Satyendra Nath Bose
National Centre
for Basic Sciences

CENTRE FOR BASIC SCIENCES 1986
S. N. BOSE NATIONAL
1894-1974
विज्ञानेन परिपश्यन्ति धीराः

BOSE FEST 2023

Abstract Booklet

BOSE FEST 2023: List of Oral Presentations

Sl. No.	Name	Title
1	Abhik Ghosh Moulick	Molecular insights into the binding of fatty acids with α-Lactalbumin at the molten globule (MG) state
2	Abhinandan Das	IONIC LIQUIDS & ITS IMPACT ON PROTEINS
3	Achintya Low	The Role of Phonons in Anomalous Hall Effect in Kagome Ferromagnet Fe3Sn
4	Anirban Mukherjee	Dynamic correlations in the conserved Manna sandpile
5	Ardhendu Pal	Study of Λ-doublet splittings of NO using cavity ring-down spectroscopy at 5.2 μm
6	Ariful Hoque	Variations in CO–to–H2 Column Density Ratio in Star-forming Filaments
7	Arunanshu Panda	Anomalous Hall effect in layered ferromagnet ZnMnSb
8	Ashadul Halder	Global 21-cm brightness temperature in viscous dark energy models
9	Banik Rai	Transport properties of tr-Cr5Te8
10	Biswajit Pabi	Role of molecular orientation on electron transport in a single molecular junction
11	Chandradip Khamrai	Effect of relative time-scale on steady state measure of a coupled driven system.
12	Deepshikha Das	Optimum transport in a periodically driven lattice gas with short-ranged interaction
13	Dibyendu Maity	Accelerating Protein Conformational Space Exploration with Autoencoders and VAEs
14	Diya Ram	Magnetic Activity of M-dwarfs: Optical and NIR Spectroscopic Studies
15	Indrajit Ghose	Neutrino oscillation caused by spacetime geometry
16	Indrani Kar	ARPES and its application in the study of some TMDCs
17	Koushik Pradhan	Robust half-metallicity and Topological Properties in square-net Potassium Manganese Chalcogenides
18	Krishnendu Patra	Perturbing the bond disproportionated state in NdNiO3
19	Manjari Dutta	Explicit existence of the Berry phase for harmonic oscillators in noncommutative space
20	Manodip Routh	Ground-state phase diagram of antiferromagnetic spin–1/2 coupled trimer chain
21	Milan Sil	Exploring noble gas species in the radiation-dominated region
22	Monalisa Chatterjee	Singlet quantum phases and magnetization of the frustrated spin-1/2 ladder with ferromagnetic (F) exchange in legs and alternating F–AF exchange in rungs
23	Nishant Garg	Relation between filaments and clumps in a few Galactic star-forming regions
24	Prashant Kundu	Kinetics of Initial Charge Separation in the Photosynthetic Reaction

Sl. No.	Name	Title
		Centers of Rhodobacter sphaeroides
25	Pratap Kumar Pal	Magnon–Magnon Coupling in Ni80Fe20 Nanocross Array
26	Premashis Kumar	Nonequilibrium thermodynamic signature of chimeras in the chemical reaction network
27	Ram Krishna Patra	On Composition of Multipartite Quantum Systems: Perspective From Quantum Information Theory
28	Ria Saha	Contrasting hydration dynamics in presence of Guanidinium ions and its possible effect on protein (de)stability
29	Riju Pal	Unusual Magneto-transport and Anomalous Hall Effect in Two-dimensional van der Waals Ferromagnet Fe4GeTe2
30	Rik Naranjan Mukherjee	Enthalpic and Entropic Contributions in the Mixing Thermodynamics of Deep Eutectic Solvents: The Effect of Incorporating Interactions
31	Ritwick Sarkar	Activity driven transport
32	Riya Barick	Neutrino Oscillations induced by chiral geometry.
33	Samrat Sen	Certifying beyond quantumness of locally quantum no-signaling theories through a quantum-input Bell test
34	Shiladitya Karmakar	Excited-state spin trapping in Iron(II) spin crossover complexes: A light effect
35	Shinjini Paul	Why does the charge transfer energy vary in some nickelates?
36	Siddhartha Biswas	Characterization and Identification of the pre-main sequence stars in the H II region Sh2-87
37	Soham Saha	CeOx as Surface Passivation and Hole Transfer Catalyst Layer Boosting Solar Water Oxidation of ZnFe2O4 Nanorods Photoanode
38	Soham Sen	Virtual transitions in an atom-mirror system in the presence of two scalar photons
39	Soumen Mandal	Study of photonic spin Hall shift in monolayer MoS2 via quantum weak measurement
40	Suchetana Mukhopadhyay	All-Optical Probing of Giant Interfacial Spin Transparency at a Topological Insulator/ Ferromagnet Interface
41	Sudipta Chatterjee	Disorder-induced crossover of Mott insulator to weak Anderson localized regime in an argon-irradiated NdNiO3 film
42	Sudipta Mitra	Molecular Thermodynamic Origin of Substrate Promiscuity in the Enzyme Laccase: Toward A Broad- Spectrum Degrader of Dye Effluents
43	Sumana Pyne	Alteration of lipid hydration during Polyethylene Glycol induced lipid fusion
44	Suravi Pal	External field induced mixing and demixing of a binary colloid
45	Tanmoy Chakraborty	Current Fluctuations of models of interacting self-propelled particles : microscopic approach

Molecular insights into the binding of fatty acids with α-Lactalbumin at the molten globule (MG) state

Abhik Ghosh Moulick, Jaydeb Chakrabarti

Department of Physics of Complex Systems, S N Bose National Centre for Basic Sciencs, JD Block, Sector 3, Kolkata – 700106

Abstract of the Oral Presentation

A molten globule (MG) state is an intermediate state of protein observed during the unfolding of the native structure. In MG states milk protein α-Lactalbumin (aLA) binds with oleic acid (OLA). This MG-aLA-OLA complex, popularly known as XAMLET performs cytotoxic activities against cancer cell lines. Earlier study shows that the MG state of protein behaves as an IDP where the disorder is induced by external denaturing conditions like low pH. It is known that the inherently dynamic nature of IDPs plays a key role in rapid ligand recognition. However, the microscopic understanding of ligand recognition ability in MG state of protein is not yet explored. Motivated by this, we explore binding of bovine aLA with OLA using all atom molecular dynamics(MD) simulations. We find the binding mode between MG-aLA and OLA using the conformational thermodynamics method. We also estimate the binding free energy using the umbrella sampling (US) method for both MG state and neutral state. We find that the binding free energy obtained from US is comparable with earlier experimental results. The microscopic understanding of protein-ligand binding gives an in-depth understanding of facilitating the discovery, design, and development of drugs.

References:

1. D. Barrick and R. L. Baldwin, The molten globule intermediate of apomyoglobin and the process of protein folding, Protein Science, vol. 2, no. 6, pp. 869–876, 1993.

2. P. A. Jennings and P. E. Wright, Formation of a molten globule intermediate early in the kinetic folding pathway of apomyoglobin, Science, vol. 262, no. 5135, pp. 892–896, 1993.

3. A. G. Moulick and J. Chakrabarti, Conformational fluctuations in the molten globule state of α-lactalbumin, Phys. Chem. Chem. Phys., vol. 24, pp. 21348–21357, 2022.

4. A. Das, J. Chakrabarti, and M. Ghosh, Conformational contribution to thermodynamics of binding in protein-peptide complexes through microscopic simulation,Biophysical journal, vol. 104, no. 6, pp. 1274–1284, 2013.

5. S. Brandt, F. Sittel, M. Ernst and G. Stock, J. Phys. Chem. Lett., 2018, 9, 2144–2150.

6. A. G. Moulick, J. Chakrabarti, Microscopic understanding of fatty acid binding with α-lactalbumin at molten globule state (Manuscript under preparation).

IONIC LIQUIDS & ITS IMPACT ON PROTEINS

Prayasee Baruah,[a] Dhiman Ray,[a] Ibemhanbi Konthoujam,[b] Abhinandan Das,[c] Suman Chakrabarty,[c] Kripamoy Aguan[b] and Sivaprasad Mitra *[a]

Centre for Advanced Studies, Department of Chemistry, North-Eastern Hill University, Shillong 793 022, India
Department of Biotechnology & Bioinformatics, North-Eastern Hill University, Shillong 793 022, India
Department of Chemical, Biological & Macromolecular Sciences, S. N. Bose National Centre for Basic Sciences, Kolkata 700106, India

Abstract of the Oral Presentation

Ionic liquids are a broad class of molten salts having wide range of applications. Ionic liquids exhibit several unique properties such as high electrochemical stable window, high conductivity, high thermal stability and other properties highly exploitable in biological and industrial processes. Interaction of proteins with ionic liquids can lead to several therapeutic opportunities. Naturally occurring Lysozyme in bodily fluids serves as a drug carrier, Studying interaction of Lysozyme with phenolic drug ellagic acid (EGA) in presence of ionic liquids IMD, PYD and MOR help us understand drug modulation in ionic liquids. Additionally, two each of pyridinium, morpholinium and imidazolium based ionic liquids and their effect on important enzymes such as AChE and CS help in exploring therapeutic interventions in the field of drug discovery and application.

References:

New J. Chem., 2022,46, 20419-20432

The Role of Phonons in Anomalous Hall Effect in Kagome Ferromagnet Fe_3Sn

Achintya Low, Susanta Ghosh, Soumya Ghorai, and Thirupathaiah Setti

Department of Condensed Matter and Material Physics
S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-3,
Salt Lake,
Kolkata-700106

Abstract of the Oral Presentation

The anomalous Hall effect (AHE) in which the anomalous Hall resistivity scales with the magnetization of the sample, usually occurs in ferromagnet. AHE can arise because of two qualitatively different microscopic mechanisms: extrinsic processes due to scattering effects and an intrinsic mechanism connected to the Berry curvature. Usually, the extrinsic skew scattering contribution of AHE is much less-than the intrinsic one. Here, we report on the successful growth of the high-quality Fe_3Sn single crystals and a thorough Study on its magnetic and electrical transport properties. We see a large anomalous Hall effect which has both intrinsic and temperature dependent extrinsic skew scattering contribution. A strong inelastic phonon scattering is observed in temperature dependent longitudinal resistivity data which has an impact on the skew scattering anomalous Hall resistivity.

References:

1. *Nagaosa, Naoto, et al. "Anomalous Hall effect." Reviews of modern physics 82.2 (2010): 1539*

2. *Sales, Brian C., et al. "Ferromagnetism of Fe_3Sn and alloys." Scientific reports 4.1 (2014): 1-6.*

3. *Chen, Taishi, et al. "Large anomalous Nernst effect and nodal plane in an iron-based kagome ferromagnet." Science advances 8.2 (2022): eabk1480.*

Dynamic correlations in the conserved Manna sandpile

Anirban Mukherjee and Punyabrata Pradhan

Department of Physics of Complex Systems, S. N. Bose National Centre for Basic Sciences, JD block, Sector -III, Salt Lake, Kolkata - 700106

Abstract of the Oral Presentation

We study dynamic correlations for current and mass, as well as the associated power spectra, in the one-dimensional conserved Manna sandpile. We show that, in the thermodynamic limit, the variance of cumulative bond current up to time T grows subdiffusively as $T^{1/2-\mu}$ with the exponent $\mu \geq 0$ depending on the density regimes considered and, likewise, the power spectra of current and mass at low frequency f varies as $f^{1/2+\mu}$ and $f^{-3/2+\mu}$, respectively; our theory predicts that, far from criticality, $\mu = 0$ and, near criticality, $\mu = (\beta + 1)/2\nu_{perp}z > 0$ with β, ν_{perp} and z being the order-parameter, correlation-length and dynamic exponents, respectively. The anomalous suppression of fluctuations near criticality signifies a "dynamic hyperuniformity", characterized by a set of fluctuation relations, in which current, mass and tagged-particle displacement fluctuations are shown to have a precise quantitative relationship with the density-dependent activity (or, its derivative). In particular, the relation, $D_s(\bar{\rho}) = a(\bar{\rho})$ between the self-diffusion coefficient $D_s(\bar{\rho})$, activity $a(\bar{\rho})$ and density $\bar{\rho}$ explains a previous simulation observation [Eur. Phys. J. B 72, 441 (2009)] that, near criticality, the self-diffusion coefficient in the Manna sandpile has the same scaling behavior as the activity.

References:

1. *Anirban Mukherjee and Punyabrata Pradhan, " Dynamic correlations in the conserved Manna sandpile", Phys. Rev. E 107, 024109 (2023).*

Study of Λ-doublet splittings of NO using cavity ring-down spectroscopy at 5.2 µm

Ardhendu Pal, Soumyadipta Chakraborty, Biswajit Panda and Manik Pradhan

S.N.Bose National Centre for Basic Sciences

Abstract of the Oral Presentation

The study of the spectroscopic features of nitric oxide (NO) is of great interest due to its paramagnetic nature. The Λ-type doublet is especially important to investigate because it provides a variety of spectroscopic information [1]. The spectroscopic features of the Λ-type doubling of the fine structure lines of NO in the mid-infrared fingerprint region, specifically the ($^2\Pi_{1/2}$, 1)↔($^2\Pi_{1/2}$, 0) and ($^2\Pi_{3/2}$, 1)↔($^2\Pi_{3/2}$, 0) vibrational transitions, were investigated in this study. The rotationally resolved Λ-type doublet of NO in the R-branch was measured using a high-resolution continuous-wave external-cavity quantum cascade laser (cw-EC-QCL) coupled with cavity ring-down spectroscopy (CRDS), involving parity sub-states e and f corresponding to $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ states, respectively [2]. The spectroscopic parameters, such as the Λ-type doublet splitting and the Λ-type doubling constants, were determined for both states. In the presence of three perturbing gases, the pressure broadening effect on Λ-type doublets and the dependence of pressure broadening coefficients on the rotational quantum number J of NO were also investigated. Lastly, the vibrational transition dipole moment value and the Herman-Wallis coefficients were determined from the experimental data. These spectroscopic parameters, obtained through experiments, enhance our fundamental understanding of this diatomic molecule.

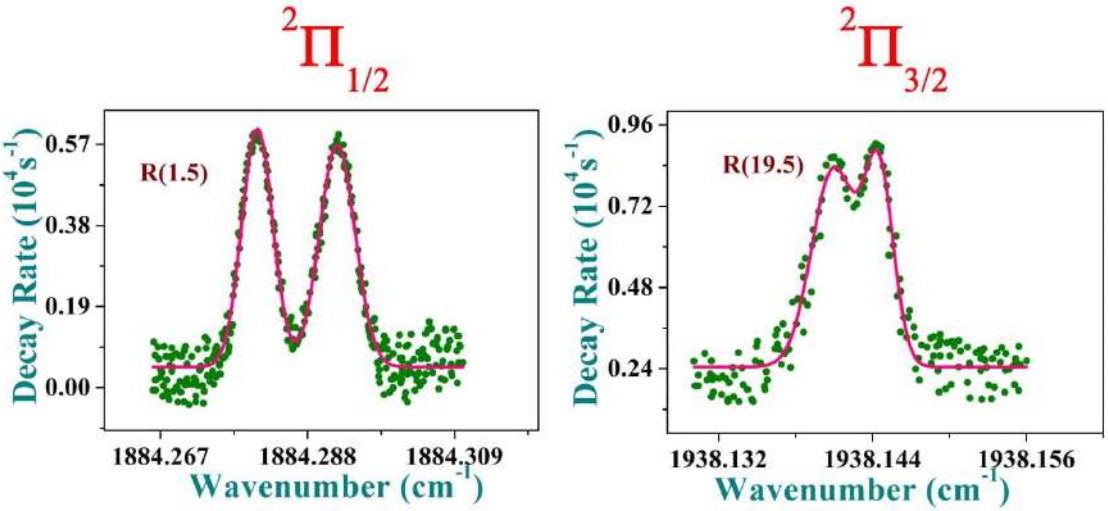


Fig. 1 Λ-doublet spectra of NO for respective state.

References:

[1] Hinkley, R. K., J. A. Hall, T. E. H. Walker, and W. G. Richards. "Λ doubling in 2Π states of diatomic molecules." Journal of Physics B: Atomic and Molecular Physics (1968-1987) 5, no. 2 (1972): 204.

[2] Geuzebroek, F. H., M. G. Tenner, A. W. Kleyn, H. Zacharias, and S. Stotle. "Parity assignment of Λ-doublets in NO X 2Π12." Chemical physics letters 187, no. 5 (1991): 520-526.

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

Ariful Hoque, Tapas Baug

S. N. Bose National Centre for Basic Sciences

Abstract of the Oral Presentation

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 Galactic 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 dependency on the density of the medium. We also find that the abundance ratio decreases linearly as temperature of the cloud increased.

Anomalous Hall effect in layered ferromagnet ZnMnSb

Arunanshu Panda, Nitesh Kumar

Department of Condensed Matter and Materials Physics,
S. N. Bose National Centre for Basic Sciences, Kolkata, West Bengal 700106, India.

Abstract of the Oral Presentation

Materials with layered crystal structure are of particular interest. These materials are ideal candidates for device applications as their structure may allow for exfoliation and easy integration into layered heterostructures, which opens a new route in exploring intrinsic magnetism in the 2D limit. 2D magnetism has been observed in many hexagonal and trigonal materials. Here we report electronic and magnetic properties of layered ZnMnSb single crystals. It has a transition temperature is near room temperature (~298 K) and these room temperature ferromagnets are important for device application. Anomalous Hall effect (AHE) in ZnMnSb was observed up to 275 K but the temperature dependent resistivity measurement doesn't show metallic nature, which is quite surprising because to get AHE, the material should be conducting and it should have finite spontaneous magnetization. This non-metallicity behavior may be due to the disorderness in the compound, to confirm that we have done annealing of our sample. Resistivity measurements of annealed sample shows metallic behavior and we are looking for how annealing affects the anomalous Hall conductivity of the single crystals.

References:

[1] M. Yessik, "The magnetic structure of Mn2P," Philos. Mag., vol. 17, no. 147, pp. 623–632, 1968, doi: 10.1080/14786436808217748.

[2] V. Johnson and W. Jeitschko, "Ferromagnetic anti-PbFCl-type ZnMnSb," J. Solid State Chem., vol. 22, no. 1, pp. 71–75, 1977, doi: 10.1016/0022-4596(77)90190-6.

[3] D. Xiong and Y. Zhao, "Related content Magnetic Properties of MnZnSb," Jpn. J. Appl. Phys., vol. 32, 1993.

[4] S. N. Guin et al., "2006301 (1 of 8) 2D-Berry-Curvature-Driven Large Anomalous Hall Effect in Layered Topological Nodal-Line MnAlGe," Adv. Mater, vol. 33, 2021, doi: 10.1002/adma.202006301.

[5] T. Graf, C. Felser, and S. S. P. Parkin, "Simple rules for the understanding of Heusler compounds," Prog. Solid State Chem., vol. 39, no. 1, pp. 1–50, May 2011, doi: 10.1016/J.PROGSOLIDSTCHEM.2011.02.001.

[6] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, "Anomalous Hall effect," Rev. Mod. Phys., vol. 82, no. 2, pp. 1539–1592, May 2010, doi: 10.1103/REVMODPHYS.82.1539/FIGURES/47/MEDIUM.

[7] P. A. E. Murgatroyd et al., "Chemically Controllable Magnetic Transition Temperature and Magneto-Elastic Coupling in MnZnSb Compounds," Adv. Funct. Mater., vol. 31, no. 17, p. 2100108, Apr. 2021, doi: 10.1002/ADFM.202100108.

Global 21-cm brightness temperature in viscous dark energy models

Ashadul Halder, Shashank Shekhar Pandey, A.S. Majumdar

S.N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt lake city, Kolkata-700106, India

Abstract of the Oral Presentation

We investigate the global 21-cm brightness temperature in the context of viscous dark energy (VDE) models. The bulk viscosity of dark energy perturbs the Hubble evolution of the Universe which could cool baryons faster, and hence, alter the 21-cm brightness temperature. An additional amount of entropy is also produced as an outcome of the viscous flow. We study the combined contribution of Hawking radiation from primordial black holes, decay and annihilation of particle dark matter and baryon-dark matter scattering in the backdrop of VDE models towards modification of the 21-cm temperature. We obtain bounds on the VDE model parameters which can account for the observational excess of the EDGES experiment (-500^{+200}_{-500} mK at redshift $14 < z < 20$) due to the interplay of the above effects. Moreover, our analysis yields modified constraints on the dark matter mass and scattering cross-section compared to the case of the ΛCDM model.

Transport properties of tr-Cr_5Te_8

[1]Banik Rai, [2]Rana Saha, [1]Nitesh Kumar

[1]S. N. Bose National Centre for Basic Sciences, Kolkata-700106, India
[2]Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale) 06120, Germany

Abstract of the Oral Presentation

Research in 2-D magnetic materials has gained quite a good pace in recent days owing to their potential applications in spintronics and next-generation data-storing devices. A potential 2-D magnet is one which has, apart from high T_C, magnetic textures like skyrmions. Magnetic skyrmions are topologically protected and hence can be used for carrying information robustly in memory and logic devices. Skyrmions in a magnetic system can be stabilized via various mechanisms viz. the magnetic dipolar interactions, Dzyaloshinki-Moriya interactions (DMI), frustrated exchange interactions, and four-spin exchange interactions. In particular, DMI-induced skyrmions are observed only in non-centrosymmetric magnets.

We have studied magnetic and transport properties on the bulk sample of one such skyrmion hosting compound—the quasi-2-D ferromagnet tr-Cr_5Te_8. We have performed Lorentz transmission electron microscopy (LTEM) experiments, wherein we have observed Néel-type skyrmions in our compound. Through various arguments, we have tried to establish the fact that the compound crystallizes in the non-centrosymmetric space group *P*3*m*1 instead of the previously reported centrosymmetric *P*-3*m*1. We have also observed hump-like features in the Hall resistivity curve which was not seen before in this compound. Following the observation of similar features in the magnetization curve, we have ruled out the possibility of the presence of THE.

Role of molecular orientation on electron transport in a single molecular junction

Biswajit Pabi and Atindra Nath Pal

Department of Condensed Matter and Materials Physics

Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Sector III, Block JD, Salt Lake, Kolkata700106, India

Abstract of the Oral Presentation

The basic components of a single molecular junction include metallic electrodes, molecular backbone, and metal-molecular interface. While the role of electrodes and the metal/molecule interface have been investigated to some extent, the understanding of the influence of molecular conformation is limited. In this talk, I would like to present the detailed transport behavior of a Ferrocene-based single molecular junction prepared in a mechanically controllable break junction setup. Firstly, we observe that Ferrocene can bind directly with Au and Ag and form stable molecular junctions. Interestingly, temperature-dependent transport reveals interesting conductance features, while at room temperature we observe a significantly high conductance conformation, at low temperatures (77K and 4.2K) conductance histogram exhibits two stable conformations. The DFT-based calculations and Molecular dynamics simulations indicate that two different orientations of Ferrocene molecule inside the junction (parallel and perpendicular to the electrodes) are energetically possible conformations and may lead to two different conductance peaks. Additionally, the two Cp rings of Ferrocene show a rotation at room temperature, forbidding the formation of a chemically stable bond between the Cp ring and Au electrodes, leading to only high conductance conformation (perpendicular geometry) at room temperature. Furthermore, one more possibility of a single molecular junction is that it can be gated by simple mechanical means. Specifically, the charge can be transferred between the electrodes and its molecular bridge when the interelectrode distance is modified, leading to variations in the electronic transport properties of the junction. I will discuss how ferrocene molecular junctions can experience either clear mechanical gating or none, depending on the orientation of the junctions. Overall, our findings establish the significant importance of molecular orientation, one of the key factor for ferrocene-based junctions.

References:

1. Resonant transport in a highly conducting single molecular junction via metal-metal bond

Biswajit Pabi, Štepán Marek, Adwitiya Pal, Puja Kumari, Soumy Jyoti Ray, Arunabha Thakur, Richard Korytár, and Atindra Nath Pal. (To be submitted soon)

2. Temperature dependent conformational accessibility of ferrocene based molecular junction.

Biswajit Pabi, Debayan Mondal, Tal Klein, Adwitiya Pal, Arunabha Thakur, Priya Mahadevan and Atindra Nath Pal. (To be submitted soon)

3. Structural regulations for mechanical gating of molecular junction

Biswajit Pabi, Jakub Šebesta, Richard Korytár, Oren Tal and Atindra Nath Pal. (Under review)

Effect of relative time-scale on steady state measure of a coupled driven system.

Chandradip Khamrai and Sakuntala Chatterjee

Department of Physics of Complex Systems, S. N. Bose National Centre for Basic Sciences

Abstract of the Oral Presentation

We study a coupled driven diffusive system [1] with two species of particles advected by a fluctuating potential energy landscape. As a result of two-way coupling between the landscape and the particles, the system shows an interesting phase diagram as the coupling parameters are varied. In the disordered phase, the landscape and the particles show no long-ranged order. However, the steady state does not satisfy the product measure in general as there are short-ranged correlations present in the system whose exact form is not known. From simulations we have observed that these local short-ranged correlations change systematically with a relative time scale introduced in the dynamics. There is a critical time scale for which the product measure holds. By using the concept of bunchwise balance and irreducible sequence introduced in [2] we can prove the product measure exactly and explain the qualitative change in the short range correlations as the relative time-scale differs from the critical value. The recently developed formalism of nonlinear fluctuating hydrodynamics (NLFH) [3] is being extensively used to study coupled driven systems with multiple conserved quantities. In principle, this formalism requires the knowledge of the exact expression of locally conserved current in terms of local density of the conserved components. Within this formalism we have been able to obtain an exact expression [4] for the critical time-scale at which product measure holds.

References:

[1] Large compact clusters and fast dynamics in coupled nonequilibrium systems by Shauri Chakraborty, Sukla Pal, Sakuntala Chatterjee and Mustansir Barma, Phys Rev E Rapid Comm 93, 050102(R) (2016).

[2] Light and heavy particles on a fluctuating surface: Bunchwis balance, irreducible sequences, and local density-height correlations by Samvit Mahapatra, Kabir Ramola, and Mustansir Barma, Physical Review Research, 2(4):043279, 2020.

[3] Fibonacci family of dynamical universality classes by Vladislav Popkov, Andreas Schadschneider, Johannes Schmidt, and Gunter M Schütz, Proceedings of the National Academy of Sciences, 112(41):12645–12650, 2015.

[4] Effect of relative time-scale on steady state measure of a coupled driven system by Chandradip Khamrai and Sakuntala Chatterjee, (manuscript in preparation).

Optimum transport in a periodically driven lattice gas with short-ranged interaction

Deepsikha Das, Punyabrata Pradhan and Sakuntala Chatterjee

Physics of Complex Systems, S.N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata 700106, India

Abstract of the Oral Presentation

We study a model of hardcore particles with nearest neighbour interaction moving on a one dimensional ring lattice in presence of a time-periodic external potential generated by periodic movement of a defect in the lattice. Using numerical simulations and mean-field calculations we have derived the conditions for optimal transport, i.e. maximum possible particle current in the system and find that the presence of nearest neighbour interaction considerably affects the current. We observe that a repulsive interaction generally enhances the current, while attractive interaction suppresses it. We show that a moving defect always induces current in the direction opposite to that of the defect movement, while bulk diffusion causes a current in the same direction of the defect movement. Interplay between the periodicity of the external drive and particle diffusion, causes net current to reverse its direction on variation of particle density, defect velocity and interaction strength. For small particle density, current becomes maximum when the repulsion is strongest. However, for large particle density, when the system is overcrowded, very strong repulsion blocks certain transitions and reduces the current. Optimum transport is therefore obtained when the interaction is strongly repulsive but not assuming its highest possible strength.

Accelerating Protein Conformational Space Exploration with Autoencoders and VAEs

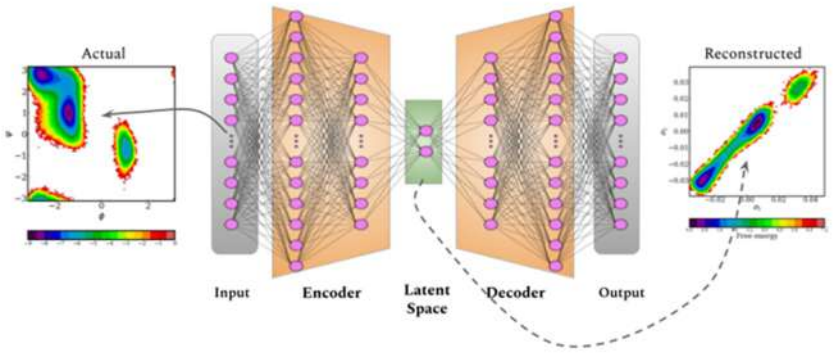
Dibyendu Maity, Suman Chakrabarty

S.N. Bose National Centre for Basic Sciences

Abstract of the Oral Presentation

Molecular dynamics (MD) simulations are a crucial tool for exploring the conformational space of proteins. However, extensive sampling of protein conformations is computationally demanding and time-consuming, primarily due to the high energy barriers that impede efficient sampling of configurational space. Biased sampling using prespecified collective variables (CVs) can be employed to drive the simulation; however, identifying suitable CVs that capture important collective dynamical motions remains a challenge.Recently, autoencoders have emerged as a type of artificial neural network that can learn suitable CVs in MD simulations. By learning nonlinear CVs that are explicit and differentiable functions of atomic coordinates, autoencoders can offer a faster approach for exploring protein conformational space in MD simulations. Autoencoders can simultaneously discover and directly accelerate along data-driven CVs[1], thus enabling more efficient sampling of configurational space.

This study presents the use of variational autoencoders (VAEs), a type of deep learning model, to identify suitable CVs in MD simulations. The results show that VAEs[2] outperform traditional autoencoders in identifying good CVs and representing the complex high-dimensional input in a lower-dimensional encoded representation. The study also highlights the importance of selecting efficient feature-engineered input, as machine learning models are sensitive to it.The use of autoencoders and VAEs in MD simulations presents a promising avenue for improving the efficiency of exploring protein conformational space. The presented approach can facilitate efficient exploration of protein conformational space in MD simulations, enabling the generation of unsampled protein conformations and the acceleration of sampling processes to explore hidden spaces in the conformational landscape.



References:

[1] Chen, W., & Ferguson, A. L. (2018). Molecular enhanced sampling with autoencoders: On-the-fly collective variable discovery and accelerated free energy landscape exploration. In Journal of Computational Chemistry (Vol. 39, Issue 25, pp. 2079–2102). Wiley. https://doi.org/10.1002/jcc.25520

[2] Tian, H., Jiang, X., Trozzi, F., Xiao, S., Larson, E. C., & Tao, P. (2021). Explore Protein Conformational Space With Variational Autoencoder. In Frontiers in Molecular Biosciences (Vol. 8). Frontiers Media SA. https://doi.org/10.3389/fmolb.2021.781635

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

Diya Ram, Soumen Mondal

Department of Astrophysics and High Energy Physics

Abstract of the Oral Presentation

M dwarfs are the most numerous stars in our Galaxy, amounting to about two-thirds (~70%) in number and about 40% 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 $M_{\odot}$ and have effective temperatures of 2500 - 4000 K. Due to their convective interiors and rotation, they have relatively strong magnetic fields and are capable of producing very strong flares, are triggered by magnetic reconnection with energies up to 10^4 times or greater than the strongest flare (~10^{32}) observed on the Sun. To understand their magnetic activity, we have undertaken optical/Near-IR spectroscopic studies of a unique sample of M-dwarfs including some having strong flares and magnetic fields. Using Himalayan Faint Object spectrograph (HFOSC) and TIFR Near-IR spectrograph (TIRSPEC) instruments on the 2-m Himalayan Chandra Telescope (HCT) telescope, and TIFR-ARIES Near Infrared Spectrometer (TANSPEC) 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) are detected in the observed spectra, and are using to characterize these late-type dwarfs. We utilize Transiting Exoplanet Survey Satellite (TESS) photometric data of M-dwarfs to investigate the relationship between star-spots, stellar flares and magnetic fields, etc. Our aim is to understand the magnetic activities on those active M dwarfs by using photometric and spectroscopic data. Data analysis is on going and we will present a few preliminary results in this presentation.

References:

Bell et al 2012, PASP, 124,14B

Delfosse, X., et al., 2000, A&A, 364, 217

Newton et al 2017, ApJ, 834, 85

Shulyak et al 2019, A&A 626, A86

West et al 2011, ASPC, 448, 1407

Schöfer et al., 2019, A & A

Rajpurohit et al, 2018, A&A 620, A180

Neutrino oscillation caused by spacetime geometry

Indrajit Ghose, Riya Barick, Amitabha Lahiri

Satyendra Nath Bose National Centre for Basic Sciences, Kolkata

Abstract of the Oral Presentation

A first order theory of gravity is introduced and coupled to Quantum Mechanical Matter. It is shown that fermionic matter couples to the antisymmetric part of the connection. The antisymmetric degree of freedom can be integrated out and we get an effective theory with a four fermi interaction. After passing through a thermal background the four fermi interaction contributes to neutrino effective mass. [1] This effective mass can change the current oscillation parameters and gives a non-null conversion even for a degenerate mass spectrum. [2]

References:

1. S. Chakrabarty and A. Lahiri, "Geometrical contribution to neutrino mass matrix," Eur. Phys. J. C 79, no.8, 697 (2019) [arXiv:1904.06036 [hep-ph]]

2. I. Ghose, R. Barick and A. Lahiri, "Neutrino oscillation caused by spacetime geometry", accepted in LHEP

ARPES and its application in the study of some TMDCs

Indrani Kar and Thirupathaiah Setti

Department of Condensed Matter and Materials Physics, S N Bose National Centre for Basic Sciences, Salt Lake, JD Block, Sector III, Bidhannagar, Kolkata-700106, India

Abstract of the Oral Presentation

Transition metal dichalcogenides (TMDCs) are available with wide range of electronic properties starting from the metallic, to the semimetallic, to the semiconducting, and to the Mott insulators. This group of materials are of great research interests due to their potential applications in spintronics and optoelectronics devices. In addition, the diverse electronic properties of TMDCs include the charge density wave (CDW), spin density wave (SDW), magnetism, superconductivity, and topological properties. In recent years, band engineering is widely applied on this group of materials due to weak van der Waals forces between the layers to uncover the exotic physical properties. Thus, examining the electronic band structure of these materials is crucial for microscopic understanding of their peculiar physical properties.

Here, we performed angle-resolved photoemission spectroscopy (ARPES) studies on various TMDCs such as $ZrSe_2$, $ZrTe_2$, $TaTe_2$, and $NiTe_2$ to understand their low-energy electronic band structure in the vicinity of the Fermi level. ARPES studies on $ZrTe_2$ demonstrate free charge carriers at the Fermi level, which is further confirmed by the DFT calculations. An equal hole and electron carrier density estimated from the ARPES data, points to $ZrTe_2$ being a semimetal. The DFT calculations further suggest a band inversion between Te-*p* and Zr-*d* states at the *Γ* point, hinting at the nontrivial band topology in $ZrTe_2$. Thus, our studies suggest that $ZrTe_2$ is a topological semimetal. Also, a comparative band structure study is done on $ZrSe_2$, which shows a semiconducting nature of the electronic structure with an indirect band gap of 0.9 eV between *Γ(A)* and *M(L)* high-symmetry points. From this comparative study between $ZrTe_2$ and $ZrSe_2$ we conclude that the metal-chalcogen bond length plays a crucial role in tuning the electronic properties from semiconductor ($ZrSe_2$) to a topological semimetal ($ZrTe_2$). From the ARPES studies on $TaTe_2$ which is one of the charge density wave (CDW) materials from the group V TMDCs, we find that the Fermi surface topology of $TaTe_2$ is quite complicated compared to its isovalent compounds such as TaS_2, $TaSe_2$, and isostructural compound $NbTe_2$. Most importantly, we discover that the surface electronic structure of *1T'*-$TaTe_2$ has more resemblance to the *2H*-$TaTe_2$, while the bulk electronic structure has more resemblance to the hypothetical *1T*-$TaTe_2$. These experimental observations are thoroughly compared with the DFT calculations performed on *1T* -, *2H*-, and *2H* (monolayer)/*1T* -$TaTe_2$. We further notice that the Fermi surface topology is temperature independent up to 180 K, confirming that the *2H* phase on the surface is stable up to 180 K and the CDW order is not due to the Fermi surface nesting. Also, our ARPES data on $NiTe_2$ clearly show a surface Dirac point observed at a binding energy of 1.45 eV which is consistent with an earlier theoretical prediction. Thus, our results for the first time experimentally show that $NiTe_2$ is a topological TMDC. Our ARPES data further suggest a metallic nature of $NiTe_2$. We find that overall, the electronic structure of $NiTe_2$ has similarities with the other topological TMDCs like $PdTe_2$, $PtTe_2$, and $PtSe_2$.

References:

1. Indrani Kar, Joydeep Chatterjee, Luminita Harnagea, Y. Kushnirenko, A. V. Fedorov, Deepika Shrivastava, B. Büchner, P. Mahadevan, and S. Thirupathaiah, Metal-chalcogen bond-length induced electronic phase transition from semiconductor to topological semimetal in ZrX_2(X=Se and Te), Phys. Rev. B 101, no. 16 (2020): 165122.

2. Indrani Kar, Kapildeb Dolui, Luminita Harnagea, Yevhen Kushnirenko, Grigory Shipunov, Nicholas C. Plumb, Ming Shi, Bernd Büchner, and Setti Thirupathaiah, Experimental Evidence of a Stable 2H Phase on the Surface of Layered 1T'-$TaTe_2$, J. Phys. Chem. C 125, no. 1 (2021): 1150-1156.

3. Indrani Kar, Luminita Harnegea, Soma. Banik, Surjeet Singh, and Setti Thirupathaiah, Observation of surface Dirac state in transition metal dichalcogenide $NiTe_2$ using ARPES, AIP Conference Proceedings 2265, no. 1 (2020): 030361.

Robust half-metallicity and Topological Properties in square-net Potassium Manganese Chalcogenides

Koushik Pradhan[1], Prabuddha Sanyal[2], and Tanusri Saha-Dasgupta[1]

[1]*S.N.Bose National Center for Basic Sciences, JD Block, Sector-III, Kolkata-700106*

[2]*Moulana Abul Kalam Ajad University of Technology, XG5V+27R, Haringhata Farm, West Bengal 741249*

Abstract of the Oral Presentation

Combining ab-initio and model Hamiltonian approaches, we investigate the electronic, magnetic and topological properties of Potassium Manganese chalcogenides that host square nets of Mn and chalcogen atoms. Our analysis establishes these compounds to be robust half-metallic, ferromagnets. The origin of ferromagnetism in these compounds is found to be based on kinetic energy-driven double-exchange mechanism, first proposed for Sr_2FeMoO_6, a double-perovskite compound. Presence of finite spin-orbit coupling at chalcogen sites, triggers non-trivial topology of the chalcogen-derived bands at the conducting channel, dominating the electronic structure close to the Fermi level. This puts the studied compounds in the class of topological half-metals with appreciable values of anomalous Hall conductivity, opening up the application possibility in topological quantum spintronics. Cleavability of these layered compounds makes the situation further promising.

References:

1. K. Pradhan, P. Sanyal, and T. Saha-Dasgupta (manuscript under communication)

Perturbing the bond disproportionated state in NdNiO3

Krishnendu Patra[1], Sagar Sarkar[2], Priya Mahadevan[1]

S N Bose National Center for Basic Science

Pohang University of Science and Technology

Abstract of the Oral Presentation

The rare-earth nickelates with the exception of LaNiO3 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. One route adopted is to explore carrier doping by doping at the rare earth site. Both electron and hole doping are found to tune the effective charge transfer energy, with the latter increasing it and providing a route to tune to a positive value, where we do not expect a bond disproportionated state. 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.

References:

1. B. Mandal et al., arXiv 1701.06819.

Explicit existence of the Berry phase for harmonic oscillators in noncommutative space

Manjari Dutta[1], Shreemoyee Ganguly[2], Sunandan Gangopadhyay[1]

[1] *S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700106, India*

[2] *University of Engineering and Management (UEM), Newtown, Kolkata 700156, India*

Abstract of the Oral Presentation

This work is devoted to finding the explicit existence of the Berry phase for harmonic oscillators in time dependent noncommutative space. In this regard, two time dependent periodic model systems are considered in time dependent noncommutative space. While the first model contains a scale invariant term in the original Hamiltonian from the beginning, the second model is a system in which the scale invariant term appears due to a shift of variables from the noncommutative space to the commutative space. Then Lewis invariant technique is employed to obtain the generic form of Berry's geometric phase under adiabatic approximation. Finally, the existence of the Berry phase is tested explicitly for both systems. Our study reveals that an apparent existence of Berry phase in a generic form may not always lead to a non zero Berry phase.

References:

1. Berry M V 1984 Proc. R. Soc. Lond. A 392 45

2. Berry M V 1985 J. Phys. A: Math. Gen. 18 15

3. Mezincescu L Star Operation in Quantum Mechanics hep-th/0007046

4. Biswas S, Nandi P and Chakraborty B 2020 Phys. Rev. A 102 022231

5. Dittrich W and Reuter M 1991 Phys. Lett. A 155 94

6. Lewis H R Jr. and Riesenfeld W B 1969 J. Math. Phys. 10 1458

7. Dey S and Fring A 2014 Phys. Rev. D 90 084005

8. Ermakov V 1880 Univ. Izv. Kiev. 20 1

9. Pinney E 1950 Proc. Am. Math. Soc. 1 681

Ground-state phase diagram of antiferromagnetic spin−1/2 coupled trimer chain

Manodip Routh[1], Sudip Kumar Saha[1], Aslam Parvej[2], and Manoranjan Kumar[1]

1Department of Condensed Matter and Materials Physics, S.N. Bose National Centre for Basic Sciences, Kolkata 700098, India.

2Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Abstract of the Oral Presentation

The ground state properties of a spin-1/2 coupled trimer chains are investigated using density-matrix renormalization group (DMRG) technique. We consider only the nearest-neighbor (NN) exchange as trimerized interaction, i.e., NN exchange interaction at every 3rd NN bond along the spin chain is J_1' and $J_1' < J_1$ ($J_1$is the NN exchange between other neighboring spin-1/2). The next nearest-neighbor (NNN) exchange interactions J_2 is uniform in our study and the Hamiltonian is in unit of $J_1 (J_1 = 1)$. We restrict our study for antiferromagnetic (AF) interactions ($J_1, J_1', J_2 > 0$) and our calculations are limited for the range $0 < J_1' < 1$ and $0 < J_2 < 1$. The main goal of this manuscript is to demonstrate the phase diagram of spin-1/2 trimerized chain based on ground state properties with a special attention on the phase transition between gapless trimer phase to gapped dimer phase. At small intratrimer exchange limit ($0 < J_1' < 0.4$) three distinct phases are found: spin fluid (SF) phase at small J2, trimerized phase with high spin ground state at intermediate values of J2 and gapped spiral phase at large J2. However, large intratrimer exchange limit ($0.4 < J_1' < 1$) does not support the trimer phase. The SF and spiral phases still persist at this limit at small and large J2, respectively, and in between these phases a gapped dimer phase occurs.

References:

1. Z. G. Soos, A. Parvej, and M. Kumar, J. Phys.: Condens. Matter 28, 175603 (2016).

2. G. Giri, D. Dey, M. Kumar, S. Ramasesha, and Z. G. Soos, Phys. Rev. B 95, 224408 (2017)

3. B. Gu, G. Su, and S. Gao, Phys. Rev. B 73, 134427 (2006).

4. B. Gu and G. Su, Phys. Rev. B 75, 174437 (2007).

5. R. R. Montenegro-Filho, E. J. P. Silva-J´unior, and M. D. Coutinho-Filho, Phys. Rev. B 105, 134423 (2022).

Exploring noble gas species in the radiation-dominated region

Milan Sil[1], Ramkrishna Das[1], Ruchi Pandey[2], Ankan Das[3]

[1]*Department of Astrophysics and High Energy Physics, S. N. Bose National Centre for Basic Sciences*
[2]*Astronomy and Astrophysics Division, Physical Research Laboratory*
[3]*Institute of Astronomy Space and Earth Science*

Abstract of the Oral Presentation

Two noble gas molecular cations, argonium (ArH^+) and hydro-helium or helenium (HeH^+), are discovered toward the two radiation-dominated environments in space: the Crab nebula supernova remnant and the planetary nebula (NGC 7027), respectively. The elemental abundance of neon is lower than helium but higher than that of argon. However, the neonium cation (NeH^+) is yet to be identified in space. Here, I would like to show some modeling results of the noble gas chemistry containing hydride cations. The chemical evolution of these species under the diffuse and exotic environment (the Crab nebula filamentary region) is studied. The intrinsic line surface brightness is calculated to find a favorable parameter space that can explain the observational features for the condition suitable in the Crab filamentary region. The possibility of detecting some hydride cations in the Crab nebula environment is also highlighted. As an ongoing work, I will also show some modeling results of some Nova ejecta, where HeH^+ abundance is in the observed range, and some rotational transition could be proposed to observe using NASA James Webb Space Telescope (JWST).

References:

Sil, M., Das RK, Pandey, R., & Das, A (in preparation)

Singlet quantum phases and magnetization of the frustrated spin-1/2 ladder with ferromagnetic (F) exchange in legs and alternating F–AF exchange in rungs

Monalisa Chatterjee, [1] Manoranjan Kumar, [1] and Zoltán G. Soos [2]

[1] *S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata 700106, India*

[2] *Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA*

Abstract of the Oral Presentation

The magnetization M(h) is used to identify three singlet quantum phases of the ladder with isotropic exchange interactions. The Dimer phase with frustrated F exchanges in rungs and legs has a first-order M(h) transition at 0 K from singlet to ferromagnetic at the saturation field h_s. The Haldane-DAF phase with strong F exchange in rungs and net AF exchange between rungs has continuous M(h) and is adiabatically connected to the S = 1 Heisenberg AF chain. The AF phase with strong F exchange in legs and net AF exchange between legs has continuous M(h) and is adiabatically connected to the spin-1/2 $J_1 - J_2$ model with $J_1 > 0$ and $J_2 < 0$. All three singlet phases have finite gaps to the lowest triplet state.

References:

1. D. Dmitriev, V. Krivnov, and A. Ovchinnikov, Eur Phys J B : Condensed Matter and Complex Systems 14, 91 (2000).

2. K. Hida, K. Takano, and H. Suzuki, J. Phys. Soc. Japan 82, 064703 (2013).

3. S. Sahoo, D. Dey, S. K. Saha, and M. Kumar, J. Condens. Matter Phys. 32, 335601 (2020).

4. S. R. White, Phys. Rev. Lett. 69, 2863 (1992).

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

Nishant Garg, Tapas Baug

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

Abstract of the Oral Presentation

Even though filamentary structure of Galactic molecular clouds was 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 graviationally unstable clumps.

Kinetics of Initial Charge Separation in the Photosynthetic Reaction Centers of *Rhodobacter sphaeroides*

Prasanta Kundu and Gautam Gangopadhyay

S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata-700106, India. E-mail: prasanta.kundu@bose.res.in

Abstract of the Oral Presentation

Photosynthesis that efficiently converts light energy into chemical energy is initiated by transferring an electron from the photoexcited donor to a suitable acceptor. In the reaction center of photosynthetic bacterium *Rhodobacter sphaeroides*, during the early stage of photosynthesis, an electron is transferred from a pair of bacteriochlorophylls to the bacteriopheophytin through an adjacent bridging chlorophyll. The experimental study by Wang *et al*, performed on the reaction centers of wild type and 14 different mutants of the bacterium, recognized the motion of the surrounding protein environment, structured by 39 tryptophan residues, with the aid of changes in the tryptophan absorption spectra at 280 nm and measured the rates of electron transfer by detecting the stimulated emission signals from the excited donor (transient absorbance changes at 930 nm).[1] Remarkably, the decay profiles at both the wavelengths were nonexponential, however, the protein's response remained essentially identical for all of the species on the timescale of electron transfer. The kinetics of primary charge separation thereby was effectively modulated by the slower dynamics of the reaction center protein, leading to dynamic disorder in the reaction pathway. Here, in this work, to yield a kinetic elucidation of the observed results, we suggest a stochastic kinetic study of the initial electron transfer reaction based on a multistate framework.[2] Our approach to the disorder-driven complex kinetics, unlike the earlier dynamic analysis,[3] remains independent of the direct use of the 280 nm data. Rather, exploiting a rational description of the reaction coordinate, effected by the relaxation of the surrounding protein environment,[4] we become able to reproduce the measured charge transfer kinetics quantitatively on account of a fairly concise but sufficient mathematical analysis.[5] Moreover, comparisons of the extracted relative free energies of electron transfer and the available independent electrochemical estimates show exact agreement for the case of selected mutants.[6,7]

References:

1. Wang, H.; Lin, S.; Allen, J. P.; Williams, J. C.; Blankert, S.; Laser, C.; Woodbury, N. W. Protein Dynamics Control the Kinetics of Initial Electron Transfer in Photosynthesis. Science 2007, 316, 747-750.

2. Kou, S. C.; Cherayil, B. J.; Min, W.; English, B. P.; Xie, X. S. Single-molecule Michaelis-Menten Equations. J. Phys. Chem. B 2005, 109, 19068-19081.

3. Kundu, P.; Dua, A. Protein Dynamics Modulated Electron Transfer Kinetics in Early Stage Photosynthesis. J. Chem. Phys. 2013, 138, No. 045104.

4. Min, W.; Luo, G.; Cherayil, B. J.; Kou, S. C.; Xie, X. S. Observation of a Power-Law Memory Kernel for Fluctuations within a Single Protein Molecule. Phys. Rev. Lett. 2005, 94, No. 198302.

5. Kundu, P. Kinetics of Initial Charge Separation in the Photosynthetic Reaction Centers of Rhodobacter sphaeroides. J. Phys. Chem. B 2022, 126, 3470-3476.

6. Lin, X.; Murchison, H. A.; Nagarajan, V.; Parson, W. W.; Allen, J. P.; Williams, J. C. Specific Alteration of the Oxidation Potential of the Electron Donor in Reaction Centers from Rhodobacter sphaeroides. Proc. Natl. Acad. Sci. U.S.A. 1994, 91, 10265−10269.

7. Williams, J. C.; Haffa, A. L. M.; McCulley, J. L.; Woodbury, N. W.; Allen, J. P. Electrostatic Interactions Between Charged Amino Acid Residues and the Bacteriochlorophyll Dimer in Reaction Centers from Rhodobacter sphaeroides. Biochemistry 2001, 40, 15403−15407.

Magnon–Magnon Coupling in $Ni_{80}Fe_{20}$ Nanocross Array

Pratap Kumar Pal[1], Sudip Majumder[1], YoshiChika Otani[2,3] and Anjan Barman[1,*]

[1]*Department of Condensed Matter Physics and Material Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700 106, India*

[2]*Center for Emergent Matter Science, RIKEN, 2-1 Hirosawa, Wako 351-0198, Japan*

[3]*Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan*

Abstract of the Oral Presentation

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 300 nm, edge-to-edge separation (S) of 200 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 phenomena 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.

References:

1. J. Chen, C. Liu, T. Liu, Y. Xiao, K. Xia, G. E. W. Bauer, M. Wu, and H. Yu, Strong Interlayer Magnon-Magnon Coupling in Magnetic Metal-Insulator Hybrid Nanostructures, Physical Review Letters 120, 217202 (2018).

2. Y. Li, W. Cao, V. P. Amin, Z. Zhang, J. Gibbons, J. Sklenar, J. Pearson, P. M. Haney, M. D. Stiles, W. E. Bailey, V. Novosad, A. Hoffmann, and W. Zhang, Coherent Spin Pumping in a Strongly Coupled Magnon-Magnon Hybrid System, Physical Review Letters 124, 1 (2020).

3. K. Adhikari, S. Sahoo, A. K. Mondal, Y. Otani, and A. Barman, Large Nonlinear Ferromagnetic Resonance Shift and Strong Magnon-Magnon Coupling in N I80 F E20 Nanocross Array, Physical Review B 101, 54406 (2020).

Nonequilibrium thermodynamic signature of chimeras in the chemical reaction network

Premashis Kumar and Gautam Gangopadhyay

S. N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata 700 106

Abstract of the Oral Presentation

Chimera, a counterintuitive emergent behavior identified as distinguishable spatial coexistence of coherent and incoherent dynamics, has been investigated in the reaction-diffusion system of a generic chemical reaction

network by implementing a modified complex Ginzburg-Landau equation in the presence of global coupling. For an arbitrary control parameter value, we have systematically acquired the evolution of central nonequilibrium thermodynamic entities corresponding to the chimera state of the system. The temporal evolution of the entropy production rate (EPR) exhibits a beat pattern, whereas the spatial EPR captures a symmetric profile associated with the incoherent regime of the chimera. More importantly, by recognizing the spatial energetics profile of the chimera state as the Gabor elementary function, we infer that the information uncertainty principle plays a guiding role in shaping the chimera energetics. Further, by alternating the amplitude and frequency ratio of the mean field, we have demonstrated transition among different possible states in this framework and differentiated these dynamic states based on their thermodynamic signatures. Investigating the dynamic states in the collective system from an energetic and entropic viewpoint would shed new light on the control and possible application of such phenomena.

References:

Kumar, P., & Gangopadhyay, G. (2022). Nonequilibrium thermodynamic characterization of chimeras in a continuum chemical oscillator system. Physical Review E, 105(3), 034208.

On Composition of Multipartite Quantum Systems: Perspective From Quantum Information Theory

Ramkrishna Patra[1], Sahil Gopalkrishna Naik[1], Edwin Peter Lobo[2], Samrat Sen[1], Govind Lal Sidhardh, Mir Alimuddin[1], Tamal Guha[3], Some Sankar Bhattacharya[4], and Manik Banik[1]

[1]*Department of Physics of Complex Systems, S. N. Bose National Center for Basic Sciences, Kolkata, India*

[2] *Laboratoire d'Information Quantique, Universite libre de Bruxelles (ULB), Av. F. D. Roosevelt 50, 1050 Bruxelles, Belgium*

[3] *Department of Computer Science, The University of Hong Kong, Pokfulam Road, Hong Kong*

[4] *International Centre for Theory of Quantum Technologies, University of Gdansk, Wita Stwosza 63, 80-308 Gdansk, Poland*

Abstract of the Oral Presentation

Figuring out the physical rationale behind natural selection of quantum theory is one of the most acclaimed quests in quantum foundational research. This pursuit has inspired several axiomatic initiatives to derive a mathematical formulation of the theory by identifying the general structure of state and effect space of individual systems and specifying their composition rules. This generic framework can allow several consistent composition rules for a multipartite system even when state and effect cones of individual subsystems are assumed to be quantum. Nevertheless, none of these compositions allow beyond quantum space-like correlations for any bipartite system. In this work, we show that such bipartite compositions can admit stronger than quantum correlations in the time-like domain and, hence, indicates pragmatically distinct roles carried out by state and effect cones. We discuss the consequences of such correlations in a communication task, which accordingly opens up a possibility of testing the actual composition between elementary quanta. The principle of information causality, proposed as a generalization of no signaling principle, has efficiently been applied to outcast beyond quantum correlations as unphysical. We show that this principle when utilized properly can provide a physical rationale for the structural derivation of multipartite quantum systems.

References:

1. *S. G. Naik, E. P. Lobo, S. Sen, R. K. Patra, M. Alimuddin, T. Guha, S. S. Bhattacharya, and M. Banik; Composition of Multipartite Quantum Systems: Perspective from Timelike Paradigm, Phys. Rev. Lett. 128, 140401 (2022).*

2. *S. Sen, E. P. Lobo, R. K. Patra, S. G. Naik, M. Alimuddin, A. D. Bhowmik, and M. Banik; Timelike correlations and quantum tensor product structure, Phys. Rev. A 106, 062406 (2022).*

3. *R. K. Patra, S. G. Naik, E. P. Lobo, S. Sen, G. L. Sidhardh, M. Alimuddin, and M. Banik; Principle of information causality rationalizes quantum composition, arXiv:2208.13996 (2022).*

Contrasting hydration dynamics in presence of Guanidinium ions and its possible effect on protein (de)stability

Ria Saha[1], Subhadip Chakraborty[1], Krishnendu Sinha[1], Partha Pyne[1], Anjan Barman[2], Suman Chakrabarty[1], Rajib Kumar Mitra[1]

[1] *Department of Chemical and Biological Sciences, S N Bose National Centre for Basic Sciences, Kolkata 700106, India;*
[2] *Department of Condensed Matter and Materials Physic, S N Bose National Centre for Basic Sciences, Kolkata 700106, India*

Abstract of the Oral Presentation

Guanidinium cation (Gdm^+) in known to serve as a potent protein denaturant over decades. It is well-known that the protein (de)stabilizing ability of Gdm^+ is dependent on the type of its counter-ion(s) [1, 2]. In spite of several theoretical as well as experimental efforts, the molecular mechanism behind such contrasting nature of Gdm^+ salts remains elusive. Here, we probe the interaction of a well-known protein denaturant GdmCl and a protein stabilizer Gdm_2SO_4 with a model molecule N-methyl acetamide (NMA) having an amide bond (similar to that in protein backbone). Electrochemical impedance spectroscopy (EIS) deciphers the effect of counterions on the activity of Gdm^+, specifically at electrode interface (in the frequency range of 1 Hz-1 MHz). Terahertz time domain spectroscopy (TTDS; 0.2-2.5THz) provides distinct information regarding the alteration of slow water-relaxation timescale during NMA-Gdm^+ interactions. We further investigate the change in NMA hydration after interactions with Gdm^+ using ATR THz-FTIR (1.5-22.5 THz, 50 to 750 cm^{-1}) spectroscopy technique. Our experimental study illustrates that the counterion-specific solvation of Gdm^+ plays a key role in protein (de)stability which is also supported by our MD simulation analysis.

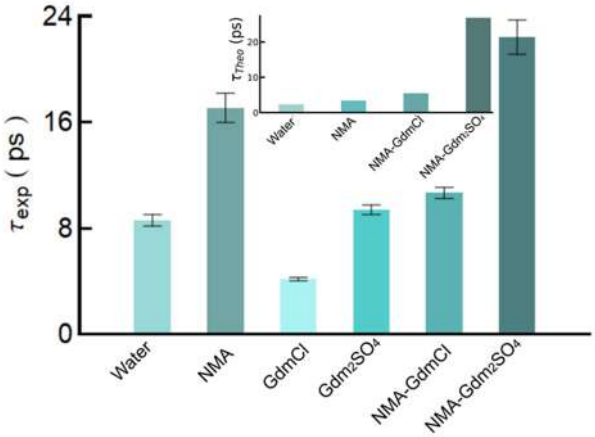


Fig. 1. Relaxation timescale (τ) (both experimental and theoretical) as a function of only water, Gdm^+ salts (at concentration 4M) solutions, and NMA (at concentration 2M) solutions in absence and presence of Gdm^+ salts; Explicitly associates with the spontaneous restructuring of the hydrogen bond network.

References:

[1] C. E. Dempsey, P. E. Mason, J. W. Brady, and G. W. Neilson, J. Am. Chem. Soc. 129, 15895 (2007).

[2] A. H. Viga, et al., J. Phys. Chem. Lett. 4, 3397 (2013).

[3] P. E. Mason, et al., J. Phys. Chem. B. 113, 3227 (2009).

[4] P. E. Mason, et al., J. Am. Chem. Soc. 131, 16689 (2009).

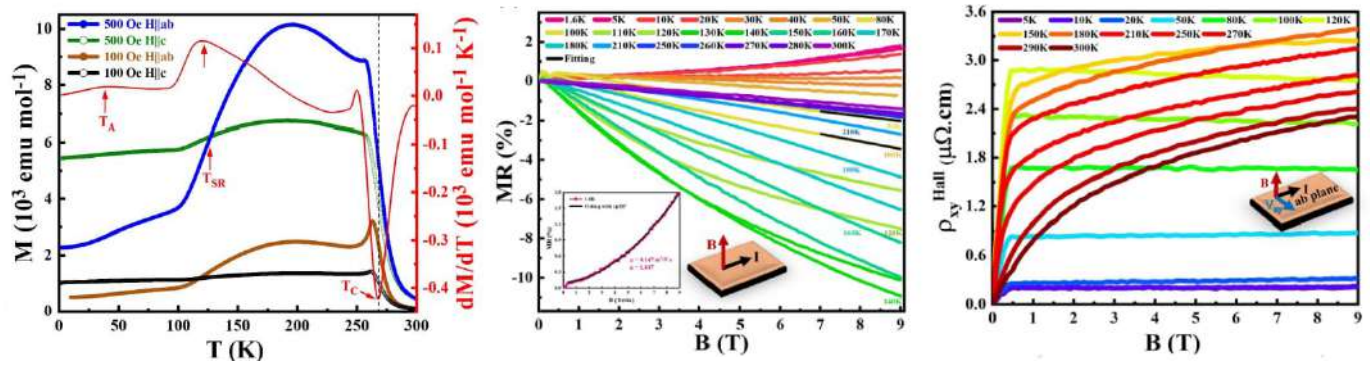
Unusual Magneto-transport and Anomalous Hall Effect in Two-dimensional van der Waals Ferromagnet Fe_4GeTe_2

Riju Pal[1], Buddhadeb Pal[1], Suchanda Mondal[2], Prabhat Mandal[1, 2] and Atindra Nath Pal[1]

[1]*Department of Condensed Matter Physics and Material Sciences,*
S. N. Bose National Centre for Basic Sciences, Block–JD, Sector–III, Salt Lake, Kolkata, 700106, India
[2]*Saha Institute of Nuclear Physics, HBNI, 1/AF Bidhannagar, Calcutta 700064, India*

Abstract of the Oral Presentation

Fe_4GeTe_2 (F4GT), an itinerant van der Waals (vdW) ferromagnet having T_C closed to room temperature (~ 270K), attracted a lot of attention due to its unique magnetic properties. In particular, it exhibits an additional transition (T_{SR}) apart from the ferromagnetic transition where the easy axis of magnetization changes from in-plane to out-of-plane direction[1]. While the nature of magnetic transition in F4GT has been investigated to some extent, the electronic transport and the role of various scattering mechanisms have not been investigated in details. Here, we have studied the magneto-transport in a multilayer (thickness ~ 95 nm) Hall bar device fabricated on 300 nm Si/SiO_2 substrate. Interestingly, the zero field four-terminal resistivity shows negligible change in resistivity near the FM transition unlike the typical metallic ferromagnet, whereas, it exhibits a dramatic fall in resistivity near the spin reorientation transition (T_{SR}). An additional anomaly in the $d\rho/dT$ curve was observed near T ~ 38K (T_Q), below which the resistivity shows quadratic temperature dependence according to the Fermi liquid behavior, further confirmed by the magnetic field dependence. The temperature dependent Hall data exhibits important consequences. The ordinary Hall coefficient changes sign near T_{SR} indicating the change in majority carriers which corresponds to the Fermi surface reconstruction associated with the spin reorientation transition. It also possesses significant anomalous Hall conductivity from ~ 123 $\Omega^{-1}cm^{-1}$ (T ≈ 5K) to the maximum value of ~ 366 $\Omega^{-1}cm^{-1}$ near T_{SR}. While the low temperature part may originate due to the intrinsic KL mechanism[2], our analysis indicates that the temperature dependent AHE is primarily appearing due to the side jump mechanism[3] as a result of the spin-flip electron-magnon scattering. In a similar manner, the magnetoresistance (MR) data also exhibits nonmonotonic behavior with a significant large negative MR (~ 11%) near T_{SR} and becomes positive below ~ 38 K. As positive MR signifies dominance of orbital effect, the negative MR reflects the reduction of electron-magnon scattering by the application of magnetic field. Our study demonstrates an interplay between magnetism and band topology and its consequence on electron transport in Fe_4GeTe_2, important for its future application in spintronic devices.



References:

1. Seo, Junho, et al. Nearly room temperature ferromagnetism in a magnetic metal-rich van der Waals metal. Science advances 6, 1 (2020): eaay8912.
2. Karplus, R. & Luttinger, J. M. Hall Effect in Ferromagnetics. Phys. Rev. 95, 1154 (1954).
3. Berger, L. Side-Jump Mechanism for the Hall Effect of Ferromagnets. Phys. Rev. B 2, 4559 (1970).

Enthalpic and Entropic Contributions in the Mixing Thermodynamics of Deep Eutectic Solvents: The Effect of Incorporating Interactions

Rik Niranjan Mukherjee[1,2], Ranjit Biswas[1], Pradip Kumar Ghorai[2]

[1]*CBS department, S N Bose National Centre for Basic Sciences*
[2]*Department of Chemical Sciences, IISER-Kolkata*

Abstract of the Oral Presentation

Theoretical modeling of solid-liquid equilibria is necessary for the appropriate choice (among numerous possible candidates) of pure components to form deep eutectic solvents with suitable physicochemical properties[1]. Thermodynamic models attempt to parameterize the non-ideality of the mixture and connect it to the liquidus temperature of the deep eutectic solvents[2]. Though the Gibbs free energy change for mixing the constituents can be related to the melting properties of the solid mixture, still the partitioning of enthalpy and entropy contribution is ambiguous. Available models pack all the interactions into the enthalpy term and only combinatorial effects are included in the entropy contribution[3]. In this work, we devise a theoretical model to identify the enthalpic and entropic contribution to the Gibbs free energy change for mixing and, then compare the effect of incorporating interaction into the enthalpy as well as entropic term. We have chosen two acetamide-based systems, one of them (acetamide+urea mixture) appeared to be well described by the ideal solution model and here incorporating interaction through simulation is redundant. But, for the acetamide+$LiNO_3$ system, we found a considerable effect of interaction in predicting the eutectic temperature.

References:

(1) *Hansen, B. B.; Spittle, S.; Chen, B.; Poe, D.; Zhang, Y.; Klein, J. M.; Horton, A.; Adhikari, L.; Zelovich, T.; Doherty, B. W.; Gurkan, B.; Maginn, E. J.; Ragauskas, A.; Dadmun, M.; Zawodzinski, T. A.; Baker, G. A.; Tuckerman, M. E.; Savinell, R. F.; Sangoro, J. R. Deep Eutectic Solvents: A Review of Fundamentals and Applications. Chem. Rev. 2021, 121 (3), 1232–1285. https://doi.org/10.1021/acs.chemrev.0c00385.*

(2) *Kollau, L. J. B. M.; Vis, M.; Van Den Bruinhorst, A.; Esteves, A. C. C.; Tuinier, R. Quantification of the Liquid Window of Deep Eutectic Solvents. Chem. Commun. 2018, 54 (95), 13351–13354. https://doi.org/10.1039/c8cc05815f.*

(3) *Kollau, L. J. B. M.; Vis, M.; van den Bruinhorst, A.; Tuinier, R.; de With, G. Entropy Models for the Description of the Solid–Liquid Regime of Deep Eutectic Solutions. J. Mol. Liq. 2020, 302, 112155. https://doi.org/10.1016/j.molliq.2019.112155.*

Activity driven transport

Ritwick Sarkar

Department of Physics of Complex Systems

Abstract of the Oral Presentation

We study the stationary state of a chain of harmonic oscillators driven by active reservoirs at the boundaries. Active reservoirs exert correlated stochastic forces on the boundary oscillators, which leads to a nonequilibrium stationary state (NESS) with a nonzero energy current flowing through the system. Three most well-known dynamics for the active force are considered here, namely, the active Ornstein-Uhlenbeck process (AOUP), run-and-tumble process (RTP), and active Brownian process(ABP). These forces have exponentially decaying two-point temporal correlations with different higher-order fluctuations. We find that irrespective of the dynamics of the driving, the velocity fluctuation at the bulk remains Gaussian with a flat kinetic temperature profile at the bulk. An "equipartition of energy" emerges in the bulk of the system—in the thermodynamic limit, the value of the bulk kinetic temperature and the bulk potential temperature are equal, irrespective of the specific dynamics of the drive. We also calculate the stationary distribution of the instantaneous energy current in the bulk which shows a logarithmic divergence near the origin with asymmetric exponential tails. The signatures of specific active driving become visible near the boundary and this is most prominent for the RTP- and ABP-driven chains. For these two cases, the boundary velocity distributions become non-Gaussian and the current distribution has a finite cutoff.

References:

1. Stationary states of activity-driven harmonic chains, Ritwick Sarkar, Ion Santra, and Urna Basu, Phys. Rev. E 107, 014123 – Published 17 January 2023.

2. Activity driven transport in harmonic chains, Ion Santra, Urna Basu, SciPost Phys. 13, 041 (2022) – Published 30 August 2022.

Neutrino Oscillations induced by chiral geometry

Riya Barick[1], Indrajit Ghose[1], Amitabha Lahiri[1]

[1]*Satyendra Nath Bose National Centre for Basic Sciences*

Abstract of the Oral Presentation

Standard Model says neutrinos are massless. But to explain neutrino oscillation phenomena, we have to take neutrinos to be massive. When neutrinos pass through a medium they interact with it via weak interaction. Interaction with a medium results in different effective masses for the neutrinos belonging to different lepton families, which can also cause neutrino oscillation, but a neutrino mass is still needed. Recently it was proposed that space time geometry can lead to chiral four-fermion interaction. The torsion is generated by the presence of fermions itself. It couples to the neutrinos with different coupling constants which are not universal but should be fixed by experimental observations. This quartic interaction will cause a neutrino mixing while propagating through fermionic matter. Thus in presence of matter we have to consider both – weak interaction (which is diagonal in the flavor basis) and torsional quartic interaction (which is diagonal in mass basis). In my talk I will discuss all this briefly and will show, by taking into account all these effects, how neutrino conversion and survival probabilities change in the presence of matter.

References:

[1] S. Chakrabarty and A. Lahiri,
"Geometrical contribution to neutrino mass matrix,"
Eur. Phys. J. C 79 no.8, 697 (2019)
doi:10.1140/epjc/s10052-019-7209-2
[arXiv:1904.06036 [hep-ph]].

[2] Riya Barick, Indrajit Ghose, Amitabha Lahiri (In preperation).

Certifying beyond quantumness of locally quantum no-signaling theories through a quantum-input Bell test

Edwin Peter Lobo,[1] Sahil Gopalkrishna Naik,[2] Samrat Sen,[2] Ram Krishna Patra,[2] Manik Banik,[2] and Mir Alimuddin[2]

1 School of Physics, IISER Thiruvananthapuram, Vithura, Kerala 695551, India

2 Department of Physics of Complex Systems, S. N. Bose National Center for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106, India

Abstract of the Oral Presentation

Physical theories constrained with local quantum structure and satisfying the no-signaling principle can allow beyond-quantum global states. In a standard Bell experiment, correlations obtained from any such beyond quantum bipartite state can always be reproduced by quantum states and measurements, suggesting the local quantum structure and no-signaling to be the axioms to isolate quantum correlations. In this Letter, however, we show that if the Bell experiment is generalized to allow local quantum inputs, then beyond-quantum correlations can be generated by every beyond-quantum state. This gives us a way to certify the beyond-quantumness of locally quantum no-signaling theories and in turn, suggests the requirement of additional information principles along with the local quantum structure and no-signaling principle to isolate quantum correlations. More importantly, our work establishes that the additional principle(s) must be sensitive to the quantum signature of local inputs. We also generalize our results to multipartite locally quantum no-signaling theories and further analyze some interesting implications.

DOI: 10.1103/PhysRevA.106.L040201

References:

[1] J. S. Bell, On the Einstein Podolsky Rosen paradox, Phys. Phys. Fiz. 1, 195 (1964).

[2] J. S. Bell, On the problem of hidden variables in quantum mechanics, Rev. Mod. Phys. 38, 447 (1966).

[3] N. D. Mermin, Hidden variables and the two theorems of John Bell, Rev. Mod. Phys. 65, 803 (1993).

[4] N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, Bell nonlocality, Rev. Mod. Phys. 86, 419 (2014).

[5] E. Schrödinger, Discussion of probability relations between separated systems, Math. Proc. Cambridge Philos. Soc. 31, 555 (1935).

[6] J. Barrett, L. Hardy, and A. Kent, No Signaling and Quantum Key Distribution, Phys. Rev. Lett. 95, 010503 (2005).

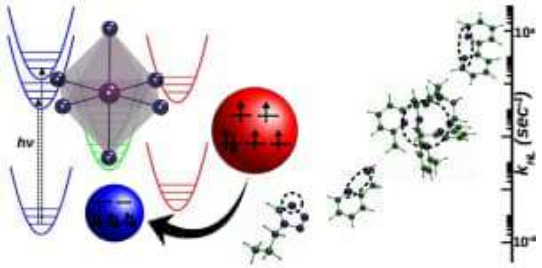
Excited-state spin trapping in Iron(II) spin crossover complexes: A light effect

Shiladitya Karmakar and Tanusri Saha-Dasgupta

Department of Condensed Matter and Material Physics, S. N. Bose National Centre for Basic Sciences, Kolkata 700106, India.
E-mail: shiladitya1995@bose.res.in

Abstract of the Oral Presentation

Spin Crossover (SCO) complex, a class of molecular materials, exhibiting switching of physical properties in response to external perturbations, have drawn considerable attention for decades due to its diverse application possibilities, ranging from data storage to molecular electronics, to photo-magnetism and nonlinear optics [1]. In 1984 Decurtins et al. [2] demonstrated that the Fe^{2+} ion in the $[Fe(ptz)_6](BF_4)_2$ (ptz = 1-propyltetrazole) complex gets converted from the stable diamagnetic low-spin (LS) state to a metastable paramagnetic high-spin (HS) state at 10K when illuminated by green light, and remains trapped in the HS state for several hours for T≤50 K. This phenomenon, named as Light-Induced Excited Spin-State Trapping (LIESST) is of potential technical use as optical switches and magneto-optical storage but it is limited by the fact that trapping to metastable HS state usually happens at rather low temperature. Microscopic understanding of this phenomenon is thus needed. Computational modeling of this interesting phenomena is however complex. In our study, we attempt so by application of time-dependent density functional theory (TDDFT). Our findings reveal that TDDFT is a reasonable approach to estimate the low temperature relaxation rates $k_{HL}(T->0)$ of real complexes, consisting of several tens to hundreds of atoms and has the advantage of computationally inexpensive nature compared to that of multi-reference approaches.[3] We apply our method to study the 14 order of magnitude jump in relaxation rate of Fe(II) SCO complexes coordinated by mono-dentate, bi-dentate and multi-dentate ligands.[4] The calculated rate constants are found to be in excellent agreement with measured values. The trend is rationalized in terms of the change in metal-ligand covalency, numerically estimated by the crystal orbital Hamiltonian population, thus influencing the back donation or delocalization of the electrons from the low-lying Fe(II)-centered molecular orbital to the empty low-lying ligand-centered π* antibonding molecular orbitals.[5]



Acknowledgements: Prof. Debashree Ghosh, IACS and Dr. Pradip Chakraborty, IIT-KGP

References:

1. M. A. Halcrow, Spin-crossover materials: properties and applications, John Wiley & Sons, 2013

2. S. Decurtins, P. Gütlich, C. Köhler, H. Spiering and A. Hauser, Chem. Phys. Lett., 1984, 105, 1–4

3. S. Karmakar, D. Ghosh and T. Saha-Dasgupta, Int. J. Quantum Chem., 2020, 120, e26122

4. A. Hauser, A. Vef and P. Adler, J. Chem. Phys., 1991, 95, 8710–8717

5. S. Karmakar, P. Chakraborty and T. Saha-Dasgupta, Phys. Chem. Chem. Phys., 2022, 24, 10201–10209

Oral presentation will be based on Refs.[3] and [5].

Why does the charge transfer energy vary in some nickelates?

Shinjini Paul and Priya Mahadevan

Department of Condensed Matter and Material Physics,
S. N. Bose National Centre For Basic Sciences. Salt Lake, Sector -III, Kolkata-700106

Abstract of the Oral Presentation

Zaanen, Sawatzky and Allen classified insulators into Mott-Hubbard insulators ($U < \Delta$) and Charge transfer insulators ($U > \Delta$) [1]. Most of the superconducting elements were cuprates and they have a lower Δ than U. In 2019, the discovery of high temperature superconductivity in $Nd_{1-x}Sr_xNiO_2$ [2] has raised much interest in the nickelates among the researchers. Recently it has been claimed that infinite layer nickelates lie in the Mott-Hubbard regime . Earlier work has been done on charge transfer energy of the the nickelates, varying Ni-O-Ni dimensionality in divalent nickelates [3].Here in this project we have studied the electronic structure of some nickelates and analysed the variation of Δ. We observe the changes in charge transfer energy for different dimensionality and valency of the transition metallic ion for some nickelates and tried to analyse the possible reason behind these variations.

References:

[1] J. Zaanen, G. A. Sawatzky and J. W. Allen ; Phys. Rev. Lett. Vol. 55, 418-421 (1985).

[2] Li, D., Lee, K., Wang, B.Y. et al. Nature 572, 624–627 (2019).

[3] K. Maiti, P. Mahadevan, D. D. Sarma ; Phys. Rev. B Vol. 59, 12457(1998).

Characterization and Identification of the pre-main sequence stars in the H II region Sh2-87

Siddhartha Biswas[1*], Soumen Mondal[1], Alik Panja[1], Somnath Dutta[2], Ramkrishna Das[1]

[1] *S. N. Bose National Centre for Basic Sciences, Kolkata-700 106, India*

[2] *Institute of Astronomy and Astrophysics, Academia Sinica, Taipei 10617, Taiwan*

Abstract of the Oral Presentation

H II regions are regarded as the effective tracers of the star-formation activity and different zones of the H II regions serve as the place of the second-generation star-formation. The main objective of our work is to classify and characterize the pre-main-sequence stars (PMSs) associated with the H II region Sh2-87 (S87), ($\alpha_{(2000)} = 19^h\ 46^m\ 20.7^s$, $\delta_{(2000)} = +24^\circ\ 35'\ 15''$) which belongs to the Vulpecula OB association (Vul OB 1), with other neighbours such as S88 and S89 (Billot et al. (2010)). Here, we have utilized our own new spectroscopic observational data from the 2-m Himalayan Chandra Telescope (2-m HCT) as well as several archival catalogues, e.g., IPHAS, SPITZER, WISE, UKIDSS, 2MASS. Low-resolution spectroscopic observations of a few bright stars from 2-m HCT reveal the presence of a few massive (early-B) sources. From the H, K photometry of UKIDSS, we have generated the K band extinction map of this region by using the nearest-neighbourhood method of Gutermuth et al. (2008), which shows a huge variation indicating the non-uniform distribution of extinction. From the mid-infrared (SPITZER, ALLWISE) colour–colour criteria we have identified 82 Class II and 6 class sources. Using the near-infrared (UKIDSS) colour excess, 133 young members are also identified. The presence of a significant number of PMS suggests active star-formation activity toward this region. Additionally, a significant number of Hα emitters, detected from IPHAS photometry implies strong ionization activity. Therefore, from the multi-wavelength datasets, an overall census of PMS will be presented here.

References:

Billot N., Noriega-Crespo A., Carey S., Guieu S., Shenoy S., Paladini R., Latter W., 2010, ApJ, 712, 797

Gutermuth R. A., et al., 2008, ApJ, 674, 336

CeO_x as Surface Passivation and Hole Transfer Catalyst Layer Boosting Solar Water Oxidation of $ZnFe_2O_4$ Nanorods Photoanode

Dipanjan Maity[1], Debashish Pal[2], Soham Saha[1], Pooja Punetha[3], Debasish Sarkar[4], Debasis De[5], Gobinda Gopal Khan[2], Kalyan Mandal[1]

[1] *Department of Condensed Matter Physics and Material Sciences, S. N. Bose National Centre for Basic Sciences, Block JD, Sector-III, Salt Lake, Kolkata, West Bengal 700 106, India*

[2] *Department of Material Science and Engineering, Tripura University (A Central University), Suryamaninagar, Agartala, Tripura 799 022, India*

[3] *Department of Materials Engineering, Indian Institute of Science, CV Raman Rd, Bengaluru, Karnataka 560012, India*

[4] *Department of Physics, Malaviya National Institute of Technology, Jaipur, Rajasthan 302 017, India*

[5] *Energy Institute, Bengaluru, (Center of Rajiv Gandhi Institute of Petroleum Technology), International Airport Road, Vidyanagar, Bengaluru 562 157, Karnataka, India*

Abstract of the Oral Presentation

Solar assisted Photoelectrochemical (PEC) water splitting is one of the most elegant ways of capturing and storing solar energy in an eco-friendly manner. Among materials that can enable such a task, metal oxide semiconductors are an attractive choice due to their extremely good stability and abundance. Zinc Ferrite ($ZnFe_2O_4$ or ZFO) is a spinel ferrite, which in addition to fulfilling the above two conditions, also has a narrow band gap (≈2 eV) enabling it to absorb most of the visible spectrum, but like other ferrites, suffers from severe photocarrier recombination and poor conductivity. In this work, we couple reduced $ZnFe_2O_4$ with CeO_x catalyst as a hole transport layer to reduce the surface charge recombination on the photoanode surface significantly. The $ZnFe_2O_4/CeO_x$ nano-heterostructure photoanode exhibits a current density of 0.64 mA cm^{-2} at 1.23 V versus RHE under AM 1.5 G illumination, which corresponds to >167% increase over that of the $ZnFe_2O_4$ NRs photoanode. The CeO_x coupling reduces the onset potential cathodically by 180 mV over the $ZnFe_2O_4$ NRs photoanode. The $ZnFe_2O_4/CeO_x$ nano-heterostructure photoanode also exhibits excellent charge transfer efficiency (≈64% at 1.23 V vs RHE) and photostability. The results indicate the superior catalytic performance of oxygen vacancy defect-rich CeO_x in the PEC process. This work demonstrates the multifunctional role of CeO_x as a surface passivation overlayer, hole transfer layer, and efficient oxygen evolution reaction catalyst.

References:

1) Maity, D., Pal, D., Saha, S., Punetha, P., Sarkar, D., De, D., Khan, G. G., Mandal, K., CeO_x as Surface Passivation and Hole Transfer Catalyst Layer Boosting Solar Water Oxidation of $ZnFe_2O_4$ Nanorods Photoanode. Adv. Mater. Interfaces 2023, 10, 2201645. https://doi.org/10.1002/admi.202201645

*2) Kim, J.H, Jang, Y.J, Choi, S.H, Lee, B.J, Kim, J.H, Park, Y.B, Nam, C.M, Kim, H.G*and Lee, J.S. A multitude of modifications strategy of ZnFe2O4 nanorod photoanodes for enhanced photoelectrochemical water splitting activity. J. Mater. Chem. A, 2018, 6, 12693.*

3) Liu, Y, Xia, M, Yao, L, Mensi, M, Ren, D, Grätzel, M, Sivula, K, and Guijarro, N. Spectroelectrochemical and Chemical Evidence of Surface Passivation at Zinc Ferrite (ZnFe2O4) Photoanodes for Solar Water Oxidation. Advanced Functional Materials. 2021, 31, 2010081.

4) Ahmed, M.G, Zhang, M, Tay, Y.F, Chiam, S.Y and Wong, L.H. Surface Modification of Hematite Photoanodes with CeOx Cocatalyst for Improved Photoelectrochemical Water Oxidation Kinetics. ChemSusChem 10.1002/cssc.202001135.

Virtual transitions in an atom-mirror system in the presence of two scalar photons

Ashmita Das , Soham Sen , and Sunandan Gangopadhyay

A. Das (PDRA-III), Soham Sen (JRF), Dr. S. Gangopadhyay (Associate Professor)

Abstract of the Oral Presentation

We examine the virtual transition of an atom-mirror system with the simultaneous emission of two scalar photons, where the atom and the mirror admit a relative acceleration between them. For the single photon emission, the literature [A. A. Svidzinsky et al., Phys. Rev. Lett. 121, 071301 (2018)] dictates that the transition probabilities of two individual systems, such as an atom accelerating with respect to the mirror and its reverse, turn out to be equivalent under the exchange of the frequencies of atom and the field. Addressing the observational merit of such excitation process, a detectable probability (P ~ 10^(-2)) is also reported in the above literature. In the present manuscript our finding dictates that the simultaneous emission of dual photon instead of one, destroys the equivalence between the transition probabilities as reported in the above literature.

OTM

References:

1. *A. Das, S. Sen, and S. Gangopadhyay, Phys. Rev D 107 (2023) 025009.*

Study of photonic spin Hall shift in monolayer MoS_2 via quantum weak measurement

Soumen Mandal , Akash Das, and Manik Pradhan

S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata 700 106, India

Abstract of the Oral Presentation

Photonic spin Hall shift, the photonic version of electronic spin Hall effect, took place when a linearly polarized optical beam with a finite transverse extent interacts at a particular optical interface, then the reflected or refracted ray dissociate by a distance as right and left circular polarization. The distance between them is known as photonic spin Hall shift (PSHS) [1]. We report the experimental evidence of the PSHS in monolayer MoS_2 for a fundamental Gaussian beam using quantum weak measurement formalism. We have revealed the dependence of PSHS over a large range of angles of incidence, post-selection angles along with the mode of polarization of the incident light [2]. We also found a unique signature linking angular position at which spin Hall shifts (zero crossing) with the discontinuity in the phase difference of reflection coefficient further establishing the connection between PSHS to the geometric phases of 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.

References:

[1] O. Hosten and P. Kwiat, "Observation of the spin Hall effect of light via weak measurements," Science 319, 787–790 (2008)

[2] A Das, S Mandal, M Pradhan , "Signature of the photonic spin Hall effect in monolayer MoS_2 via weak measurement" JOSA B 39 (7), 1822-1828 (2022)

All-Optical Probing of Giant Interfacial Spin Transparency at a Topological Insulator/ Ferromagnet Interface

Suchetana Mukhopadhyay[1,2], Pratap Kumar Pal[1],Subhadeep Manna[2], Chiranjib Mitra[2], Anjan Barman[1*]

[1]*Department of Condensed Matter and Materials Physics, S.N. Bose National Center for Basic Sciences, Block-JD, Sector III, Salt Lake, Kolkata, 700106, India*

[2]*Department of Physical Sciences, Indian Institute of Science Education and Research, Mohanpur, West Bengal, 741252, India*

[*]*Email: abarman@bose.res.in*

Abstract of the Oral Presentation

The rise of three-dimensional topological insulators as a uniquely attractive playground for the observation and control of various spin-orbit effects has ushered in the promising field of topological spintronics. In order to fully exploit their potential as efficient spin-orbit torque generators, it is crucial to investigate the efficiency of spin injection and transport at various topological insulator/ferromagnet interfaces and identify the key parameters for their optimization. In this work, all-optical time-resolved magneto-optical Kerr effect magnetometry is used to demonstrate efficient spin pumping in Sub/$BiSbTe_{1.5}Se_{1.5}$(BSTS)/$Co_{20}Fe_{60}B_{20}$(CoFeB)/SiO_2 thin film heterostructures. From the observed modulation of Gilbert damping parameter with BSTS thickness, the intrinsic spin mixing conductance of the BSTS/CoFeB interface is extracted and the spin diffusion length in BSTS is determined, revealing that pure spin current can penetrate significantly into the BSTS film. Moreover, the damping variation with different CoFeB layer thickness is modeled to extract the effective spin-mixing conductance. It is found that in the "perfect spin-sink" regime when BSTS thickness far exceeds the spin diffusion length, an interfacial spin transparency as high as 0.9 is attainable in these heterostructures, which can promote such systems as scintillating candidates for spin-orbitronic devices.

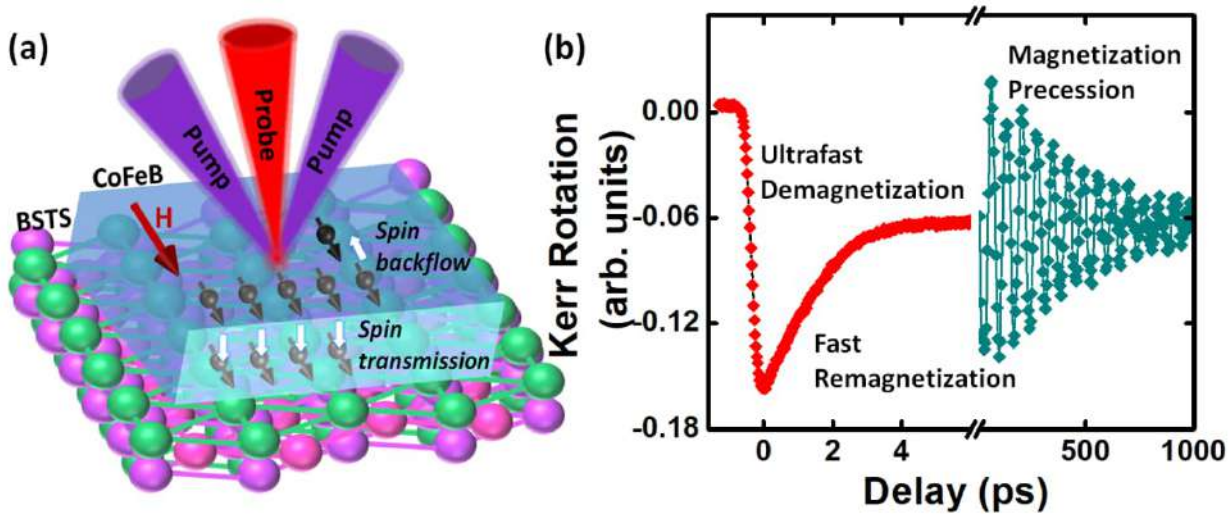


Figure 1. (a) A schematic of sample structure and TR-MOKE measurement geometry. (b) Time-resolved Kerr rotation data for the Sub/BSTS(25 nm)/CoFeB(10 nm)/SiO_2(3 nm) thin film showing three distinct temporal regimes.

Disorder-induced crossover of Mott insulator to weak Anderson localized regime in an argon-irradiated $NdNiO_3$ film

Ravindra Singh Bisht[1], Sudipta Chatterjee[1], Sreyan Raha[2], Achintya Singha[2], D. Kabiraj[3], D. Kanjilal[3], and A. K. Raychaudhuri[4]

[1]*Department of Condensed Matter and Materials Physics, S.N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700106, India*

[2]*Department of Physics, Bose Institute, 93/1, Acharya Prafulla Chandra Road, Kolkata 700009, India*

[3]*Materials Science Division, Inter University Accelerator Centre, Aruna Asaf Ali Marg, New Delhi 110067, India*

[4]*CSIR-Central Glass and Ceramic Research Institute, 196 Raja S.C. Mullick Road,*

Abstract of the Oral Presentation

We show that an introduction of disorder in a controlled way using 1 MeV argon (Ar) ion irradiation, suppresses the correlation driven metal-insulator transition (MIT) in $NdNiO_3$ films. The films make a crossover to a heavily disordered conductor governed by weak localization (WL) and at even higher disorder, an Anderson localized state. We show that the pristine films of $NdNiO_3$ exhibit an MIT with the conduction process being governed by variable range hopping (VRH). For disorder up to 1% of the displaced atoms or lower, the insulating state arising from a gap in the density of states (DOS) at the Fermi level (E_F) as in a Mott insulator is suppressed and the conduction in the film shows a WL behavior with finite conductivity at temperature $T \rightarrow 0$. This behavior is expected in a disordered conductor that does not have a gap in DOS at E_F. At higher fluences the conductivity reduces substantially but the electrical conduction shows a power-law temperature dependence with a small but finite zero temperature conductivity σ ($T = 0$) which is expected in a solid with electrons that are Anderson localized. A similar experiment was performed on the La substituted $NdNiO_3$ films ($Nd_{1-x}La_xNiO_3$) with $x = 0.3$ that are grown in the same way. La substitution in $NdNiO_3$ suppresses the temperature driven transition and leads to a metallic state with critical composition at $x \approx 0.3$. The pristine as well as films irradiated with lowest fluence shows metallic or marginally metallic behavior grown on $LaAlO_3$ and $SrTiO_3$ substrates, respectively. However, at higher fluences they too exhibit a convergence in electronic transport and σ shows a power-law temperature dependence at low T with σ ($T = 0$) $\neq 0$. Evidence of suppression of correlated behavior can also be seen in the irradiated films where the non-Gaussian nature of resistance fluctuation at $T \approx T_{MI}$, a signature of correlated electron systems, is suppressed on irradiation that leads to collapse of the MIT [1, 2]. Evidence for progressing disordering of the films on irradiation were observed in Raman spectroscopy as well as x-ray studies that show the basic integrity of the NiO_6 octahedra is preserved and the structure retains its crystallinity.

References:

1. S. Chatterjee, R. S. Bisht, V. R. Reddy, and A. K. Raychaudhuri, Phys. Rev. B 104, 155101 (2021).

2. R. S. Bisht , S. Chatterjee, S. Raha, A. Singha, D. Kabiraj, D. Kanjilal, and A. K. Raychaudhuri, Phys. Rev. B 105, 205120 (2022).

Molecular Thermodynamic Origin of Substrate Promiscuity in the Enzyme Laccase: Toward A Broad- Spectrum Degrader of Dye Effluents

Sudipta Mitra, Arnab Sil, Ranjit Biswas and Suman Chakrabarty

S.N. Bose National Centre for Basic Sciences

Abstract of the Oral Presentation

Industrial dye effluents have emerged as significant health hazard. Laccases found in white rot fungi can degrade an assortment of dyes. Here we explore the molecular thermodynamic origin of the substrate promiscuity in laccases using a combination of steady state UV-Visible absorption spectroscopy, molecular docking and molecular dynamics (MD) simulation studies on the interaction of laccase with five dye molecules with varying charge, size and shape. The spectroscopic studies confirm that all these dyes can be degraded by laccase. Using MD simulations we have demonstrated the presence of various distinct conformations of a loop in the protein active site that can accommodate the wide range of dye molecules. We have also shown that the diverse selection of dye molecules may exhibit surprisingly similar binding affinity due to cancellation of different thermodynamic factors. Our results highlight the potential of laccase as a multi-purpose degrader for industrial dye effluents.

References:

1. J. Phys. Chem. Lett. 2023, 14, 1892−1898 .

2. Arregui, L et al. Laccases: Structure, Function, and Potential Application in Water Bioremediation. Microb. Cell Fact. 2019, 18, 1– 33.

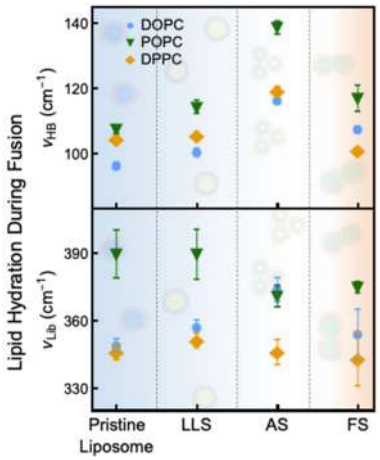
Alteration of lipid hydration during Polyethylene Glycol induced lipid fusion

Sumana Pyne, Partha Pyne, Rajib Kumar Mitra*

Department of Chemical and Biological Sciences, S N Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106, India

Abstract of the Oral Presentation

Membrane fusion is one of the most ubiquitous phenomena of life, a key event in intracellular membrane trafficking e.g. egg fertilization, viral entry, intracellular transport, neurotransmission through cell etc.[1,2] In living cells, several proteins like SNAP Receptor (SNARE), SM protein, Rab protein etc. facilitate membranes for intracellular fusion.[3] Polyethylene glycols (PEG) have also been commonly used to fuse membranes in absence of proteins.[4] In the present study we deploy THz FTIR spectroscopy (1.5-13.5 THz frequency domain) to explore the hydration behavior of three lipids (1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC), 2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine (POPC) and 1,2-Dipalmitoyl-sn-glycero-3-phosphocholine (DPPC)) with different aliphatic tails as they undergo fusogenic transition in the presence of PEG (average molecular weight 4000). We use dynamic light scattering and electron microscopy to monitor the lipid fusion process and the results confirm the formation of different intermediate steps of the liposomes during the fusion process: bilayer aggregation, destabilization and finally lipid fusion. THz-FTIR results conclude that liposomes get dehydrated in presence of PEG during the fusion pathway. It has also been observed that change in hydration depends on the particular intermediate state(s).



References:

(1) Jahn, R.; Lang, T. Membrane Fusion. Cell 2003, 112, 519–533.

(2) Jahn, R.; Sudhof, T. C. Membrane Fusion and Exocytosis. Annu. Rev. Biochem. 1999, 68, 863–911.

(3) Südhof, T. C.; Rothman, J. E. Membrane Fusion: Grappling with SNARE and SM Proteins. Science 2009, 323, 474–477.

(4) Lentz, B. R. PEG as a Tool to Gain Insight into Membrane Fusion. Eur. Biophys. J. 2007, 36, 315–326.

External field induced mixing and demixing of a binary colloid

Suravi Pal[1], Jaydeb Chakrabarti[1], and Srabani Chakrabarty[2]

[1]*Physics of complex systems, S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata 700106, India*

[2]*Department of Physics, Lady Brabourne College, P-1/2, Suhrawardy Ave, Beniapukur, Kolkata-700017, India*

Abstract of the Oral Presentation

We explore the rich phase behaviour shown by a binary phase seperated colloidal system under external spatially periodic modulation. We perform Monte Carlo simulation on a binary mixture of big and small repulsive Lennard-Jones particles with diameter ratio 1:2. We characterise structure by isotropic and anisotropic pair correlation function, cluster size distribution, bond angle distribution, and demixing order parameter. We observe that there is a tendency of mixing among the two species under external modulation which gets enhanced with increasing potential strength. The smaller particles tend to form hexagonal order among themselves, as reflected in bond angle distribution after being subjected to external modulation. The phase transition from demixed to mixed state is observed through the demixing order parameter and the specific heat.

References:

[1] Kaplan P D, Yodh A G, and Pine D J 1992 Phys. Rev. Lett. 68 393

[2] Ristenpart W D, Aksay,I A and Saville D A 2003 Phys. Rev. Lett. 90 128303

[3] Crocker J C, Matteo J A, Dinsmore A D, and Yodh A G 1999 Phys. Rev. Lett. 82 4352

[4] Varga I, Kun F, and Pal K F 2004 Phys. Rev. E 69 030501(R)

[5] Capellmann R F, Khisameeva A, Platten F and Egelhaaf S U 2018 J. Chem. Phys. 148 114903

Current Fluctuations of models of interacting self-propelled particles : microscopic approach

Tanmoy Chakraborty and Punyabrata Pradhan

Department of Physics of Complex Systems

Abstract of the Oral Presentation

We calculate the fluctuation of the time-integrated or cumulative bond current Q(X,T) up to time T in a prototypical one-dimensional model, having variable-range hopping, which mimics passive diffusion and the ballistic motion of hard-core active, or self-propelled, particles with a persistence length. We have developed a closure scheme that enables us to precisely determine the fluctuation using density-current and density-density correlations. Our analysis captures the short-time ($T<<L^2$) sub-diffusive growth ~ $\sqrt{T}$ as well as the linear or diffusive growth of the fluctuation at longer times $T>>L^2$. Although the system violates detailed balance at the microscopic level, we have recovered an equilibrium-like Green-Kubo relationship linking the current fluctuation with the linear response function or the conductivity. Remarkably, in the limit of infinite persistence length, tuning the density causes the steady-state fluctuation to diverge, revealing the dynamical origin of the previously observed condensation transition of the system [1].

References:

1. Hydrodynamics, superfluidity, and giant number fluctuations in a model of self-propelled particles, Tanmoy Chakraborty, Subhadip Chakraborti, Arghya Das, and Punyabrata Pradhan, PHYSICAL REVIEW E 101, 052611 (2020).

BOSE FEST 2023: List of Posters Presentations

Sl. No.	Name	Title
P1	Amrita Mondal	An Insight into Ultrafast Solution Dynamics in Li-ion Battery Electrolyte Using Streak Camera
P2	Anirban Paul	Molecular dynamics investigation of the dynamical response of interfacial water near DPPC bilayer to Hyaluronic acid
P3	Anish Das	Shadow of black hole immersed in plasma as viewed by a co-moving observer
P4	Anyesh Saraswati	Electrical transport study and possible charge density wave-mediated electrical magneto-chiral anisotropy in a flat-band kagome anti-ferromagnet FeGe
P5	Arnab Chakraborty	Chiral Torsion and Parity Violation
P6	Arnab Mukherjee	Unruh quantum Otto engine in the presence of a reflecting boundary
P7	Bikash Chandra Mishra	A Thiazole-linked Covalent Organic Framework for Lithium- Sulphur Batteries
P8	Biswajit Panda	Simultaneous detection of dual-species (CH4 / N2O) using wavelength modulation spectroscopy for atmospheric monitoring and breath diagnostics applications.
P9	Chandan Kumar	Investigation of the Magnon Mode Reversal in Bicomponent Magnonic Crystal.
P10	Dayal Das	Fabrication of Artificially Stacked Van-der-Waals Heterostructures
P11	Gesesew Reta Habtie	Optical spectroscopy of the fastest classical nova, V1674 Her
P12	Govind Lal Sidhardh	Exploring superadditivity of coherent information of noisy quantum channels through genetic algorithms
P13	Indrani Bhattacharya	The Underlying Mechanism of Reduction in Elevated Serum Creatinine Level by Anti-Oxidants: A Spectroscopic Investigation
P14	Indrayani Patra	Probing ortho and para nuclear-spin isomers of NH3 using cavity ring-down spectroscopy
P15	Ishita Jana	Improvement of Leakage, Electric and Magnetic Properties in Cobalt doped Gallium Ferrite
P16	J Sridhar Mohanty	Giant room temperature magnetocaloric response in (MnNiSi)1-x(FeNiGa)x system
17	Kanchan Meena	TIME REVERSED STATES IN BARRIER TUNNELING
18	Krishnendu Sinha	Regulation of RhoA GTPase by Phosphorylation of RhoGDI
19	Manoj Gupta	Interplay of hopping pathways, spin-orbit coupling and interaction in quarter filled t2g orbitals on honeycomb lattice
20	Narayan Chandra Maity	Ultrafast solvation dynamics through the eyes of streak camera
21	Neeraj Kumar	Breaking of Universal Nature of Central Critical Charge in Black Hole Thermodynamics
22	Rahul Karmakar	Reverse Osmosis of binary mixture through polymeric membrane
23	Ramesh Pramanik	Chemotactic response to spatio-temporal variation in attractant environment

Sl. No.	Name	Title
24	Sahil Gopalkrishna Naik	Distilling nonlocality in quantum correlations
25	Saikat Mitra	Growth, Charecterization and dielectric studies of two dimensional organic-inorganic halide perovskite.
26	Samir Rom	Interplay of Magnetism and Unconventional Topology in LaCoO3/SrIrO3 Heterostructure
27	Sanuja Kumar Khuntia	Density functional theory based Predictive Model for Low-Dimensional Organic-Inorganic Halide Perovskites
28	Sayan Ghosh	Ground state properties & Quantum Phase Diagram for spin-1/2 antiferromagnetic kagome stripe chain
29	Sayan Routh	Magnetoresistance in the critical region of weak-itinerant ferrimagnet FeCr2Te4 single crystal
30	Shobhan Dev Mandal	Effect of receptor clustering on E.coli chemotaxis: Sensing versus adaptation
31	Sourabh Saha	Quantum Phase Diagram of The One dimensional Extended Hubbard Model with Polarization
32	Sreya Pal	Active Acousto-Plasmo-Magnonics in a Two-dimensional Artificial Magnonic Crystal
33	Subhankar De	“Formation of atomic point contact using mechanically controlled break junction.”
34	Susanta Ghosh	Observation of Spin-reorientation Transition and Large Anomalous Hall Effect at Elevated Temperatures in Mn3Ge Weyl Semimetal.

An Insight into Ultrafast Solution Dynamics in Li-ion Battery Electrolyte Using Streak Camera

Amrita Mondal and Ranjit Biswas*

S. N. Bose National Centre for Basic Sciences, Block- JD, Sector- III, Salt Lake, Kolkata-700106, West Bengal, India.

Abstract of the Poster Presentation

The LiTFSI-Glyme electrolyte solutions behave like solvate ionic liquid (SIL) at equimolar mixture (1:1) of LiTFSI and triglyme (G3) [1,2]. The ultrafast dynamics of a standard fluorescent probe, trans-2-[4-(dimethylamino)styryl] benzothiazole (DMASBT) has been investigated in LiTFSI-G3 electrolyte medium (mole ratio between LiTFSI and G3: 0.1 to 1) at room temperature by employing a sub-picosecond resolved streak camera providing a temporal resolution of about ~400 fs. The excited state average fluorescence lifetimes of DMASBT in the electrolyte solutions are found to be ~ sub-100 ps. In contrast, this lifetime is few times faster than the lifetimes measured with TCSPC setup that has time-resolution of ~ 20 ps. Critical comparison between lifetime emission decays of DMASBT recorded with streak camera and TCSPC indicates that streak camera is more accurate to report time-resolved fluorescence features than TCSPC for short-lifetime and low-quantum yield fluorophore like DMASBT in multi-component mixtures [3,4]. The time-correlated solvent response function, $S(t)$, of DMASBT in 1:1 mixture of Li-salt:Glyme, is measured to be bi-exponential with two well-separated time-components: τ_1 ~20 ps and τ_2 ~90 ps. Interestingly, the average solvation time varies in between ~12-70 ps with changing the mole ratio of LiTFSI to G3. Dynamic Stokes shift measurements in the present electrolyte systems with varying salt concentration (mole ratio :0.1-1) report ~200-400 cm^{-1} dynamic shifts which is ~40-50% of the estimated total dynamic Stokes shift. A strong spatial heterogeneity has been detected from excitation wavelength dependent steady state emission study of DMASBT in the solutions and the extent of heterogeneity increases with increasing salt content in the media. These heterogeneous domains relax in ~ 100 to sub-100 ps.

References:

1. Phys. Chem. Chem. Phys., 2014, 16, 8761-8772.

2. Phys. Chem. Chem. Phys., 2015, 17, 126—129.

3. Biochemistry., 1991, 30, 26, 6517–6527.

4. Appl. Phys. Lett., 2003, 83, 4658-4660.

Molecular dynamics investigation of the dynamical response of interfacial water near DPPC bilayer to Hyaluronic acid

Anirban Paul, Jaydeb Chakrabarti

Dept. of Physics of Complex Systems.

Abstract of the Poster Presentation

Hyaluronic acid (HA) is a long, highly hydrophilic polyanion that is overexpressed in cells and body fluids during pathogenic situations. Previous studies have shown that water molecules mediate the interaction between HA and lipid molecules[1]. Although HA is known to provide orientational ordering and restricted dynamics to its proximal water molecules[2], no theoretical study of HA's significance in water dynamics near lipid vesicles has been reported. We take DPPC bilayer and HA of different sizes and concentrations in our all-atom molecular dynamics simulation. Our findings suggest that at the HA-DPPC bilayer interface, HA can restrict the translational and rotational diffusion of water. When HA concentration is changed in the system, the effect becomes more noticeable. However, the effect is minor for the range of HA sizes we consider in our study.

References:

[1] Paul Smith, Robert M Ziolek, Elena Gazzarrini, Dylan M Owen, and Christian D Lorenz. On the interaction of hyaluronic acid with synovial fluid lipid membranes. Physical Chemistry Chemical Physics, 21(19):9845–9857, 2019.

[2] Johannes Hunger, Anja Bernecker, Huib J Bakker, Mischa Bonn, and Ralf P Richter. Hydration dynamics of hyaluronan and dextran. Biophysical journal, 103(1):L10–L12, 2012.

Shadow of black hole immersed in plasma as viewed by a co-moving observer

Anish Das[1], Ashis Saha[2], Sunandan Gangopadhyay[1]

[1]*Department of Astrophysics and High Energy Physics, SNBNCBS, Kolkata, India*
[2]*Department of Physics, University of Kalyani, Kalyani, India*

Abstract of the Poster Presentation

In our studies of compact objects such as black holes, we assume them to be eternally fixed to a point in space-time. But in reality, the universe is undergoing an accelerating expansion. In order to take this into account, we assume that the expansion is driven by the cosmological constant Λ (which is related to Hubble constant H_0). To make the situation more realistic, we immerse the black hole in a dust-like plasma (with pressure P=0). We have calculated the angular shadow size (α) from the point of view of a co-moving observer and found that the shadow size decreases with increase in distance r_0 from the black hole but never reduces to zero and remains finite. Also, we used the observational results of M 87^* and Sgr A^* to constrain the plasma parameter.

References:

1. A. Das, A. Saha and S. Gangopadhyay Shadow of Kottler black hole in the presence of plasma for a co-moving observer Class. Quantum Grav. 40 (2023) 015008.

Electrical transport study and possible charge density wave-mediated electrical magneto-chiral anisotropy in a flat-band kagome anti-ferromagnet FeGe

Anyesh Saraswati[1], Mahima Singh[1], Nitesh Kumar[1]

[1]*S. N. Bose National Center for Basic Sciences, Sector III, Block JD, Salt Lake, Kolkata –700106*

Abstract of the Poster Presentation

Kagome materials have been a very interesting group of compounds in recent fields of research in condensed matter physics. They exhibit a large number of exotic properties and cascade of different phases such as presence of flat bands with localized electrons, inherent charge density wave and superconductivity. In this poster, we present the electrical transport and characterization studies such as EDS and XRD on a kagome anti-ferromagnet FeGe. With charge density waves occurring in an identical manner to that of AV3Sb5 (A= Cs, Rb, K), and the presence of electrical magneto-chiral anisotropy in previously reported compound CsV3Sb5 experimentally, FeGe gives us a lot of scope to study the aforementioned phenomena, which is basically a non-reciprocal chiral transport in compounds with no center of inversion as well as broken time reversal symmetry. In addition to this, we also expect a reversible chirality, which can be modulated by reversing the sign of the applied magnetic field. With the TCDW =110K discovered in FeGe, there is a good scope of studying the magneto-chiral anisotropy effect in it which is something we are planning to commence in the upcoming weeks.

References:

1. *Guo, C, et al. "Switchable chiral transport in charge-ordered kagome metal CsV3Sb5." Nature 611 (2022) 461-466.*
2. *Teng, X, et al. "Discovery of charge density wave in a kagome lattice antiferromagnet." Nature 609 (2022) 490-495.*
3. *Rikken, G. L. J. A., J. Fölling, and P. Wyder. "Electrical magnetochiral anisotropy." Physical review letters 87 (2001) 236602.*
4. *Yin, Jia-Xin, et al. "Discovery of charge order and corresponding edge state in kagome magnet FeGe." Physical Review Letters 129 (2022) 166401.*

Chiral Torsion and Parity Violation

Arnab Chakraborty and Amitabha Lahiri

S.N. Bose National Centre for Basic Sciences

Abstract of the Poster Presentation

In the framework of the Einstein-Cartan theory of gravitation, coupling of spin-1/2 matter fields to gravity leads to a four-fermion interaction term. The most general such interaction involves chirally coupled fermions. This interaction is parity-violating due to the presence of a mixed parity current-current term. We consider the contribution of the torsional four-fermion interaction to parity-violating electron scattering (PVES) processes. We calculate the left-right asymmetry and compare with measurements of this parameter to arrive at bounds for the chiral coupling constants.

References:

[1] S. Chakrabarty and A. Lahiri, Geometrical contribution to neutrino mass matrix, Eur. Phys. J. C 79, 697 (2019).

[2] P. L. Anthony et al. (SLAC E158 Collaboration), Precision Measurement of the Weak Mixing Angle in Møller Scattering, Phys. Rev. Lett. 95, 081601 (2005).

[3] D. Wang et al. (PVDIS), Nature 506, 67 (2014).

[4] L. Freidel, D. Minic, and T. Takeuchi, Quantum gravity, torsion, parity violation, and all that, Phys. Rev. D 72, 104002 (2005).

Unruh quantum Otto engine in the presence of a reflecting boundary

Arnab Mukherjee; Sunandan Gangopadhyay; A. S. Majumdar

S.N. Bose National Centre for Basic Sciences, JD Block, Sector-III, Salt Lake City, Kolkata 700106, West Bengal, India.

Abstract of the Poster Presentation

In this study, a new model of relativistic quantum analogue of the classical Otto engine has been introduced in the presence of a perfectly reflecting boundary. A single qubit acts as the working substance interacting with a massless quantum scalar field, with the boundary obeying the Dirichlet condition. Using the notion of the Unruh effect quantum vacuum plays the role of a thermal bath. It is noted that the presence of the reflecting boundary dramatically alters the qubit's response function. We observe that three distinct cases namely, the intermediate boundary regime, the near boundary regime, and the far boundary regime emerge from the nature of the vacuum correlation function. As anticipated, as the reflecting boundary reaches infinity, the vacuum correlation in the far boundary regime approaches that of the Unruh quantum Otto engine (UQOE). The qubit's critical excitation probability and the work output of the engine are both decreased as a result of the reflecting boundary's effects. Surprisingly, it is also observed that despite the lower work output, the efficiency of the engine remains unaffected even in the presence of the boundary.

References:

[1] E. Arias, T. R. de Oliveira and M. S. Sarandy, The unruh quantum otto engine, JHEP 02 (2018) 168.

[2] F. Gray and R. B. Mann, Scalar and fermionic Unruh Otto engines, JHEP 11 (2018) 174.

[3] A. Mukherjee, S. Gangopadhyay and A. S. Majumdar, Unruh quantum Otto engine in the presence of a reflecting boundary, JHEP 09 (2022) 105.

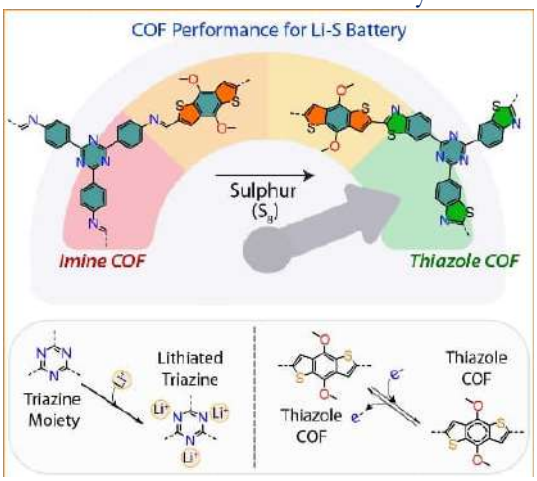
A Thiazole-linked Covalent Organic Framework for Lithium- Sulphur Batteries

Bikash Mishra,[a] Michael Traxler,[b] Jérôme Roeser,[b] Bidhan Kumbhakar,[a] Shuang Li,[b] Arne Thomas,[b] and Pradip Pachfule*[a,b]

Department of Chemical and Biological Sciences, S. N. Bose National Centre for Basic Sciences, Kolkata - 700106, India.
Email: ps.pachfule@bose.res.in
Department of Chemistry/Functional Materials, Technische Universität Berlin, Hardenbergstraße 40, 10623 Berlin, Germany.

Abstract of the Poster Presentation

Lithium-sulphur (Li-S) batteries are a promising alternative power source, as they can provide a higher energy density than current lithium-ion batteries.[1,2] Porous materials are often used as cathode materials as they can act as a host for sulphur in such batteries.[3,4] Recently, covalent organic frameworks (COFs) have also been used, however they typically suffer from stability issues resulting in limited and thus insufficient durability under practical conditions and applications.[5] Herein, we report the synthesis of a crystalline and porous imine-linked triazine-based dimethoxybenzene-functionalized COF (TTT-DMTD) incorporating high-density redox sites. The imine linkages were further post-synthetically transformed to yield a robust thiazole-linked COF (THZ-DMTD) by utilizing a sulphur-assisted chemical conversion method, while maintaining the crystallinity. As a synergistic effect of its high crystallinity, porosity and the presence of redox-active moieties, the thiazole-linked THZ-DMTD exhibited a high capacity and long-term stability (642 mAh g^{-1} at 1.0 C; 78.9% capacity retention after 200 cycles) when applied as a cathode material in a Li-S battery.



References:

[1] J. B. Goodenough, K.-S. Park, J. Am. Chem. Soc. 2013, 135, 1167-1176; [2] M. S. Whittingham, Chem. Rev. 2004, 104, 4271-4302; [3] D. Luo, M. Li, Q. Ma, G. Wen, H. Dou, B. Ren, Y. Liu, X. Wang, L. Shui, Z. Chen, Chem. Soc. Rev. 2022, 51, 2917-2938; [4] J. Kim, A. Elabd, S.-Y. Chung, A. Coskun, J. W. Choi, Chem. Mater. 2020, 32, 4185-4193; [5] F. Haase, B. V. Lotsch, Chem. Soc. Rev. 2020, 49, 8469-8500.

Simultaneous detection of dual-species (CH_4 / N_2O) using wavelength modulation spectroscopy for atmospheric monitoring and breath diagnostics applications.

Biswajit Panda*, Ardhendu Pal, Soumyadipta Chakraborty and Manik Pradhan

Department of Chemical and Biological Sciences, S. N. Bose National Centre for Basic Sciences, Salt Lake, JD block, Sector III, Kolkata-700106, India.

**Correspondence to: biswajit96@bose.res.in*

Abstract of the Poster Presentation

We have designed and developed at 7.8 μm mid-IR region by coupling a room-temperature operated continuous wave (CW) external-cavity quantum cascade laser (EC-QCL) with an astigmatic multipass cell. We have utilized wavelength modulation spectroscopy with a second harmonic detection strategy (*2f*-WMS) for the simultaneous and real-time quantitative measurements of nitrous oxide (N_2O) and methane (CH_4) in ambient air and human exhaled breath in parts per billion (ppb) levels via extremely narrow single QCL scan of ~ 0.06 cm^{-1}. The high-resolution rotational-vibrational interference-free *2f*-WMS spectra of CH_4 and N_2O centred at 1297.8192 cm^{-1} and 1297.8314 cm^{-1}, respectively, were acquired with 0.20 s data acquisition time in the optimized experimental conditions. The experimental system has achieved minimum detection limits of 6 ppb for N_2O and 30 ppb CH_4, thus opening its broad applications in environmental monitoring and non-invasive biomedical diagnostics.

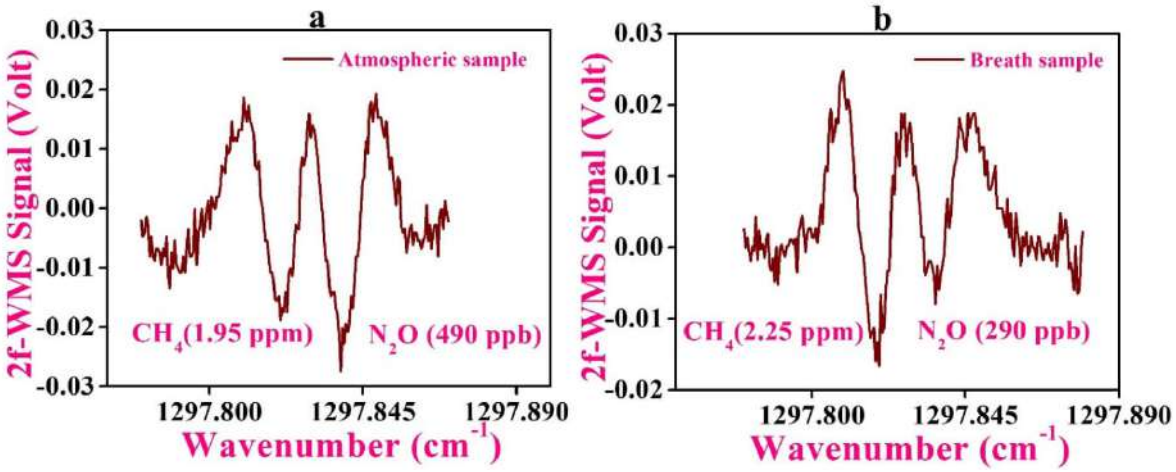


Figure-1. Measurements of CH_4 and N_2O concentrations in (a) atmosphere and (b) human breath at optimized experimental conditions.

References:

[1] B. Panda, A. Pal, S. Chakraborty, and M. Pradhan. Infrared Physics & Technology, 125, (2022), 104261.

[2] A. Maity, M. Pal S. Maithani, G.D. Banik, M. Pradhan, Laser Phys. Lett. 15, (2018), 045701.

Investigation of the Magnon Mode Reversal in Bicomponent Magnonic Crystal.

Chandan Kumar, Pratap Kumar Pal, Prof. Anjan Barman

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

Abstract of the Poster Presentation

The bicomponent magnonic crystals (BMCs) have emerged as a key component in tailoring the exotic properties of the propagating spin waves (SWs). The contrasting magnetic properties of the two different material and the inter-elemental exchange interaction, provides a rich control over spin wave tunability [1]. Here, we observe the anisotropic nature of magnon modes as well as magnon mode reversal [2] in the BMC comprising of circular and square shaped $Ni_{80}Fe_{20}$ embedded in $Co_{50}Fe_{50}$ matrix using the broadband ferromagnetic resonance technique and micromagnetic simulation. Creation and annihilation of distinct localized magnon modes have been observed due to change of in-plane orientation (Φ) of bias magnetic field on both the samples i.e., the square as well as circular shaped-BMC as show in Fig.1(g), (h) for $\Phi = 0^o$. Further, magnon mode reversal phenomena have been periodically modulated by Φ due to periodic modulation of demagnetizing field at the (inter-elemental) interfaces for both samples. These results lead us to deliver a superior control over spin wave tunability which has potential application in spin wave filter, waveguide, spin-wave-based computation and signal processing.

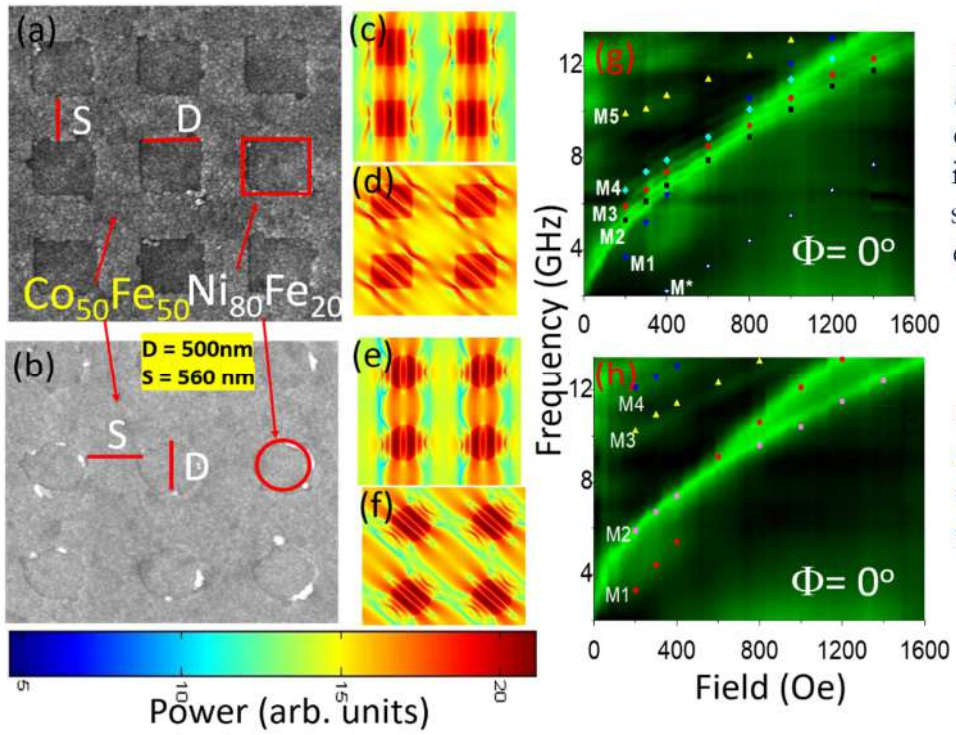


Fig. 1. (a) and (b) represents SEM image of square and circular shaped BMC where D is diameter of circular BMC or side of square BMC and S is edge to edge separation. Power profile for magnon mode M1 at $\Phi = 0^o$ and $\Phi = 45^o$ have been represented by (c), (d) for square and (e), (f) for circular BMC. Bias field dependent SW absorption spectra at $\Phi = 0^o$ have been represented by (g), (h) for square and circular BMC respectively.

References:

[1] S. Choudhury, S. Saha, R. Mandal, S. Barman, Y. Otani, A. Barman, ACS Appl. Mater. Interfaces 2016, 8, 18339.

[2] S. Mamica, J. Magn. Magn. Mater. 2022, 546, 168690.

Fabrication of Artificially Stacked Van-der-Waals Heterostructures

Dayal Das, Gaurab Samanta, Shubhadip Moulick, Shubhrasis Mukherjee and Atindra Nath Pal

Department of Condensed Matter and Material Physics, SNBNCBS

Abstract of the Poster Presentation

The mechanical exfoliation of Graphene[1] by using a scotch tape has produced a huge scope for exploring various two-dimensional layered materials. Two-dimensional materials like graphene, TMDCs (MoS_2, WS_2 etc.)have shown a lot of promises due to their excellent electronic and optical properties. These materials exhibit various exotic properties, such as MoS_2 (a semiconductor), WTe_2 (topological insulator), hBN (an insulator), $NbSe_2$ (superconductor), CrI_3 (ferromagnet). Not only that, we can create various Van-der-Waals heterostructures with such 2D materials by putting one material on top of each other. As there are no physical bonds b/w the layers, it is possible to stack arbitrarily different 2D materials together. This offers a lot of degrees of freedom in fabricating the heterostructures based on these 2D materials.

Here, in this poster we try to explain the details of fabrication process of such Van der Waals heterostructures.

References:

*(1) K. S. Novoselov, 1 A. K. Geim, 1; * S. V. Morozov, 2 D. Jiang, 1; Y. Zhang, 1 S. V. Dubonos, 2 I. V. Grigorieva, 1 A. A. Firsov2. Electric Field Effect in Atomically Thin Carbon Films. Science (80-.).2004, 306 (22), 666–669. https://doi.org/10.1126/science.1102896.*

Optical spectroscopy of the fastest classical nova, V1674 Her

G. R. Habtie[1], R. Pandey[2], N. M. Ashok[2], R. Das[1]

[1]S N Bose National Centre for Basic Sciences, Kolkata, India;
[2]Physical Research Laboratory, Ahmedabad, State of Gujarat, India

Abstract of the Poster Presentation

We present the optical spectra of the fastest classical nova, V1674 Her from day -0.032 to +28.924. By analyzing the optical light curve, we computed the ever-smaller t_2 and t_3 values of ~ 0.904 and ~1.935 d in V band. The distance is calculated to be 4.97 kpc in V band. The overall spectral and photometric evolutions affirm that the nova is extremely fast and the brightness decline sharply. The pre-maxima stage of the nova was dominated by very strong P Cygni profiles and a continuum level tilted toward the blue side. In addition, the strength of Balmer lines and some other neutral emission lines appeared less prominent than spectral lines after, compared with spectra after outburst. During the early decline phase, the tilted continuum level become flat and the less the prominent Balmer lines becomes extremely broad and strong. Same situation extended during the nebular and coronal phases, except the slight decrement in line width and change on the structure of the profiles. The best-fit model predicts the temperature and luminosity of the central ionizing source from day 10.0 to 28.9 to be in the range of 1.99 - 2.34 x 10^5 K and 1.26 - 3.16 x 10^{38} erg s^{-1}, respectively. During both the nebular and coronal phases, the elements He, O, N, and Ne, found to be overabundance of but Fe appeared overabundant during the nebular phase only. The estimated ejecta mass from the best fit model parameters is ~ 3.74 x$10^{-5}M_0$.

References:

1. Albanese I., Farina A., Andreoli V., Ochner P., Reguitti A., 2021, The Astronomer's Telegram, 14718, 1

2. Anupama G. C., Kamath U. S., 2012, Bulletin of the Astronomical Society of India, 40, 161

3. Anupama G. C., et al., 2013, A&A, 559, A121

4. Shore S. N., 2008, Optical and ultraviolet evolution, 2 edn. Cambridge University Press, p. 194–231, doi:10.1017/CBO9780511536168.011

5. Shore S. N., Sonneborn G., Starrfield S., Riestra-Gonzalez R., Ake T. B.,1993, AJ, 106, 2408

6.Starrfield S., Iliadis C., Hix W. R., 2016, PASP, 128, 051001

7. Starrfield S., Bose M., Iliadis C., Hix W. R., Woodward C. E., Wagner R. M., 2020, ApJ, 895, 70

Exploring superadditivity of coherent information of noisy quantum channels through genetic algorithms

Govind Lal Sidhardh, Mir Alimuddin, and Manik Banik

S. N. Bose National Center for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106, India

Abstract of the Poster Presentation

Machine learning techniques are increasingly being used in fundamental research to solve various challenging problems. Here we explore one such technique to address an important problem in the quantum communication scenario. While transferring quantum information through a noisy quantum channel, the utility of the channel is characterized by its quantum capacity. Quantum channels, however, display an intriguing property called superadditivity of coherent information. This makes the calculation of quantum capacity a hard computational problem involving optimization over an exponentially increasing search space. In this work, we first utilize a neural network *Ansatz* to represent quantum states, and then we apply an evolutionary optimization scheme to address this problem. We find regions in the three-parameter space of qubit Pauli channels where coherent information exhibits this superadditivity feature. We characterized the quantum codes that achieve high coherent information, finding several nontrivial quantum codes that outperform the repetition codes for some Pauli channels. For some Pauli channels, these codes display very high superadditivity of the order of 0.01, much higher than the observed values in other well-studied quantum channels. We further compared the learning performance of the neural network *Ansatz* with the raw *Ansatz* to find that in the three-shot case, the neural network *Ansatz* outperforms the raw representation in finding quantum codes of high coherent information. We also compared the learning performance of the evolutionary algorithm with a simple particle swarm optimization scheme, and we show empirical results indicating comparable performance, suggesting that the neural network *Ansatz* coupled with the evolutionary scheme is indeed a promising approach to finding nontrivial quantum codes of high coherent information.

Article: Phys. Rev. A 106, 012432

References:

1. *Johannes Bausch and Felix Leditzky New J. Phys. 22 023005 (2002)*
2. *Devetak, I., Shor, P.. Commun. Math. Phys. 256, 287–303 (2005).*
3. *Felix Leditzky, Debbie Leung, and Graeme Smith Phys. Rev. Lett. 121, 160501 (2018)*

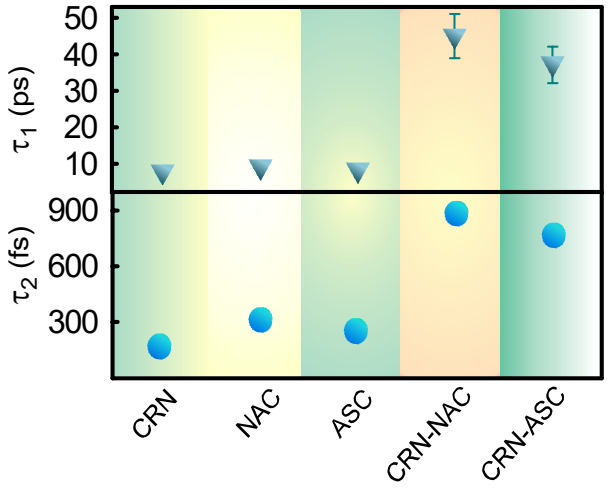
The Underlying Mechanism of Reduction in Elevated Serum Creatinine Level by Anti-Oxidants: A Spectroscopic Investigation

Subhadip Chakraborty, Indrani Bhattacharya and Rajib Kumar Mitra

Department of Chemical and Biological Sciences
S N Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106
email: indrani.bhattacharya92@gmail.com

Abstract of the Poster Presentation

A combined Terahertz (THz) and Infrared (IR) spectroscopic study has been conducted to understand the mechanism of reduction in the elevated serum creatinine (CRN) level by two anti-oxidants: N-acetyl cysteine (NAC) and Ascorbic acid (ASC). FTIR measurements in the mid IR region coupled with quantum chemical calculations (at B3LYP/6-311G++(d,p) level) reveal that both NAC and ASC form H-bonded complexes with CRN and readily undergoes a barrier-less proton transfer process to form creatinium ion which has larger solvation energy compared to bare CRN. This helps in the excretion of the excess serum creatinine from human body through urine. The same result is reflected in the ATR-FTIR study in the THz frequency region where a blue shift is observed in the H-bond stretching of water for both the CRN-NAC and CRN-ASC systems compared to the corresponding monomers implying a stronger hydration associated with the complexes. The observed reorganization from H-bonded complexes to proton-transfer species also correlates with the results obtained from THz-Time Domain Spectroscopic (TTDS) measurement where a sharp rise in the 'waiting time' (τ_1) is observed for both CRN-NAC/ASC systems which is also an indication of stronger hydration. Furthermore, from quantum chemical calculation it is found that hydration catalyses the formation of creatinium ion and results in a proton hopping within the water network in the medium. This also corroborates well with the TTDS results where a striking increases in the 'switching time' (τ_2) is noticed due to the non-availability of the donor site during the switching process as a result of proton hopping.



References:

1. *S. Holt, D. Goodier, R. Marley, D. Patch, A. Burroughs, B. Fernando, D. Harry, K. Moore, Lancet 353, 294-295, 1999.*
2. *D. Gangopadhyay, M. Das, K. K. Singh, R. K. Singh, P. Tandon, J. Raman Spectrosc. 51, 1056-1066, 2020.*
3. *T. Rehman, J. Fought, R. Solomon, Clin J Am Soc Nephrol. 3, 1610–1614, 2008.*

Probing ortho and para nuclear-spin isomers of NH_3 using cavity ring-down spectroscopy

Indrayani Patra, Soumyadipta Chakraborty, Manik Pradhan

Department of Chemical and Biological Sciences, S. N. Bose National Centre for Basic Sciences, Kolkata, India

Abstract of the Poster Presentation

Ammonia ($^{14}NH_3$) is one of the most fundamental molecules in nature and it has major significance in interstellar environment, atmospheric chemistry, and biomedical sciences [1,2]. The rotational levels of NH_3 are described by two quantum numbers J (total angular momentum) and K (projection of J along the molecular symmetry axis) and due to relative orientations of the hydrogen spins two distinct nuclear spin-isomers of ammonia exist: *ortho*-NH_3 and *para*-NH_3 [3]. In this work, we captured some rovibrational spectra of ammonia molecule ($^{14}NH_3$) in gas-phase using a high-resolution continuous wave quantum cascade laser (QCL) coupled cavity ring-down spectroscopy (CRDS). Here, ${}^{\Delta K}\Delta J\,(J'', K'') = {}^{Q}Q\,(3,3)$ and ${}^{R}Q\,(2,1)$ lines representing the examples of ortho and para transitions in the fundamental ν_4 and overtone $2\nu_2$ inversion-vibration bands of $^{14}NH_3$ are probed experimentally in the mid-infrared (6.2 μm) molecular fingerprint region at room temperature. This work illustrates the fundamental spectroscopic properties of ammonia molecule and signifies the potential of QCL-CRDS as a tool for high-resolution molecular spectroscopy [4].

References:

[1] Ricci, Peter P., and Otto J. Gregory. "Sensors for the detection of ammonia as a potential biomarker for health screening." Scientific Reports 11, no. 1 (2021): 1-7.

[2] Ho, Paul TP, and Charles H. Townes. "Interstellar ammonia." Annual Review of Astronomy and Astrophysics 21, no. 1 (1983): 239-270.

[3] Maret, Sebastien, Alexandre Faure, Emanuele Scifoni, and Laurent Wiesenfeld. "On the robustness of the ammonia thermometer." Monthly Notices of the Royal Astronomical Society 399, no. 1 (2009): 425-431.

[4] Maithani, Sanchi, Santanu Mandal, Abhijit Maity, Mithun Pal, and Manik Pradhan. "High-resolution spectral analysis of ammonia near 6.2 μm using a cw EC-QCL coupled with cavity ring-down spectroscopy." Analyst 143, no. 9 (2018): 2109-2114.

Improvement of Leakage, Electric and Magnetic Properties in Cobalt doped Gallium Ferrite

Ishita Jana

SNSBCBS, Salt lake, Kolkata, 700106

Abstract of the Poster Presentation

$GaFe_{1-x}Co_xO_3$ (GFCO, $0 \leq x \leq 0.1$) polycrystals were synthesized using the sol-gel technique. The effects of cobalt (Co) substitution at the iron (Fe) sites of $GaFeO_3$ (GFO) on the microstructure, magnetoelectric properties, and dielectric properties are investigated. Rietveld refinement of the XRD data indicates that all the samples are prepared in the orthorhombic phase containing an additional secondary cubic phase, resulting in increased lattice distortion. For Co = 5%, leakage current density decreases by approximately 4 orders, and higher substitution leads to deterioration of properties with larger leakage current. It has been proposed that the role of Co substitution can be reduced by hopping between Fe^{3+} and Fe^{2+} as well as suppressing the oxygen vacancies. This is supported by higher dielectric constant and lower dielectric loss tangent with a large difference in grain resistance and grain boundary resistance. Two-phase-like magnetic behavior in magnetic hysteresis with increased magnetization and two magnetic transition temperatures (T_C) are observed in the doped samples. Therefore, GFCO samples are promising materials with potential applications in magnetoelectric and multiferroic devices.

References:

1. *Z. Xia et al., "Co Incorporation on Structure, Conductivity and Magnetism of GaFeO3," Wuji Cailiao Xuebao/Journal of Inorganic Materials, vol. 36, no. 3, pp. 319–324, Mar. 2021, doi: 10.15541/jim20200183.*

2. *T. C. Han, Y. C. Lee, and Y. T. Chu, "Effect of cobalt doping on site-disorder and magnetic behavior of magnetoelectric GaFeO3 nanoparticles," Appl Phys Lett, vol. 105, no. 21, p. 212407, Nov. 2014, doi: 10.1063/1.4902874.*

Giant room temperature magnetocaloric response in $(MnNiSi)_{1-x}(FeNiGa)_x$ system

Subrata Ghosh, Saheli Samanta, J Sridhar Mohanty, and Kalyan Mandal

Magnetism Laboratory, Department of Condensed Matter Physics and Material Sciences, S. N. Bose National Centre for Basic Sciences

Abstract of the Poster Presentation

The topic of energy-efficient technology is interested in materials having associated magnetic and structural change. In the $(MnNiSi)_{1-x}(FeNiGa)_x$ (x = 0.16, and 0.17) hexagonal system, the coincidence of magnetic and structural transitions near room temperature is observed, leading to a magneto-structural transition (MST) from a high temperature paramagnetic hexagonal phase to a low temperature ferromagnetic orthorhombic phase, which is accompanied by a significant change in magnetization and a significant change in unit cell volume. The alloys with x = 0.16 and 0.17 are observed to exhibit gaint isothermal magnetic entropy changes (S_M) across MST of 26.2 and 63.2 $Jkg^{-1}K^{-1}$ and relative cooling power (RCP) of about 268.8 and 357.1 Jkg^{-1} for the magnetic field change (ΔH) of 50 kOe. In addition, the material at x = 0.17 exhibits a significant adiabatic temperature change (T_{ad}) of around 13 K caused by ΔH of 50 kOe, which is substantially inferred from the specific heat capacity (c_p) measurement under zero field conditions. Thus, the utilisation of these low - cost materials with large magnetocaloric reactions as magnetic refrigerants is extremely suitable for solid-state cooling systems that operate at room temperature.

References:

- *S. Ghosh, S. Samanta, J S. Mohanty, Giant room temperature magnetocaloric response in $(MnNiSi)_{1-x}(FeNiGa)_x$ system, J. Appl. Phys. 132, 045001 (2022); https://doi.org/10.1063/5.0098679.*
- *J. Chen, H. G. Zhang, E. K. Liu, M. Yue, Q. M. Lu, W. H. Wang, G. H. Wu, and J. X. Zhang, Wide Temperature Window of Magnetostructural Transition Achieved in Mn 0.4 Fe 0.6 NiSi 1−x Ga x by a Two-Step Isostructural Alloying Process, AIP Adv. 6, 056220 (2016).*
- *C. L. Zhang, D. H. Wang, Z. D. Han, B. Qian, H. F. Shi, C. Zhu, J. Chen, and T. Z. Wang, The Tunable Magnetostructural Transition in MnNiSi-FeNiGe System, Appl. Phys. Lett. 103, 132411 (2013).*

TIME REVERSED STATES IN BARRIER TUNNELING

Kanchan Meena & P. Singha Deo

S. N. Bose National Centre for Basic Sciences, 700106, Kolkata

Abstract of the Poster Presentation

Tunneling, though a physical reality, is shrouded in mystery. Wave packets cannot be constructed under the barrier and group velocity cannot be defined. The tunneling particle can be observed on either side of the barrier but its properties 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. A general scheme is developed to derive this expression for any arbitrary system. One can use mesoscopic phenomena to subject the expression to several theoretical and experimental cross checks. For demonstration we consider an ideal 1D quantum ring with Aharonov–Bohm flux ϕ , connected to a reservoir. It gives clear evidence that propagation occur under the barrier resulting in a current that can be measured non-invasively and theoretically cross checked. Time reversed states play a role but there is no evidence of violation of causality. The evanescent states are known to be largely stable and robust against phase fluctuations making them a possible candidate for device applications and so formalizing the current under the barrier is important.

References:

1. P. Singha Deo, Mesoscopic Route to Time Travel, Springer, 2021.

2. Kanchan Meena, P. Singha Deo, Adv Theo Comp Phy, 5, 458, 2022.

3. Kanchan Meena, P. Singha Deo, Physica E 149 (2023) 115680.

Regulation of RhoA GTPase by Phosphorylation of RhoGDI

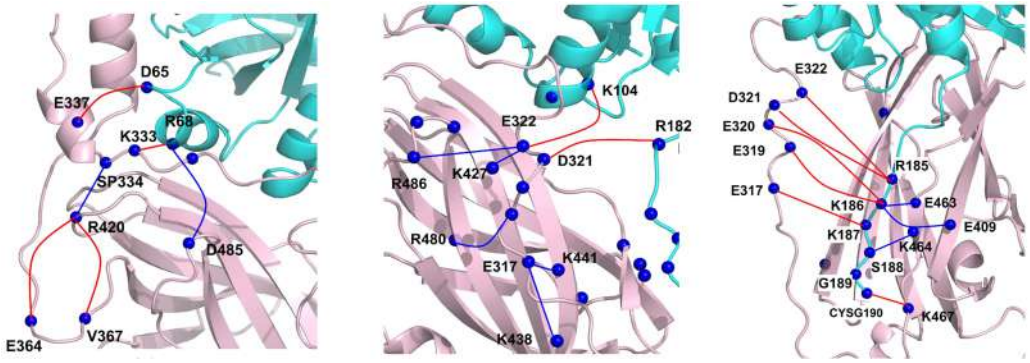
Krishnendu Sinha, Suman Chakrabarty

S.N.Bose National Centre for Basic Sciences

Abstract of the Poster Presentation

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] 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[2] (but not RhoA). On the other hand, phosphorylation of SER-34[3] or SER-96[4] by protein kinase Cα (PKCα) selectively releases RhoA (but not Rac1 or cdc42).

We have performed atomistic molecular dynamics 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. After phosphorylation we have observed major structural changes particularly in the positively charged polybasic region (PBR) of RhoA and negatively charged N-terminal region of GDI. Binding energy calculation shows a significant decrease in binding energy between RhoA and GDI. Due to phosphorylation, the number of contacts between the PBR 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.



References:

1) Hall, A. Rho Family GTPases. Biochemical Society Transactions, 2012, 40, 1378–1382. https://doi.org/10.1042/bst20120103.

(2) Garcia-Mata, R.; Boulter, E.; Burridge, K. The "Invisible Hand": Regulation of RHO GTPases by RHOGDIs. Nature Reviews Molecular Cell Biology, 2011, 12, 493–504. https://doi.org/10.1038/nrm3153.

(3) Dovas, A.; Choi, Y.; Yoneda, A.; Multhaupt, H. A. B.; Kwon, S.-H.; Kang, D.; Oh, E.-S.; Couchman, J. R. Serine 34 Phosphorylation of Rho Guanine Dissociation Inhibitor (RhoGDIα) Links Signaling from Conventional Protein Kinase C to RhoGTPase in Cell Adhesion. Journal of Biological Chemistry, 2010, 285, 23296–23308. https://doi.org/10.1074/jbc.m109.098129.

(4) Knezevic, N.; Roy, A.; Timblin, B.; Konstantoulaki, M.; Sharma, T.; Malik, A. B.; Mehta, D. GDI-1 Phosphorylation Switch at Serine 96 Induces RhoA Activation and Increased Endothelial Permeability. Molecular and Cellular Biology, 2007, 27, 6323–6333. https://doi.org/10.1128/mcb.00523-07.

Interplay of hopping pathways, spin-orbit coupling and interaction in quarter filled t_{2g} orbitals on honeycomb lattice

Manoj Gupta[1], Basudeb Mondal[2], Subhro Bhattacharjee[2], Tanusri Saha-dasgupta[1]

[1]*SN Bose National Centre for Basic Sciences, Kolkata, Salt Lake, Sector-III, Bidhan Nagar, Kolkata, West Bengal 700106.*

[2]*International Centre for Theoretical Sciences(ICTS), Survey No. 152, Shivakote, Hesaraghatta Hobli, Bengaluru-560 089, India*

Abstract of the Poster Presentation

In search of spin-orbital liquid phase Yamada et. al.[1] proposed an SU(4) symmetric model Hamiltonian on α-$ZrCl_3$ layered Honeycomb lattice. The Hamiltonian is derived under certain limits i.e. an infinite spin-orbit coupling (SOC) limit, large crystal field, and dominant indirect hopping via ligands on an uniform Honeycomb lattice. In this work, combining the ab-initio calculations and model Hamiltonian approach, we have studied the electronic structure and interplay of electronic hopping on honeycomb lattice of MX_3, where, M=Ti, Z, Hf ans X=F, Cl, Br. Our first principle calculations on real materials show the dominance of direct d-d hopping in contrast to assumption in Ref[1]. This calls for the revision of the proposal of spin-orbital liquid state of α-$ZrCl_3$. We studied the magnetic and phonon instabilities as well as topological properties which suggest these materials can host exciting properties although they differ from initial proposal. Further the phase diagram of the model interpolating different parameter regions have been studied.

References:

[1] Yamada, Masahiko G., Masaki Oshikawa, and George Jackeli. "Emergent SU (4) symmetry in α zrcl3 and crystalline spin-orbital liquids." Physical Review Letters 121.9 (2018): 097201

Ultrafast solvation dynamics through the eyes of streak camera

Narayan Chandra Maity, Jayanta Mondal, Ranjit Biswas*

SNBNCBS

Abstract of the Poster Presentation

Photophysical study has been performed to explore the solvation dynamics/stokes shift dynamics of Coumarin 153 (C153)[1] and trans-2-[4-(dimethylamino)styryl] benzothiazole (DMASBT)[2] in two polar protic solvents, namely ethylene glycol (EG) and glycerol having similar dielectric constant ($\varepsilon_0 \sim 41-42$ at 293K) but in different viscosity ($\eta_{EG} = 18.2$ cP and $\eta_{glycerol} = 1502$ cP at 293 K). Steady state absorption and emission spectra of polarity sensitive, C153 are similar in both solvents whereas viscosity sensitive DMASBT red shift has been observed in absorption spectra of glycerol with respect to ethylene. Time resolved fluorescence measurements were carried out in two-dimensional streak camera (2DSC)[3,4] with ~2.5 ps temporal resolution and time correlated single photon counting (TCSPC) technique with ~85 ps temporal resolution. Viscosity sensitive probe, DMASBT is showed four times elongated average fluorescence lifetime in viscous glycerol than ethylene glycol whereas C153 showed nearly same lifetime in both the solvent due to their similar polarity. Dynamic fluorescence Stokes shift measurements of DMASBT and C153 were observed similar stoke shift magnitude (362 cm^{-1} and 310 cm^{-1}) and solvation response time in EG. But Solvation dynamics of C153 in glycerol show larger stokes shift dynamic with longer solvent response time than DMASBT.

References:

1. *M.L. Horng, J.A. Gardecki, A. Papazyan, M. Maroncelli, J. Phys. Chem. 99 (1995) 17311–17337.*
2. *M. Kondo, X. Li, M. Maroncelli, J. Phys. Chem. B. 117 (2013) 12224–12233.*
3. *Masayuki Komura , Atsushi Yamagishi , Yutaka Shibata , Ikuko Iwasaki , Shigeru Itoh, Biochimica et Biophysica Acta. 1797 (2010) 331–338*
4. *A. J. Campillo, S. L. Shapiro, IEEE J. Quantum Electron, 9 (1983) 585-603.*

Breaking of Universal Nature of Central Critical Charge in Black Hole Thermodynamics

Neeraj Kumar, Soham Sen, Sunandan Gangopadhyay

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

Abstract of the Poster Presentation

The inclusion of the cosmological constant as one of the thermodynamic variables has led us to new understandings of black hole thermodynamics, especially in understanding the phase structure of AdS black holes. Owing to the holographic correspondence, the first law in bulk can further be written including the central charge of the boundary field theory. Free energy analysis shows that the behaviour of black holes is analogous to the Vander Waals fluid. At the point of second-order phase transition, the critical value of the central charge is shown to be 'universal' in [1]. We investigated the universality in Born-Infeld AdS black holes [2] and for black holes in Gauss-Bonnet gravity [3]. Universal nature breaks for both cases. Explicit calculations have also confirmed that the universal nature breaks for space time with dimensions greater than 4. Thus, the universal nature of the central critical charge is a generic property of Einstein's gravity theory in 3+1 dimensions.

References:

• *W. Cong, D. Kubizk, and R. B. Mann; Phys. Rev. Lett. 127, 091301 2021.*
• *N. Kumar, S. Sen, and S. Gangopadhyay; Phys. Rev. D 106, 026005 2022.*
• *N. Kumar, S. Sen, and S. Gangopadhyay; Phys. Rev. D 107, 046005 2023.*

Reverse Osmosis of binary mixture through polymeric membrane

Rahul Karmakar, Jaydeb Chakrabarti

Department of Physics of Complex Systems

Abstract of the Poster Presentation

Pressure-driven Reverse Osmosis(RO), an out of equilibrium technique, are widely used nowadays both in industry and household purposes like water desalination. In RO, solvent is forced by pressure drops through a semipermeable membrane. Experiments show that changing relative interaction of membrane matrix with mixture changes permeation of solvent, solute rejection and fouling inside the membrane. Here we model RO process through a polymeric membrane. We attach two LJ reservoir on two sides of solveated membrane. One reservoir contains binary mixture of large solute and small solvent. Other reservoir contains pure solvent. We study separation of this binary mixture through polymeric membrane where solvent is driven by force from mixed side to the pure side. We tune relative interaction strength which is defined by ratio of interaction between solute particles and two polymeric network beads. We observe that with increase in relative interaction strength, we get increase in separation where solvent accumulates in the pure side. We also observe fouling of solute inside the membrane increases with increase in relative interaction strength with the membrane. Finaly, we change relative interaction strength of solvent with membrane keeping solute interaction fixed. We observe reduce in fouling with optimum recovery rate of solvent and rejection of solute for higher relative interaction strength.

Chemotactic response to spatio-temporal variation in attractant environment

Ramesh Pramanik and Sakuntala Chatterjee

Department of Physics of Complex Systems, S. N. Bose National Centre for Basic Sciences, Kolkata- 700106

Abstract of the Poster Presentation

Chemotaxis is a property in which a cell migrates in response to the external chemical environment. An Escherichia Coli responds to its environment by performing a run-tumble motion. In our work, we are interested in how the chemotactic response of the cell is affected by spatiotemporal variation of the extracellular chemical environment.In particular, we consider an attractant profile, where the spatial gradient varies periodically in time with time period T. Our numerical simulations show that the chemotactic response of the cell varies non-monotonically with T. For $T \to 0$ and $T \to \infty$ the response is similar but at an intermediate T, it shows a minimum. We explain this interesting observation from an interplay between sensing and adaptation modules of intracellular signaling network.

References:

'Chemotactic response to spatio-temporal variation in attractant environment', Ramesh Pramanik and Sakuntala Chatterjee(manuscript in preparation)

Distilling nonlocality in quantum correlations

Sahil Gopalkrishna Naik[1], Govind Lal Sidhardh[1], Samrat Sen[1], Arup Roy[2], Ashutosh Rai[3,4], Manik Banik[1]

[1]*Department of Physics of Complex Systems, S. N. Bose National Center for Basic Sciences, Kolkata, India*
[2] *Department of Physics, A B N Seal College Cooch Behar, West Bengal 736101, India*
[3] *School of Electrical Engineering, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea*
[4] *Institute of Physics, Slovak Academy of Sciences, 845 11 Bratislava, Slovakia*

Abstract of the Poster Presentation

Nonlocality, as established by seminal Bell's theorem, is considered to be the most striking feature of correlations present in space like separated events. Its practical application in device independent protocols, such as, secure key distribution, randomness certification etc., demands identification and amplification of such correlations observed in quantum world. In this letter we study the prospect of nonlocality distillation, wherein, by applying a natural set of free operations (called wirings) on many copies of weakly nonlocal systems, one aims to generate correlations of higher nonlocal strength. In the simplest Bell scenario, we identify a protocol, namely logical OR-AND wiring, that can distil nonlocality to significantly high degree starting from arbitrarily weak quantum nonlocal correlations. As it turns out, our protocol has several interesting facets: (i) it demonstrates that set of distillable quantum correlations has non zero measure in the full eight dimensional correlation space, (ii) it can distil quantum Hardy correlations by preserving its structure, (iii) it shows that (nonlocal) quantum correlations sufficiently close to the local deterministic points can be distilled by a significant amount. Finally, we also demonstrate efficacy of the considered distillation protocol in detecting post quantum correlations.

References:

S. G. Naik, G. L. Sidhardh, S. Sen, A. Roy, A. Rai, and M. Banik; Distilling nonlocality in quantum correlations, arXiv:2208.13976(2022).

Growth, Charecterization and dielectric studies of two dimensional organic-inorganic halide perovskite.

Saikat Mitra

SRF, S N Bose National Centre For Basic Sciences

Abstract of the Poster Presentation

In this poster presentation I will show growth, charecterization and dielectric spectroscopy study of two dimensional halide perovskite. We know three-dimensional halide perovskite has got research interest boost in last decade due to its tunable band-gap, high diffusion length of minority charge carriers, high mobility of electrons and holes and low exciton binding energy. Due to these above mentioned features it finds applications in solar cell, photo-detectors, scintillating detection, gas sensing etc. But three dimentional perovskite halide suffers from stability issues due to humidity which stops it for comercial application. In this situation many researchers have turned their attention to two dimentional halide perovskite. We know that for being 3d perovskite few conditons needs to be satisfied i.e goldsmith tolerance factor, $t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$ (where if perovskite formula is ABX_3 then r_A is radius of A atom, r_B is radius of B atom and r_X is radius of X atom) has to be $0.8 \leq t \leq 1$ and octahedral factor $\mu(= \frac{r_B}{r_X}) > 0.41$. Now if value of A radius increases then tolerance factor may exceed 1 and the structure will no longer be 3d perovskite. One such class of perosvkite is Ruddleson-popper perovskite with general formula $(RNH_3)_2PbX_4$ where R is alkyl or aromatic group and X is halide groups. Here I have taken organic cation to be butylammonium ($C_4H_9NH_3$) and halide anion as bromine. After synthesis of the material, I have charecterized the material by various techniques i.e X-ray diffraction, FESEM, HRTEM etc to ensure its proper phase formation. Then I have done dielectric spectroscopic studies in which I will show dielectric relaxations and negative dielectric constant and anomalous behavour of capacitance.

References:

(1) Y. Fu, H. Zhu, J. Chen, M. P. Hautzinger, X. Y. Zhu and S. Jin, Nat. Rev. Mater., 2019, 4, 169–188.

(2) S. Masi, A. Rizzo, R. Munir, A. Listorti, A. Giuri, C. Esposito Corcione, N. D. Treat, G. Gigli, A. Amassian, N. Stingelin and S. Colella, Adv. Energy Mater., 2017, 7, 1602600.

(3) J. Zhou and J. Huang, Adv. Sci., 2018, 5, 1700256.

(4) J. Li, Z. Han, Y. Gu, D. Yu, J. Liu, D. Hu, X. Xu and H. Zeng, Adv. Funct. Mater., 2020, 31, 2008684.

(5) J. Song, T. Fang, J. Li, L. Xu, F. Zhang, B. Han, Q. Shan and H. Zeng, Adv. Mater., 2018, 30, e1805409.

(6) C. Chen, L. Gao, W. Gao, C. Ge, X. Du, Z. Li, Y. Yang, G. Niu and J. Tang, Nat. Commun., 2019, 10, 1927.

(7) J. Mater. Chem. C, 2021, 9, 6498

Interplay of Magnetism and Unconventional Topology in LaCoO3/SrIrO3 Heterostructure

Samir Rom[1], Santu Baidya[2], Subhro Bhattacharjee[3], and Tanusri Saha-Dasgupta[1]

[1)]S.N. Bose National Centre for Basic Sciences, JD Block, Sector III, Salt Lake, Kolkata 700106, India.

[2)]Materials Research Centre, Indian Institute of Science, Bangalore 560012, India.

[3)]International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru 560089, India.

Abstract of the Poster Presentation

Employing first-principles calculations, we investigate the magnetic and topological properties of LaCoO3/SrIrO3 heterostructure [1], which has been recently synthesized [2]. Our study unravels transfer of polar charge from SrIrO3 to LaCoO3, thereby reducing the Co valence from 3+ towards 2+, supporting the experimental findings. Our study further reveals stabilization of intermediate spin-state of Co and strong ferromagnetic Co-Co coupling in LaCoO3 block of the heterostructure. This, in turn, is found to induce ferromagnetism in the pseudo-tetragonally structured SrIrO3 in heterostructure geometry. Thus the heterostructure geometry supports ferromagnetic ground state, in contrast to non-magnetic nature of both LaCoO3 and SrIrO3 in bulk form. Interestingly, the band-structure of ferromagnetic, tetragonal structured SrIrO3 is found to exhibit unconventional topology, manifested as C=2 double Weyl points, which provides microscopic understanding of the observed anomalous Hall effect. Our finding of C=2 double Weyl points, belonging to class of charge-2 Dirac points, opens up the possibilities of material realization of unconventional topological properties beyond the conventional Dirac and C=1 Weyl points.

Acknowledgements: TS-D acknowledges J.C.Bose National Fellowship (grant no. JCB/2020/000004) for funding. S. B. acknowledges funding from Max Planck Partner group Grant at ICTS, Swarnajayanti fellowship grant of SERB-DST (India) Grant No. SB/SJF/2021-22/12 and the Department of Atomic Energy, Government of India, under Project No. RTI4001. TS-D and S.B. would like to thank Vajra grant (SERB/F/373/2022023) for the collaboration. The authors thank Saumya Mukherjee for bringing the problem into our notice and valuable discussions.

References:

1. *Appl. Phys. Lett. 122, 021602 (2023).*
2. *Adv. Mater. 34, 2109163 (2022).*

Density functional theory based Predictive Model for Low-Dimensional Organic-Inorganic Halide Perovskites

Sanuja Kumar Khuntia, Debayan Mondal and Priya Mahadevan*

Department of Condensed Matter Physics and Material Science
S. N. Bose National Centre for Basic Science, Kolkata,
West Bengal, India
**E-Mails: priya@bose.res.in*

Abstract of the Poster Presentation

In most synthesized organometallic perovskites nitrogen (ammonium) based molecules have been used as A-site cations so far but recently there is a trend of using phosphorus base molecules due to its lower electronegativity and having a unique band structure which leads to different optoelectronic properties. Our research is based on investigating the electronic and structural properties of these newly synthesized phosphonium-based hybrid halide perovskites. Using first principle density functional theory-based simulations, we have predicted the ground state structure of these 1D rod-like phosphonium-based hybrid halide perovskites. Different types of nonlocal, weak van der Waals (vdW) interactions have been tested to predict the structural properties correctly. Finally, it was found that the simulated XRD, spontaneous polarization, and electronic band gap have quite a good match with the experimental results. In the future, we

believe that we are able to predict the structural and electronic properties of new 1D and 2D perovskite using this methodology.

Ground state properties & Quantum Phase Diagram for spin-1/2 antiferromagnetic kagome stripe chain

Sayan Ghosh[a], Sudip Kumar Saha[a] and Manoranjan Kumar[a*]

[a]*S.N. Bose National Centre for Basic Sciences, JD Block, Sector-III, Saltlake City, Kol-700106*

Abstract of the Poster Presentation

In last few decades, quantum phase transitions (QPD) are vividly exploring in the context of condensed matter physics. In 2D frustrated quantum magnets, quantum spin liquid (QSL), like resonating valence bond (RVB) which is dimer pairings that resonate throughout the lattice may appear. In this poster presentation, we are going to explore the spin-1/2 ground state properties on kagome stripe chain (KSC) which is the one dimensional version of kagome lattice (Figure 1). Recent studies show 15 different kinds of magnetization plateaus can be achieved from KSC with some external magnetic field[1] and presence of QSL phase has been proven[2]. For exploring ground state we took our Hamiltonian,

$$H=\sum_{r=1}^{N/5} J_1\left(S_{r,1}.S_{r,4}+S_{r,2}.S_{r,5}\right)+J\left(S_{r,1}.S_{r,3}+S_{r,2}.S_{r,3}+S_{r,3}.S_{r,4}+S_{r,3}.S_{r,5}\right)+J_2\left(S_{r,4}.S_{r+1,1}+S_{r,5}.S_{r+1,2}\right)$$

where J_1, J_2 and J are three interactions and J is always fixed at unity. 'r' is number of unit cell. We use Exact Diagonalization (ED) and Density Matrix Renormalization Group (DMRG)[3] at zero temperature with periodic boundary condition (PBC) to explore the g.s. properties. By varying J_1 and J_2, we have found nine different phases from this model- Hexagonal, Uniform chain, Dimer, Two up & two down, Antiferromagnetic (AFM), Quasi long range ordered (QLRO) along the leg & middle spins, Short range ordered (SRO) along the leg & middle spins. We construct an effective model by taking each five site unit cell as an effective spin and they are connecting via J_2. In perturbative limit of J_2 we have found two phases- Two up & two down and AFM which we have also found from numerical calculations.

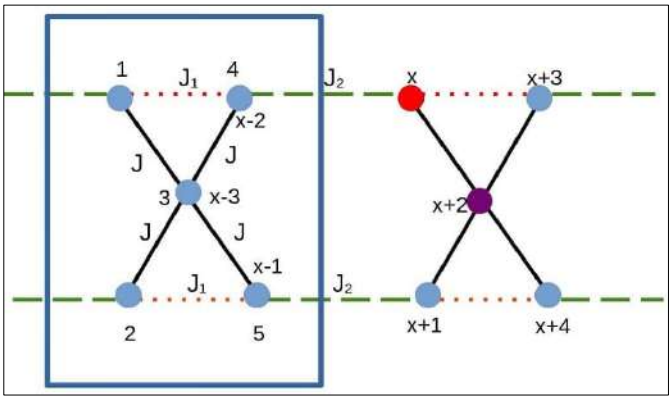


Figure 1: Structue of KSC. x is the numbering of that particular site. Boxed portion denotes 'r' unit cell. Red and purple sites are reference sites for calculation

References:

[1] Katsuhiro Morita, Shigetoshi Sota & Takami Tohyama. Magnetic phase diagrams of the spin- 21 Heisenberg model on a kagome-strip chain: Emergence of a Haldane phase. PHYSICAL REVIEW B 104, 224417 (2021)

[2] Katsuhiro Morita, Shigetoshi Sota & Takami Tohyama. Resonating dimer–monomer liquid state in a magnetization plateau of a spin-12 kagome-strip Heisenberg chain. Commun. Phys. 4, 161 (2021)

[3] White S.R. Density-matrix algorithms for quantum renormalization groups. Phys. Rev. B, 48 (1993)

Magnetoresistance in the critical region of weak-itinerant ferrimagnet FeCr2Te4 single crystal

Sayan Routh, Indrani Kar, Achintya Low, Susanta Ghosh and Tushar Kanti Bhowmik

Department of Condensed Matter and Materials Physics, S N Bose National Centre for Basic Sciences, Kolkata, West Bengal-700106, India

Abstract of the Poster Presentation

We measured a comprehensive study on the magnetic and electrical transport properties of weak-itinerant ferrimagnet $FeCr_2Te_4$ single crystal. We notice a magnetic transition from paramagnetic to ferrimagnetic ordering at ≈123 K. Temperature dependent magnetoresistance shows a minima in the vicinity of the Curie temperature (T_c). From the Hall resistivity measurement, we have seen that anomalous Hall effect (AHE) is dominated by the extrinsic skew scattering mechanism. Our study suggests that the carrier concentration is also related to the magnetoresistance behavior near (T_c).

References:

1. *Liu Y, Tan H, Hu Z, Yan B and Petrovic C 2021 Phys. Rev. B 103(4) 045106*
2. *Liu Y, Koch R J, Hu Z, Aryal N, Stavitski E, Tong X, Attenkofer K, Bozin E S, Yin W and Petrovic C 2020 Phys. Rev. B 102(8) 085158*

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

Shobhan Dev Mandal and Sakuntala Chatterjee

Department of Physics of Complex Systems S. N. Bose National Centre for Basic Sciences

Abstract of the Poster Presentation

The cooperative behavior of receptor dimers forming densely packed clusters is recently found to be a significant source of fluctuation in E. coli chemotaxis pathway. Highly dense large clusters can sense the nutrient concentration more efficiently, which enhances the chemotactic performance. But large clusters increase the fluctuation also, which causes adaptation module to respond strongly. Therefore, a competition develops between sensing and adaptation. At very large cluster size adaptation wins the competition resulting decrease in the sensitivity of chemoreceptors. Hence chemotactic efficiency deteriorates resulting 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 concentration gradient and direction of cell movement. In weak gradient for both uphill and downhill runs, after initial demethylation we see late time methylation and change in methylation level gets amplified as cluster size increases. In strong gradient uphill runs also show similar behaviour in methylation dynamics whereas the downhill runs show highly non-trivial dependence of methylation level on cluster size due to sensing and adaptation interplay[2]. In another study we see faster switching rate of receptor

activity enhances chemotactic performance. Variation of activity for small and large value of switching rate is significantly different in downhill runs and this asymmetry causes the enhancement[3].

References:

[1] Effect of receptor clustering on chemotactic performance of E. coli: Sensing versus adaptation, by Shobhan Dev Mandal and Sakuntala Chatterjee, Phys. Rev. E Letters 103, L030401(2021).

[2] Effect of receptor cooperativity on methylation dynamics in bacterial chemotaxis with weak and strong gradient, by Shobhan Dev Mandal and Sakuntala Chatterjee, Phys. Rev. E 105, 014411(2022)

[3] Effect of switching time scale of receptor activity on chemotactic performance of Escherichia coli, by Shobhan Dev Mandal and Sakuntala Chatterjee, Indian J Phys 96, 2619 (2022) .

Quantum Phase Diagram of The One dimensional Extended Hubbard Model with Polarization

Sourabh Saha, Manoranjan Kumar

S.N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata 700106, India

Abstract of the Poster Presentation

We have studied the effect of polarization in the phase diagram of the 1d extended Hubbard model. By using level-crossing method we see that one dimensional extended Hubbard model with charge dipole interaction term(P) gives six different phases for non zero values of hopping(t), whereas earlier studies showed that for t=0 it has four different phases[1]. For moderate onsite Coulomb repulsion(U) and very small values of polarization(P) the Charge Density Wave I(CDW I) to Bond Order Wave(BOW) transition is second order but BOW to Spin Density Wave(SDW) transition is Kosterlitz-Thouless type of spin gap transition. For moderate nearest neighbor Coulomb repulsion(V) and moderate P, a triplet phase comes in between SDW and Ferroelectric phase. The intermediate phase which we called Ferroelectric phase does not have the point of inversion symmetry. Due to the lack of inversion symmetry implies that this phase is Ferroelectric. We also studied the spin density, charge density, spin-spin, charge-charge correlation for different phases and from this we can also identify the nature of spin configurations of various phases. We have calculated the spin and charge structure factor from the correlations and the change of its nature also indicates the phase transition points. M. E. Torio et al. studied this phase diagram by berry phase calculation [2] but this method cannot be applied to phases that are out of reach of the continuum limit of field theory. But our level-crossing method using Exact Diagonalization(ED) and Density Matrix Renormalization Group(DMRG) do not have such kind of limitations and it gives the desirable accurate result.

References:

1. J. van den Brink, M.B.J. Meinders, J. Lorenzana, R. Eder, and G.A. Sawatzky, Phys. Rev. Lett. 75, 4658 (1995).

2. M. E. Torio, A. A. Aligia, K. Hallberg, and H. A. Ceccatto,Phys. Rev. B 62, 6991(2000).

Active Acousto-Plasmo-Magnonics in a Two-dimensional Artificial Magnonic Crystal

Sreya Pal[1], Pratap Kumar Pal[1], Raisa Fabiha[2], Supriyo Bandyopadhyay[2,♀] and Anjan Barman[1,*]

[1]*Department of Condensed Matter and Materials Physics, S. N. Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata 700106, India*

[2]*Department of Electrical and Computer Engineering, Virginia Commonwealth University, Richmond, VA 23284, USA*

Abstract of the Poster Presentation

A significant interest in combining plasmonics and magnetism at the nanoscale gains ample momentum in both photonics and magnetism that are concerned with the resonant enhancement of light-magnetic-matter interaction in nanostructures[1]. Coupling between spin waves and other entities (acoustic waves, electromagnetic waves, etc.) in nanostructured media has emerged as an important topic of research because of the rich physics and the potential for disruptive technologies. Here, we report a new phenomenon in this family that involves coupling between spin waves and hybridized phonon-plasmon waves (tripartite mixing of magnons, phonons and plasmons). We call it *acousto-plasmo-magnonics* and study it in an artificial magnonic crystal comprising a two-dimensional periodic array of magnetostrictive nanomagnets deposited on a silicon substrate with an intervening thin film of aluminium that acts as a source of surface plasmons. Here, cavity of plasmonic material becomes responsible for nonlinear frequency generation technique such as sum-frequency and difference-frequency generation and creates frequency-comb[2]. Enhanced MOKE signal from the plasmonic samples imply the power transfer from the hybrid mode to SW modes to increase their amplitudes and confirming plasmon enhanced magneto- optical effects. Our findings also reveal the presence of parametric amplification in this system; energy is transferred from the hybridized phonon-plasmon modes to the acousto-plasmo-spin wave modes to amplify the latter (giant power amplification by a factor of ~ 200). All this opens a path to the design of novel active metamaterials with tailored and enhanced response. They may enable high-efficiency magneto-mechanical-plasmonic frequency mixing in the GHz−THz frequency regime and provide a unique avenue to study non-linear coupling, parametric amplification, and frequency comb physics.

References:

1. *A.Kimel et al., Journal of Physics D: Applied Physics 2022, 55, (46).*
2. *A.Ahmed et al., Nano Lett 2022, 22, (13), 5365-5371.*

Formation of atomic point contact using mechanically controlled break junction.

Subhankar De, Biswajit Pabi and Atindra Nath Pal.

S. N. Bose National Centre for Basic Sciences.

Abstract of the Poster Presentation

Understanding the transport characteristics at the atomic limit is the prerequisite for futuristic nano electronic applications. Among various experimental procedures, mechanically controllable break junction (MCBJ) is one of the well adopted experimental technique to study and control the atomic or molecular scale devices. Here, we present the details of the development of a piezo controlled table top MCBJ set up, working at ambient condition, along with necessary data acquisition technique and analysis of the data. We performed conductance experiment on a macroscopic gold wire, which exhibits quantized conductance plateau upon pulling the wire with the piezo. Conductance peaks up to ~ 12 G_0 ($G_0 = 2e^2/h$, e is the electronic charge and h being the plank's constant) could be resolved at room temperature. This is in line with the previous reports. This demonstrate that our custom-designed MCBJ set up is capable of measuring quantum transport of a single molecular junction at ambient condition.

References:

Biswajit Pabi and Atindra Nath Pal. "Probing metal-molecule contact at the atomic scale via conductance jumps." Physical Review B 104.12 (2021): L121407.

Observation of Spin-reorientation Transition and Large Anomalous Hall Effect at Elevated Temperatures in Mn_3Ge Weyl Semimetal.

Susanta Ghosh,[1] Achintya Low,[1] Susmita Changdar,[1] Shubham Purwar,[1] and S. Thirupathaiah[1].

[1]*Condensed Matter and Material Physics Department, S N Bose National Centre for Basic Sciences, Kolkata, 700106, West Bengal, India*

Abstract of the Poster Presentation

We report on the magnetic and Hall properties of nearly stoichiometric, magnetic Weyl semimetal, $Mn_{2.94}Ge$ single crystal. From the magnetic properties study, we identify unusual magnetic transitions below the N´eel temperature of 353 K such as the spin-reorientation (T_{SR}), ferromagnetic, and spin-glass transitions. Though the spin-reorientation and spin-glass transitions are generally observed in Mn_3Sn, these were not so far observed in Mn_3Ge. Further, consistent with the magnetic properties, the Hall effect study shows an unusual behavior around the spin-reorientation transition. Specifically, the anomalous Hall conductivity (AHC) increases with increasing temperature with a maximum at T_{SR} and then gradually decreases with increasing temperature. This observation is quite contrast to the previous reports on Mn_3Ge, where a gradual decrease in AHC was demonstrated with increasing temperature.

References:

1) *S. Ghosh, et al., Observation of Spin-reorientation Transition and Large Anomalous Hall Effect at Elevated Temperatures in Mn3Ge Weyl Semimetal (Manuscript under review).*

2) *S. Nakatsuji, N. Kiyohara, and T. Higo, Nature 527, 212 (2015).*

3) *A. K. Nayak, et al., Science advances 2, e1501870 (2016).*

4) *A. Low, S. Ghosh, S. Changdar, S. Routh, S. Purwar, and S. Thirupathaiah, Phys. Rev. B 106, 144429 (2022).*