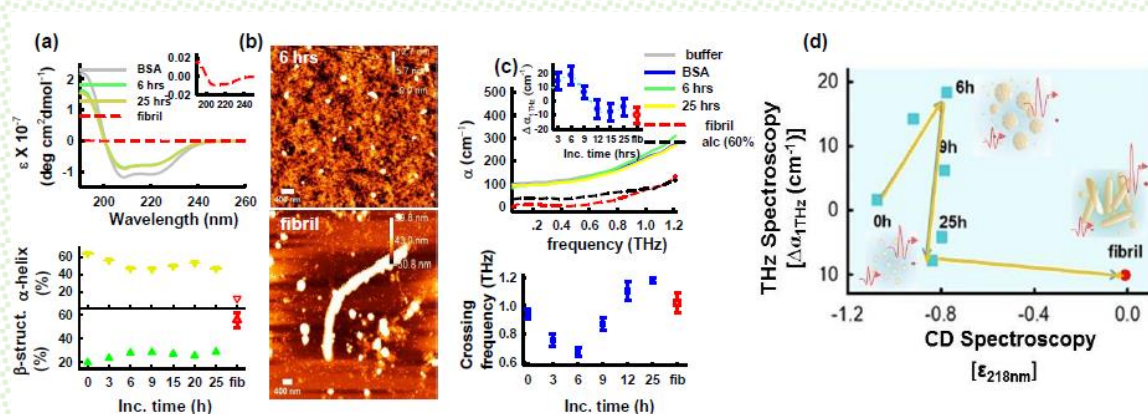
Fig. 1. (a) CD signal of BSA under different condition (upper panel) and α helix and β-structure of BSA oligomers and fibrils (lower panel). (b) AFM images after 6h incubation and fibril. (c) Absorption coefficient of water, Protein (both native, oligomer and fibril) measured using THz spectroscopy (upper panel). Circle indicates the representative crossing point, inset of c, upper panel shows the difference of absorption coefficient at 1THz. (c; lower panel) Crossing frequency at different condition. (d) Correlation between hydration (from THz spectroscopy) and structural perturbation (from CD spectroscopy).

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BOSE FEST 2021

Diffused metal-insulator transition in NdNiO3 film grown on BaTiO3: Likely evidence of electronic Griffiths phase

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In this work we have found likely evidence of electronic Griffiths phase in $NdNiO_3$ thin film which undergoes Mott transition. The investigation was carried out in the multilayer $NdNiO_3/BaTiO_3/SrTiO_3$ (NNO/BTO/STO), where a large mismatch of lattice constant of NNO with BTO leads to strain relaxation and disorder in the NNO film. NNO in the multilayer structure shows a broad Mott type MIT at a temperature T_{MI} = 160K from a high temperature bad metallic phase ($d\rho/dT < 0$) to a low temperature insulating phase. Using noise spectroscopy and impedance spectroscopy which can probe the dynamics of the co-existing phases, it was observed that in addition to the MIT at T_{MI} = 160K, there exists a new characteristics temperature T^* = 230K well above the T_{MI}, where large low frequency correlated fluctuations appear signifying appearance of a phase with slow dynamics. It is suggested that the temperature T^* may signify the onset of an electronic Griffiths phase that has been theoretically proposed for Mott transition with disorder.

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A physical explanation of soft-excess emission of Seyfert 1 AGNs

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An excess X-ray emission below 2 keV is called soft-excess, and it is detectable in a significant fraction of Seyfert 1 AGNs. The origin of this ubiquitous feature remains unclear. Several models have been proposed to explain it. In most cases, the warm Comptonization and blurred ionization reflection is suggested. In order to constrain the origin of this component, we exploit a 'bare-AGN', Ark 120, which is famous for its soft-excess emission. The spectral analysis of long-term (~15 years) X-ray observations of this source provides a reasonable understanding of the origin of soft-excess of this source. The long-term intrinsic luminosities of the soft-excess and the primary continuum show a correlation with a Pearson Correlation coefficient of 0.90. This indicates that the soft-excess and the primary continuum originate from the same physical process. From a physical model fitting, we infer that the soft-excess for Ark 120 could be due to a small number of scatterings in the Compton cloud. Using Monte-Carlo simulations, we show that indeed the spectra corresponding to fewer scatterings could provide a steeper soft-excess power-law in the 0.2-3.0 keV range. Furthermore, simulated luminosities are found to be in agreement with the observed values. Besides this, we also explore the other spectral and temporal properties of this source. Later, we applied the same method for other Seyfert 1 AGNs and found a similar type of correlation between soft-excess and the primary continuum emission.

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Topological insulators in the 1T' phase of MX$_2$ (M=Mo,W; X=S,Se,Te) revisited

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Mo and W based transition metal dichalcogenides (TMD) in the 1T' phase are known to be topological insulators [1]. This has been understood within the Kane-Mele model and is associated with the level inversion between the anion p states and the transition metal d states. However, what is surprising is that this happens across the entire series varying the anion from S to Se to Te for both Mo and W based systems. Examining various families of topological insulators, one finds that while one member of the series would be close to the point of inversion, it is not expected for every member to be close to the point of inversion and therefore become a topological insulator. In this work, we study 1H , 1T and 1T' phase of TMD extensively. We carry out ab-initio electronic structure calculations for each member of the TMD family. To quantify the electronic structure, we map the ab-initio band structure onto a tight binding model. We show that above mentioned level inversion is not specific to 1T' and also present in 1H phase. Further we identify the relevant interactions that make all the Mo and W based TMD to be topological insulators.

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Thermodynamics of Chimera

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Chimera[1, 2], a counterintuitive state identified as the spatial coexistence of synchronous and asynchronous domains, has been found in diverse theoretical and experimental setups. We have obtained a chimera state in a generic chemical oscillator having a reaction-diffusion structure by implementing a relevant complex Ginzburg-Landau equation(CGLE)[3] with global coupling. The evolution of nonequilibrium thermodynamic entities corresponding to this novel dynamical state is achieved by expounding a recently developed thermodynamic framework. Studying chimera state from an energetic and entropic viewpoint[4] would shed new light on the control and possible application of such a symmetry-breaking phenomenon.

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Long ranged order in ligand capped nanoparticles in pres- enceof temperature difference

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Aggregation of macromolecules under external drive is far from understood. An important driving situation is achieved by temperature difference that causes particle movement known as thermophoresis. Often interparticle interaction parameters show sensitivity to temperature, as it happens in ligand coated metal nanoparticle. Here we study self-assembly of nanoparticles with temperature dependent interaction parameters, using Brownian dynamics simulation. We find long range structural order in the cold region of the system with Avrami equation like crystal growth kinetics. We also show that partially ordered hot-cold interface drives the ordering in the system. Our observations might be useful in designing self- assembled structures with nanoscale particles.

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Cosmology in asymptotically safe quantum gravity

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We study different type of cosmological model at late times, taking into account quantum gravitational corrections in the formalism of the exact renormalization group flow of the effective average action for gravity. The cosmological evolution equations are derived by including the scale dependence of Newton's constant G and cosmological constant Λ. We investigate anisotropic Bianchi type-I model taking the covariant conservation of the Einstein tensor and Energy momentum tensor together. Here, we obtain the scale factors in different directions which eventually evolve into FLRW universe for radiation. However, for stiff matter we find that the universe need not evolve to the FLRW cosmology in general, but can also show Kasner type behaviour. On the other hand, we investigate the quantum corrected scale factor, energy density for FLRW cosmology by imposing just the covariant conservation of the Einstein tensor.

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A First-Principle Study of SrIrO3/LaCoO3 Perovskite Oxide n-type Interface

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Various emergent phenomena occur when we create an interface (IF) between two different crystalline materials (Heterointerfaces). The most important phenomenon is the formation of a high-mobility 2D electron gas at the junction between two materials[1] In this study, we will consider the n-type interface between semimetallic $SrIrO_3$ (SIO) and insulating $LaCoO_3$ (LCO) perovskite oxides in both superlattice and thin-film-substrate geometry. The stacking of the layers is made along the [001] direction with charge arrangements in one of the oxides like $(SrO)^0$ and $(IrO2)^0$, but have a charge on the other oxide like $(LaO)^{+1}$ and $(CoO2)^{-1}$. As a result, polar discontinuities occur at the interface. We will focus on the n-type interface (IF) with the LaO layer of LCO facing the IrO2 layer of SIO. Here we want to see how the superlattice and thin-film-substrate geometries behave in terms of charge transfer from LaO layer to IrO2 layer through the IF. Then we will explore the role of spin-orbit coupling in such interfaces.

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Quantum chemical studies on chelation in nano-bio conjugate between ZnO nanoparticle and cellular energy carrier molecules, ATP, ADP and AMP

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The microscopic understanding of the nano-bio complexes, made up of nanoparticle and biomolecules, is very important due to their wide applications in biomedical nanotechnologies. Here, we carry out quantum chemical calculations based on DFT on nano- bio conjugate between $Zn_{12}O_{12}$ cluster (ZnONP) and the energy carrier biomolecules in cellular environment, like, ATP, ADP and AMP. We focus on microscopic details of chelation by individual groups, phosphate, ribose and adenine of the ligands with ZnONP. Electronic structures and bonding interactions for ground state configurations of all complexes are presented through molecular orbital (MO) theory and natural bond orbital (NBO) analyses as well as through Raman Spectra calculations. DFT-optimized geometries and bond indices suggest presences of Zn-N(adenine) bond and multiple Zn-O(phosphate) bonds. Phosphate groups form additional O-H---O non-classical bonds with ZnO nano-cluster in all three nano-bio complexes. Kohn-Sham MOs and natural population analyses suggest that the adenine moiety forms a coordinate covalent bond (Zn-N) with ZnO cluster through adenine ⟶ ZnO charge transfer (CT), while phosphate groups from coordinate covalent bonds (Zn-O) through ZnO ⟶ phosphate CT in all nano-bio complexes, leading to the stability of bio-molecules-ZnO complex with increasing of number of phosphate groups in bio-molecules. Our results may also be important to understand how the metal oxide nanoparticles affect the cellular energy transfer reactions and the reaction pathways.

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Experimental Observation of Exchange Bias in Antiferromagnetic $Cr_{0.79}Se$ due to Itinerant Weak Ferromagnetism at Low-temperature

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Here we are showing the structural, electrical transport, and magnetic properties of antiferromagnetic transition-metal monochalcogenide $Cr_{0.79}Se$. Different from the existing off-stoichiometric compositions, $Cr_{0.79}Se$ is found to be synthesised into the same NiAs-type hexagonal crystal structure of CrSe. Resistivity data suggest $Cr_{0.79}Se$ to be a Fermi-liquid-type metal at low temperatures, while at intermediate temperatures the resistivity depends sublinearly on the temperature. Eventually, at the elevated temperatures the rate of change of resistivity rapidly decreases with temperature. Magnetic measurements suggest a transition from paramagnetic phase to an antiferromagnetic phase at a Neel temperature of 225 K. Further reduction of the sample temperature results into coexistance of weak ferromagnetism along with the antiferromagnetic phase below 100 K. As a result, below 100 K, we identify significant exchange bias due to the interaction between the ferro- and antiferromagnetic phases. In addition, from the temperature dependent X-ray diffraction measurements we observe that the NiAs-type structure is stable up to as high as 600^0C.

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Flux attachment and fractional statistics from electron-vortex interaction

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A mixture of interacting bosons and fermions at very low temperatures contains a rich variety of new physical phenomenon. Boson-Fermion mixture has been considered in theoretical models for highT_c cuprate superconductors, BCS-BEC cross over, superfluid-insulator transition, charged bose liquids, etc. We take a similar relativistic system containing charged Bosons and Fermions coupled minimally to electromagnetic field where topological vortices can appear in the scalar matter. In the symmetry broken phase of the scalar field, in presence of vortices, we dualize the phase of the bosonic field in terms of anti-symmetric 2-form field. The dual lagrangian contains terms that suggest an interaction between a non-local fermion current, termed spin current, and vorticity[1]. We then show that such an interaction, at low energies, may lead to an attachment of vortices to spin magnetic moment density of non-relativistic fermionic modes on the surfaces of a bulk sample. This attachment of fermionic spin moment density is similar to the flux attachment discussed in the context of Chern-Simons theory and FQHE. We take this analogy further and define an effective gauge field using the singular part of the bosonic phase. At low energies, this gauge field couple minimally to fermions and lead to the same flux attachment equation. Also due to minimal coupling, any fermion taken around a path containing another fermion attached to a vortex may obtain a Bohm-Aharanov phase which depends on the local average magnetic moment per particle. For an arbitrary value of this average magnetic moment, the fermions attached to vortices may obey anyonic statistics[2].

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Genuine Einstein-Podolsky-Rosen steering of three-qubit states by multiple sequential observers

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We investigate the possibility of multiple use of a single copy of three-qubit state for detecting genuine tripartite Einstein-Podolsky-Rosen (EPR) steering. A pure three- qubit state of either the Greenberger-Horne-Zeilinger (GHZ)-type or W-type is shared between two fixed observers in two wings and a sequence of multiple observers in the third wing who perform unsharp or non-projective measurements. The measurement settings of each of the multiple observers in the third wing is independent and uncorrelated with the measurement settings and outcomes of the previous observers. In such set-up, we investigate all possible types of $(2 \rightarrow 1)$ and $(1 \rightarrow 2)$ genuine tripartite EPR steering. For each case, we obtain an upper limit on the number of observers on the third wing who can demonstrate genuine EPR steering through the quantum violation of an appropriate tripartite steering inequality. We show that the GHZ state allows for a higher number of observers compared to that for W states.

Additionally, $(1 \rightarrow 2)$ genuine steering is possible for a larger range of the sharpness parameters compared to that for the $(2 \rightarrow 1)$ genuine steering cases.

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Enhanced thermoelectric properties of double transition metal MXenes

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Thermoelectric (TE) materials are the promising candidate for renewable energy harvesting technology since it can generate electricity by recovering energy from the waste heat of environmental sources utilizing Seebeck effect.[1] The efficiency of TE device depends on transport properties (of both charge carrier plus lattice) of the material and is estimated by a dimensionless quantity called figure of merit (ZT). The best TE materials available today operating near room temperature, are doped semiconductor alloys of antimony and bismuth telluride having ZT of about 1, although for practical purposes, ZT value of 3-4 is desired.[2] In recent year, significant improvement on the performance of TE devices has been achieved in nanostructured TE materials, like layered 2D materials such as, MXene, family of transition-metal (TM) carbides, nitrides and carbonitrides.[1] Jing et al. predicted that figure of merit of p-type double TM MXene $Cr_2TiC_2(OH)_2$ could reach to 3.0 at 600K.[3]

Motivated by the above, in the present study [4] we focus on Mo and Ti based ordered double TM MXenes, namely $Ti_{3-x}Mo_xC_2T_2$ (x = 0.5, 1, 1.5, 2, 2.5) with surface termination T = -O/-F/-OH that can exist in two ordered phases, o-MXene and i-MXene. Employing first-principles calculations, we analyze their thermodynamic stability with respect to 1) ordered phases by computing formation energy and bond energy and 2) competing binary phases by ternary convex hull formation. Investigation of electronic and magnetic properties results in three semiconducting MXene stable in o-phase, namely $TiMo_2C_2F_2$, $TiMo_2C_2(OH)_2$ and $Ti_2MoC_2F_2$ having narrow band-gap with antiferromagnetic ground state, while rest are found to be metallic. In order to validate our scheme of transport calculation, we first determine the electrical transport properties of passivated n-type $TiMo_2C_2$ for which experimental results are available [5] and show good agreement with experimental data for the choice of passivation with O and OH. Our calculations show superior electrical transport properties of Ti_2MoC_2 compared to $TiMo_2C_2$ with a power factor of 10^4 μW cm^{-1} K^{-2} at 300 K for a p-type carrier density of 10^{19} cm^{-3}. This leads to an exceptional ZT of 1.5 at 300 K and 3.1 at 800 K, the latter with a 27% efficiency thereby reaching close to the desired target. Our exercise should motivate experimental study of yet-to-be synthesized double TM MXene compound, Ti_2MoC_2.

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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[1, 2]. Highly densed large clusters can sense the nutrient concentration more efficiently, which enhances the chemo- tactic efficiency of the cell when clustersize increases from small value. But as clustersize increases gradually a competition develops between sensing and adaptation. We have observed a performance peak due to this competition[3]. We perform simulation in a detailed theoreti- cal model to reveal how fluctuation also increases with clustersize like chemotactic efficiency and adaptation module of the network responds to this growing fluctuation intensely by raising the methylation level of receptors, which is actually responsible for adaption. So motillity of the cell is completely regulated by methylation levels of receptors and sensitivity towards ligand concentration goes down reulting decrease in the chemotactic efficiency at large clustersize[3].

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Flicker noise in large area Graphene FET on lightly doped substrate

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We have fabricated a CVD Graphene device on a lightly doped Si/SiO$_2$ substrate (doping concentration $\approx$5 x 10^{15} cm^{-3}). a peak in the noise around the zero back-gate voltage.

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Gate tunable strong photo response from a few layered MoS₂ transistor

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Semiconducting, two-dimensional molybdenum disulfide (MoS₂) is considered to be a promising new material[1] for high sensitive photodetection[2], because of its atomically thin profile and favorable bandgap. Monolayer MoS₂ has direct optical bandgap (~ 1.8 eV), however, low absorption of incident light due to its atomic thickness limits the device performance. Here, we present systematic transport data from a few layer (~3-4 layers) MoS₂ field effect transistor with a high electrical on/off ratio (~ 10^4). The device shows huge photoresponse by the application of light (λ ~ 633 nm) with a responsivity closed to ~ 10^5 - 10^6, being one of the highest for few layered devices. We plan to improve the device performance and detection range by creating hybrid with other 2D/0D or 2D/2D TMD materials.
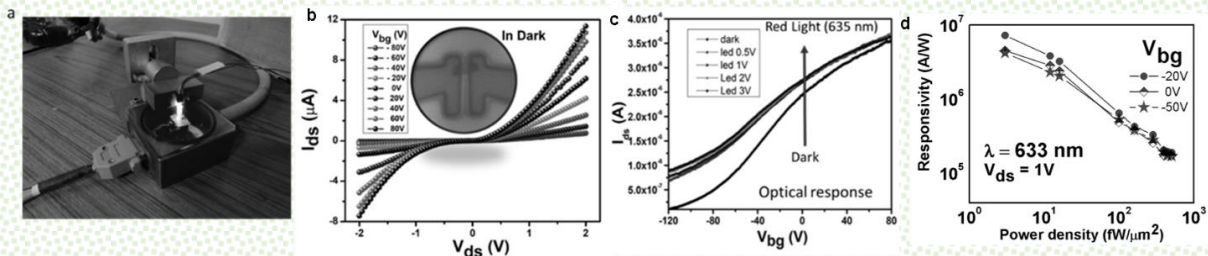
Fig. a) Optoelectronic transport measurement set up, (b) I-V characteristics at different gate voltages for a two terminal few layer MoS₂ transistor. Inset shows the device image. (c) I_{DS}-V_{bg} characteristics in dark and, in presence of red light, showing significant photo response. (d) Calculated Responsivity plotted as a function of power for three different gate voltages.

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Studies of Pre-main sequence stars in Galactic star-forming regions

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H II regions are the low-density cloud 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 (Anderson et al. 2014). Here, we are exhibiting the identification and characterization of the pre-main-sequence stars associated with the H II regions Sh2-87 and Teutsch 127. We have utilized both of our own new spectroscopic observational data and several archival catalogues, e.g., IPHAS, WISE, 2MASS. From the slit spectroscopic results, a primary classification of a few sources in the above two regions has been presented here. Using the colour-colour diagram from WISE data in the region of Sh2-87, a total of 20 Class I and 70 Class II young objects are classified within the region. In that same region, the IPHAS photometry unveils the classification of 20 Hα emitting sources. From the 2MASS data, we have classified the 50 young stellar objects in the region Teutsch 127. These multi-wavelength studies will help us for the further studies of these regions.

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Excited-state Proton Transfer in Reverse Micelles: Effect of Temperature and a Possible Interplay with Solvation

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Excited state proton transfer (ESPT) is a fundamental process of immense biophysical interest and considering the heterogeneity existing in real biological environments we investigate the process in bio-mimicking reverse micellar (RM) systems. A fundamental question in ESPT dynamics is related to its inherent coupling with the solvation process. A much-debated issue is which process precedes? This contribution addresses this fundamental question by conducting a detailed study of the ESPT process of a photo-acid D-luciferin at various temperatures in RMs composed of: anionic AOT, cationic DDAB, and neutral Igepal-520 using steady-state and time-resolved fluorescence measurements at fixed hydration, $w_0=10$. We found that with increasing temperature both solvation as well as the ESPT rate accelerates, however, the extent of the increase is RM specific, and they even not complement each other. Our study clearly identifies the pivotal role of solvation, specially in micro-heterogeneous environments, to guide the ESPT process.
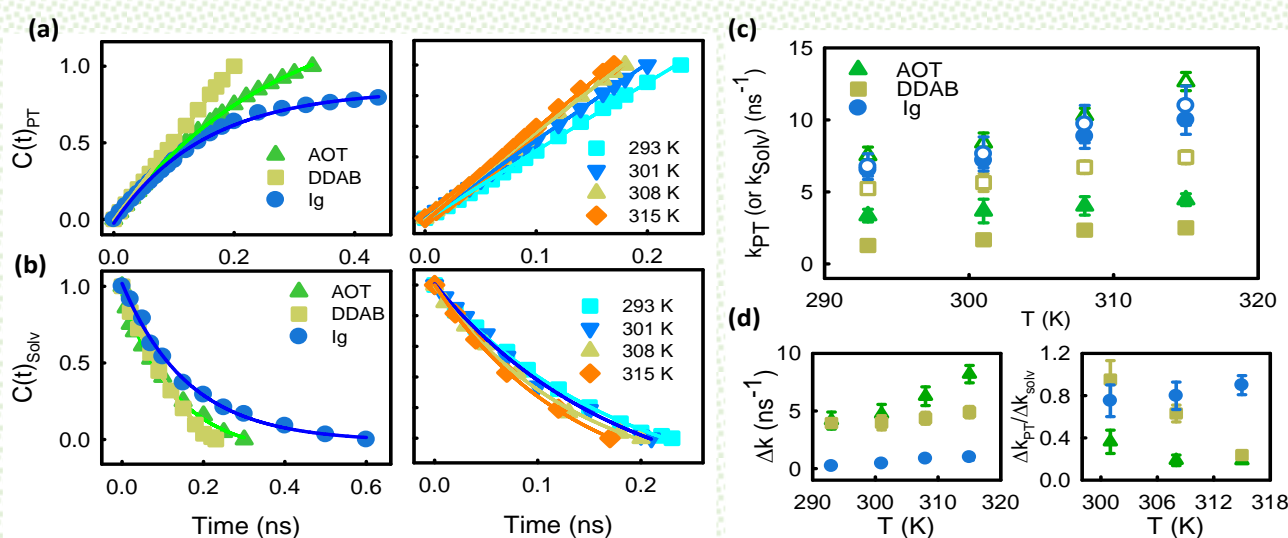
Figure: (a) *Left panel:* Proton transfer correlation function ($C(t)_{PT}$) of D-luciferin in three different RM systems as. *Right panel:* $C(t)_{PT}$ of D-luciferin in DDAB RM at different temperatures. The solid lines are exponential fits. (b) *Left panel:* ROH^* solvation correlation function ($C(t)_{Solv}$) of D-luciferin in three different RM systems as. *Right panel:* $C(t)_{Solv}$ of D-luciferin in DDAB RM at different temperatures. The solid lines are exponential fits. (c) Proton transfer rate, k_{PT} (filled symbols) and solvation rate, k_{Solv} (open symbols) of D-luciferin in three different RM systems. Note that the solvation dynamic is faster than the PT kinetics. (d) *Left panel:* Difference of solvation and proton transfer kinetics ($\Delta k=k_{Solv}-k_{PT}$) of D-luciferin as a function of temperature in three different RMs. *Right panel:* $\Delta k_{PT}/\Delta k_{solv}$ as a function of temperature in three different RMs.

Quantum phases and thermodynamics of afrustrated spin-1/2 ladder with alternateIsing–Heisenberg rung interactions

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We study a frustrated two-leg spin ladder with alternate isotropic Heisenberg and Ising rung exchange interactions, whereas, interactions along legs and diagonals are Ising-type. All theinteractions in the ladder are anti-ferromagneticin nature and induce frustration in the system.This model shows four interesting quantum phases: (i) stripe rung ferromagnetic (SRFM), (ii)stripe rung ferromagnetic with edge singlet (SRFM-E), (iii) anisotropic antiferromagnetic(AAFM), and (iv) stripe leg ferromagnetic (SLFM) phase. We construct a quantum phasediagram for this model and show that in stripe rung ferromagnet (SRFM), the same type of sublattice spins (either isotropic S-type or discrete anisotropic σ-type spins) are aligned in the same direction. Whereas, in anisotropic antiferromagnetic phase, both S and σ-type of spins are anti-ferromagnetically aligned with each other, two nearest S spins along the rung form an anisotropic singlet bond whereas two nearest σ spins form an Ising bond. In large Heisenberg rung exchange interaction limit, spins on each leg are ferromagnetically aligned, but spins on different legs are anti-ferromagnetically aligned. The thermodynamic quantities like specificheat $C_v(T)$, magnetic susceptibility $\chi(T)$ and thermal entropyS(T) are also calculated using the transfer matrix method for various phases. The magnetic gap in the SRFM and the SLFM can be noticed from $\chi(T)$ and $C_v(T)$ curves.

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Effect of Schottky barrier height and morphology of nanostructured PZT on the output power density of piezoelectric nanogenerators

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The enhancement of the output power density of piezoelectric nanogenerators to drive microelectronic devices is a great challenge due to the high internal resistance of piezoelectric materials. In this work, piezoelectric NG (PENG) has been developed on a flexible substrate, where hydrothermally grown Lead Zirconate Titanate (PZT) of different nanostructured morphologies were used as the generating material. The reduction of the internal resistance of PZT based PENGs has been achieved in two ways including i) fabrication of interdigitated electrodes (IDE) to increase the interfacial polarization and ii) lowering of Schottky barrier heights at the junction of the PZT nanostructure and the metal electrode by varying the work functions of electrode materials. Morphology-dependent piezoelectric energy harvesting characteristics show needle-shaped nanowires provide an outstanding power density. The PZT nanoneedles-based flexible PENG can deliver output power density 617 $\mu W/cm^2$ and voltage 9.5 V on the application of low mechanical pressure (~1 KPa) by tapping motion. A prototype has been developed based on this work. The work provides a complete insight into a systematic pathway that helps in solving the problems faced due to the high internal resistance of the piezoelectric nanogenerators.

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Cosmic acceleration in an extended Brans-Dicke-Higgs theory

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We consider an extended scalar-tensor theory of gravity where the action has two interacting scalar fields, a Brans-Dicke field that makes the effective Newtonian constant a function of coordinates and a Higgs field that has derivative and non-derivative interaction with the lagrangian. There is a non-trivial interaction between the two scalar fields that dictates the dominance of different scalar fields in different era. We investigate if this set-up can describe a late-time cosmic acceleration preceded by a smooth transition from deceleration in recent past. From a cosmological reconstruction technique, we find the scalar profiles as a function of redshift. We find the constraints on the model parameters from a Markov chain Monte Carlo analysis using observational data. Evolution of an effective equation of state, matter density contrast, and thermodynamic equilibrium of our Universe are studied and their significance in comparison with a LCDM cosmology is discussed.

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Physical characteristics of Wolf Rayet Stars

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Wolf Rayet (WR) stars discovered in the Cygnus Constellation by C.J.E. Wolf & G. Rayet in 1867, are massive, highly luminous and hot stars belonging to Population I class. They are basically known for their broad emission line spectra which also distinguishes them from their Main Sequence counterparts. Several spectroscopic studies of such highly evolved massive stars have concluded that due to their expanding outer envelopes they show blue-shifted UV absorption (P Cygni) profiles and due to the heavy mass-loss rates that are powered by extremely fast stellar winds, they reveal their inner layers that are rich in heavier elements and simultaneously contribute towards the chemical enrichment of the ISM and the evolution of galaxies in which they are present. As per the latest classification (van der Hucht, 2001), a total of about 227 galactic WR stars have been catalogued properly and out of which only about 30-40 of them have been studied in detail, while the recent NIR surveys have revealed several thousands of them which were previously hidden due to dust extinction. In order to study several properties of WR stars such as cause of stellar mass outflow, wind velocity structure, varying chemical and mechanical influence on the ISM, understudying dust formation & distribution etc., we have been acquiring optical and near-Infrared spectroscopic data by carrying out observations using the national observing telescopes, and have been analysing them. Also, we have been trying to model the spectra using the radiative transfer model atmosphere grids such as PoWR and have been able to estimate various physical stellar parameters. In this talk I shall briefly describe the results obtained so far.

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Strong Magnon-Magnon Coupling in Two-Dimensional Diamond Shaped Ferromagnetic Nanodots Array

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Strong coupling between magnons and different quantum particles was studied extensively for quantum electrodynamics in the past few years. However, the strongly magnon-magnon [1] couplings in a confined nanomagnet remains to be revealed. Here, we report the interaction between different magnon modes [2] in a magnetic dot array. The intermodal coupling in the strong coupling regime was approached with a maximum coupling strength of 0.745 GHz and cooperativity of 2.5. Furthermore, it is found that the coupling strength is highly dependent on the orientation of bias field. Micromagnetic simulation reveals that the compitetion between external bias field and inter dot dipolar interaction create a movement of domain in between the dot which results the anticrossing. The tunable coupling strength with the strength and orientation of bias field opens the opportunity of extremely controlled hybrid magnonic devices. This findings could greatly enrich the still evolving field of quantum magnonics.

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Crystal Structure Dependent Interfacial Spin Transparency in W/CoFeB Thin Films

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Spin pumping[1] is an efficient and extensively used method to generate pure spin current in an ferromagnet(FM)/nonmagnetic(NM) heterostructure, which can leads to the development of spin-torque based spin logic and memory devices that can overcome the drawbacks like excess power consumption and enlarged thermal fluctuation observed in conventional charged-based devices. Here we have investigated the spin pumping effect in sputter deposited W/CoFeB thin films by using femtosecond laser-based all-optical time-resolved magneto-optical Kerr effect (TR-MOKE) magnetometry [2] and underpinned the effect of crystal phase on interfacial spin transparency. W and CoFeB thickness-dependent Gilbert damping parameter is modelled using both the ballistic and diffusive spin transport theories to extract the spin-diffusion length of W, backflow factor, spin-mixing conductance and spin-flip probability parameter, which proved W to be a good spin sink material. We have isolated the contributions of spin pumping, spin memory loss (SML), and two-magnon scattering (TMS) to the Gilbert damping modulation revealing that spin pumping contribution is strongly dominant over SML and TMS, which is reconfirmed from the invariance of Gilbert damping with the Cu spacer layer thickness. We have extracted interfacial spin transparency by using both drift-diffusion model and spin Hall magnetoresistance model. We have achieved a giant interfacial spin transparency (>0.8), which is a record value of interfacial spin transparency among the NM/FM heterostructures reported till date[3]. Another key finding is the sharp change in electronic properties such as spin-mixing conductance and interfacial spin transparency with the structural phase of W with a subtle variation in its thickness which can give a guiding principle in choosing appropriate thickness and phase for optimizing the spin transparency.

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Synthesis and spectroscopic characterization of a target specific nano-hybrid for redox- buffering in cellular milieu

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A crucial balance between oxidative eustress and distress is important for maintaining redox homeostasis in the cellular milieu. Therefore, sustaining the intracellular redox buffer condition with exogenous agents could be a viable therapeutic strategy against numerous diseases where redox imbalance plays a major role. Here, we synthesized chitosan functionalized Mn_3O_4 nanoparticles (Ch-Mn_3O_4 NPs) and tested their redox buffering capability in *in-vitro* and *in-cellulo* experiments. As chitosan is stable in the gastro-intestinal (GI) tract and also easily absorbed by the intestine it can be used as a delivery material specific to the intestine. On the other hand, Mn_3O_4 NPs have redox modulatory properties. So a combination of chitosan and Mn_3O_4 NPs provide the chance for targeted redox buffering. Our detailed spectroscopic studies *in vitro* on this nanohybrid suggest ROS generation and antioxidant ability. *In cellulo* studies using adenocarcinomic human alveolar basal epithelial cells (A549) confirmed the efficacy of the nanohybrid in redox homeostasis in the cellular milieu. The cumulative outcomes of our study suggest that the Ch-Mn_3O_4 nano-hybrid has the potential to function as a target-specific redox buffering agent in both in vitro as well as *incellulo* systems.

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Magnetoelectric properties of Ba and Y co-doped Bismuth Ferrite Nanoparticles

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Barium (Ba) doping at Bismuth (Bi) site was previously reported to enhance magnetic properties of Bismuth Ferrite ($BiFeO_3$) while Yttrium (Y) doping at the same site was found to improve ferroelectric and dielectric properties. Nanostructural forms with size less than 62nm is also desirable to destroy the spin cycloid responsible for weakening of magnetoelectric behavior of $BiFeO_3$. To investigate the combined effect of Ba and Y co-doping on nanostructural forms, $Ba_{0.1}Bi_{0.9-x}Y_xFeO_3$ (x = 0.0, 0.03, 0.05 and 0.1) nanoparticles are synthesized using chemical synthesis method and their magnetoelectric and dielectric properties are studied in detail. Ferroelectric properties are enhanced for x = 0.05 while magnetic properties are unchanged. Variation of electric field-guided strain shows reduced asymmetry in co-doped samples and a peak-to-peak strain value of 67.8% in x = 0.05. Both dielectric constant and dielectric loss are observed to be maximum for this sample with a magnetodielectric factor of $\sim -1.2\%$ and magnetoelectric coupling coefficient (γ) of $\sim -1.10963 \pm 0.23193$ $(emu/g)^{-2}$.

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Transport and fluctuations in mass aggregation processes: mobility-driven clustering

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We calculate the bulk-diffusion coefficient and the conductivity in nonequilibrium conserved-mass aggregation processes on a ring. These processes involve chipping and fragmentation of masses, which diffuse on a lattice and aggregate with their neighboring masses upon contact, and, under certain conditions, they exhibit a condensation transition. We find that, even in the absence of microscopic time reversibility, the systems satisfy an Einstein relation, which connects the ratio of the conductivity and the bulk-diffusion coefficient to mass fluctuation. Interestingly, when aggregation dominates over chipping, the conductivity or, equivalently, the mobility of masses, is greatly enhanced. The enhancement in the conductivity, in accordance with the Einstein relation, results in large mass fluctuations and can induce a mobility-driven clustering in the systems. Indeed, in a certain parameter regime, we show that the conductivity, along with the mass fluctuation, diverges beyond a critical density. Therefore due to the onset of instability in the conductivity, the system undergoes a nonequilibrium condensation transition which was previously observed in [1] . Notably, the bulk-diffusion coefficient remains finite in all cases. We find our analytic results in quite good agreement with simulations.

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