REPORT

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A. Research Highlights:

- Research in Adish Dani's group has focused on two broad areas at the interface of neuroscience, cell and molecular biology: (1) They have developed single cell and spatial transcriptomics as a handle to investigate the diversity and gene expression differences between cell types of a specialized chemosensory organ using mouse models. (2) They have developed super-resolution microscopy tools to investigate the ultrastructure of a specialized ribbon synapse found in cochlear cells and alterations observed as a result of deafness. (3) They have developed tools to investigate the organization of calcium channels on the plasma membrane of the cell to understand their gating and molecular characteristics.
  [All collaborators in this work: Faculty - Adish Dani (TIFRH), Mark Rutherford (Washington University in St Louis, USA), Monika Vig (TIFRH); Students (TIFRH) - Devakinandan GVS, Sritama Dutta, Kunal Jagetiya; Research Fellows (TIFRH) - Gayatri Chandran, Nandana Nanda]

- A bis-NHC-CAAC dimer derived dicationic diradical (Anukul Jana)
  The isolation of carbon-centered diradicals was always considered to be challenging due to their synthetic difficulties as well as due to their limited stability. Recently Anukul Jana and colleagues reported the synthesis of a trans-1,4-cyclohexylene bridged bis-NHC-CAAC dimer derived thermally stable dicationic diradical. The diradical character of this compound was confirmed by EPR spectroscopy. The variable temperature EPR study suggested the singlet state to be marginally more stable than the triplet state ($2J = -5.5\ cm{-}1$ ($\Delta E_{ST} = 0.065\ kJmol^{-1}$)). The presence of the trans-1,4-cyclohexylene bridge was instrumental for the successful isolation of this dicationic diradical. Notably, in case of ethylene or propylene bridged bis-NHC-CAAC dimers, the corresponding dicationic diradicals were transient and rearranged to hydrogen abstracted products.
  [All collaborators in this work: Mithilesh Kumar Nayak, Nicolas Chrysochos, Ramakirushnan Suriya Narayanan, Ramapada Dolai, Biswarup Roy, Vishal Malik, Hemant Rawat, and Anukul Jana (TIFRH) ; Pallavi Sarkar and Swapan K. Pati (Jawaharlal Nehru Centre for Advanced Scientific Research); Benedict J. Elvers and Carola Schulzke (Universität Greifswald); Sakshi Mehta and Abhishake Mondal (Indian Institute of Science); Fangyuan Zhang and Prince Ravat (University of Würzburg; Ivo Krummenacher, Holger Braunschweig (Julius-Maximilians-Universität Würzburg); Thangavel Vijayakanth

and Ramamoorthy Boomishankar (Indian Institute of Science Education and Research Pune)

- Single molecule RNA Fluorescence in situ Hybridization to monitor differential expression of EGFR pathway genes in primary Drosophila tissue and effects of dosage on adult eye phenotypes (Aprotim Mazumder)
  Single molecule Fluorescence in situ Hybridization (smFISH) for mRNA provides a quantitative handle on gene expression. Previously Aprotim Mazumder and colleagues developed a modified method of smFISH applicable on various primary whole-mount tissues from the fruit fly Drosophila melanogaster. They used this method to investigate the links between EGFR signaling and cell proliferation. These studies have revealed an intriguing differential expression of EGFR pathway genes in the developing larval eye discs. The researchers connected changes in gene dosage of *Spitz* and *Argos* genes to final patterning of the Drosophila eye. More than absolute levels of expression, the ratio of these two gene products turned out to be a critical regulator of proper eye patterning. The researchers further used a temperature-sensitive Gal80 to systematically tune the spitz-to-argos mRNA ratio. By tuning this ratio, they identified the range to which the final eye phenotype is developmentally buffered. In this period, the researchers also investigated the more proximate outcomes of such signaling. This study provides critical insight into how specific cell types emerge during organismal development and how developmental systems may be buffered against gene expression fluctuations. This work was published in the journal PLOS Genetics.
  [All collaborators in this work: Nikhita Pasnuri, Manish Jaiswal, Krishanu Ray, Aprotim Mazumder]

- Ultrafast coherent sources in the infrared (Chaitanya Kumar Suddapalli)
  High power, tunable ultrafast near-to-mid-infrared coherent sources are interesting for variety of applications including spectroscopy and imaging. However, access to desired spectral regions in not always trivial. In this work, the researchers have demonstrated a near-infrared coherent source providing picosecond pulses at MHz repetition rates tunable specifically in the 1.3−1.5 μm region, which is otherwise inaccessible using readily available sources.
  [Collaborators in this work: ICFO-The Institute of Photonic Sciences, Spain]

- Development of atomic magnetometer with pico-Tesla sensitivity and 25 kHz bandwidth (G Rajalakshmi)
  G Rajalakshmi and colleagues demonstrated a single-beam atomic magnetometer operating at room temperature for the measurement of oscillating magnetic fields. The magnetometer functions in the nonlinear regime of magneto-optical rotation in an atomic vapour system. The system has a sensitivity of approximately 0.9 pT at 2 kHz and a large bandwidth of 24 kHz. The dynamic range of measurement is 10^6 , making the sensor effective even in Earth's field.
  [All collaborators in this work: G Rajalakshmi, P K Madhu, Sushree S Sahoo, George Kurian K K]

- Jagannath Mondal and colleagues demonstrated the role of low molecular weight cosolutes (known as osmolytes) in maintaining native electrostatic interaction between charged surfaces under salt stress. The mechanism of retaining charge density by these

osmolytes was found to be dependent of chemical structure. The effort underlined a joint in-campus collaboration via apt combination of theory and experimental techniques.
[All collaborators in this work: Susmita Sarkar, Anku Guha, T. N. Narayanan, Jagannath Mondal]

- Current Fluctuations in Interacting and Non-Interacting Particle Systems (Kabir Ramola)
  Kabir Ramola and colleagues introduced generalized "quenched" and "annealed" disorder averages for active particle systems that account for multiple degrees of freedom, including positions and velocities of particles. The researchers used this to study the fluctuations of the integrated density current across the origin up to time T in one dimensional systems of non-interacting as well as interacting active particles. They illustrated these new techniques through exact results for current fluctuations of non-interacting run and tumble particles in one-dimension. Surprisingly, quenching both positions and velocities anomalously suppresses current fluctuations. This suppression cannot be achieved through quenching the positions alone, highlighting the importance of considering multiple fields in disorder averages. Their techniques open new research areas in the fields of disordered and non-equilibrium systems, where averages over multiple fields have not been considered.

  For the interacting case, they explored a lattice model of active particles with hard-core interactions that is amenable to an exact description within a fluctuating hydrodynamics framework. For the case of uniform initial profiles, they showed that the second cumulant of the integrated current displays three regimes: an initial rise with a power 1/2, a cross-over regime where the effects of activity increase the fluctuations, and a large time behavior once again characterized by a power 1/2. In the limit of zero diffusion for the interacting system, they showed that the fluctuations also exhibit suppressed fluctuations at short times. Finally, they also showed that the results for non-interacting active particles are recovered for low densities.
  [All collaborators in this work: Stephy Jose, Rahul Dandekar, Alberto Rosso, Kabir Ramola]

- ‘Peptide hybridization’ – an innovative strategy to design peptide inhibitor of PfAMA1–PfRON2 interactions (Kalyaneswar Mandal)
  In an endeavour to develop a peptide inhibitor of PfAMA1–PfRON2 interactions, Kalyaneswar Mandal and colleagues have, very successfully, designed a unique chimeric peptide that has displayed malaria parasite growth inhibition with nanomolar IC50, which is two orders-of-magnitude better than any of its parent peptides. The peptide chimera has been prepared by fusion of the best features of two previously known peptide inhibitors. This work is highly significant, as the resultant chimeric peptide has been found to exhibit growth inhibition activity to a representative drug-resistant *P. falciparum* strain (Dd2) even better than the most common parasite strain (3D7). To understand the molecular basis of the augmented potency, the researchers computationally modelled the hybrid peptide on its receptor. The innovative peptide hybridization strategy demonstrated by the researchers will open up new possibilities to design novel peptide inhibitors for other protein-protein interaction based drug targets as well.

[All collaborators in the work: Jamsad Mannuthodikayil, Suman Sinha, Sameer Singh, Anamika Biswas, Irshad Ali, Purna Chandra Mashurabad (UoH), Wahida Tabassum (UoH), Pratap Vydyam (UoH), Mrinal Kanti Bhattacharyya (UoH) and Kalyaneswar Mandal]

- Using NMR spectroscopy to understand protein structure and dynamics (Kaustubh R Mote)
  Kaustubh R Mote and colleagues are studying actin structure and dynamics in order to understand how these ubiquitous proteins are modulated by cofactors and modulating proteins. They have been able to perform high resolution solid-state NMR experiments at fast MAS frequencies on the bacteria actin-like protein ParM, as well as express and purify MreB, a bacterial actin that determines cell shape and motility, and is an important target for potential antibiotics. Additionally, the researchers have been able to express and purify a carrier protein called SemiSWEET which will allow them to adress some of the fundamental questions in the field of membrane transport.
  The researchers have also developed new experiments to determine dynamics in proteins at very fast MAS frequencies. This method will be used to study the above two proteins. Further, they have developed several methods based on multiple acquisition techniques that speed up data acquisition in proteins under fast as well as slow-moderate MAS frequencies.
  [All collaborators in this work: Kaustubh R. Mote, V. Agarwal, P. K. Madhu, G. Pananghat (IISER Pune)]

- Bendless is essential for PINK1-Park mediated Mitofusin degradation under mitochondrial stress. (Manish Jaiswal)
  The difference in shape and size of mitochondrial has been shown to profoundly impact mitochondrial metabolic capabilities and overall cellular physiology. In a genetic screen in *Drosophila*, mutations in *lrpprc2* were recovered, which showed an increased number of globular mitochondria in contrast with the tubular network in healthy flies. Mutations in human LRPPRC2 have been identified in Leigh syndrome patients. It was found the activation of a mitochondrial quality control mechanism by the Bendless, PINK1 and Parkin proteins inhibits the fusion of globular mitochondria, and thus they remain segregated from each other in *lrpprc2* mutants. It was found that the suppression of the mitochondrial quality control mechanism in lrpprc2 mutants resulted in large globular mitochondria entering the mitochondrial network, however, with aggravated neurodegeneration. Overall, this study highlights the existence of protective responses which act by altering mitochondrial dynamics.
  [All collaborators in this work: Rajit Narayanan Cheramangalam, Tarana Anand, Priyanka Pandey (CCMB), Deepa Balasubramanian, Reshmi Varghese (CCMB), Neha Singhal, Sonal Nagarkar Jaiswal (CCMB), Manish Jaiswal]

- Role of SNARE Family Genes in Receptor Induced Calcium Influx and Signaling (Monika Vig)
  Key molecular mediators of the evolutionarily conserved process of store-operated calcium entry (SOCE) via calcium release activated (CRAC) channels were identified by the lab earlier. With the hypothesis that SNAP receptor (SNARE) proteins play an unconventional and direct role, a genetic screen was performed to identify the specific SNARE family genes involved in regulating SOCE. Several SNARE family genes were found to significantly regulate SOCE and one of them, syntaxin 1, was characterized further, in

collaboration with Adish Dani's lab (eLife 2013, MBoC 2016, eLife 2017, pLOSOne 2021). Syntaxin 1, a t-SNARE, along with other genes identified in a screen (conducted by the researchers), regulates a rare immunological disease called Familial Hemophagocytic Lymphohistiocytosis (FHLH) in humans. Therefore, in parallel, the mechanism of regulation of SOCE by Syntaxin 1 and its potential role in FHLH was also investigated using a knockout mouse model of Stx1. Further characterization is underway.
[All collaborators in this work: Faculty - Monika Vig (TIFRH) and Adish Dani (TIFRH), Students - Sritama Datta (co-supervisor for iPhD student), Kunal M Jagetiya (co-supervisor for iPhD student), Abhikarsh Gupta (pre-registration student), Atharva R Yande (pre-registration student)]

- Methods development in NMR and applications in materials. (P K Madhu)
  P K Madhu and colleagues focus on the development of methods in solid-state nuclear magnetic resonance with an aim to improve the resolution and sensitivity of the NMR spectra. This has implications in various applications and the group is interested in improving the efficiency and stability of perovskite materials, used in solar cells, and in battery materials. Solid-state NMR methods are also used in understanding residue-level structural information of TTR fibrils and oligomers which are implicated in various diseases.
  [All collaborators in this work: G. Rajalakshmi, Kaustubh Mote, Pabitra Nayak, T. N. Narayanan, and Sreejith Raran-Kurussi]

- A-site cation influence on the conduction band of lead bromide perovskites. (Pabitra K Nayak)
  Hot carrier solar cells hold promise for exceeding the Shockley-Queisser (single junction) limit. Slow hot carrier cooling is one of the most intriguing properties of lead halide perovskites and distinguishes this class of materials from other emerging semiconductor materials used in solar cells. In this work, element selectivity of high-resolution X-ray spectroscopy and density functional theory were used to uncover a previously hidden feature in the conduction band states, the σ-π energy splitting which is strongly influenced by the strength of electronic coupling between the A-cation and bromide-lead sublattice.
  [All collaborators in this work: G J Man (Uppsala University, Sweden) , Chinnathambi Kamal (Raja Ramanna Centre for Advanced Technology, Indore) , Aleksandr Kalinko (Deutsches Elektronen-Synchrotron DESY, Germany), Dibya Phuyal (KTH Royal Institute of Technology, Swden), Joydev Acharya (TIFR Hyderabd), Soham Mukherjee (Uppsala University, Sweden) , Pabitra K Nayak, Håkan Rensmo (Uppsala University, Sweden), Michael Odelius (Stockholm University, Sweden), Sergei M Butorin (Uppsala University, Sweden).

- Contrast inversion in atom scattering microscopy using large atomic cluster. (Pranav R Shirhatti)
  Atom scattering based microscopy is an emerging technique where low energy neutral atoms, are used as a soft probe for surfaces. The resulting contrast patterns obtained by detecting the scattered atoms from the surface of a given sample provides a way for imaging surfaces. In this work Pranav R Shirhatti and colleagues have explored the use of large atomic clusters of Krypton atoms as a probe (average cluster size ~ 10,000 atoms). Their work shows that using clusters one can get the well topographic contrast

(corresponding the macroscopic geometric features on a surface). Further, contrast beyond simple topographic in nature (resulting from the finer differences in atomic cluster – surface interaction and fragmentation) is also observed for atomically thin films. Clusters by the virtue of being much larger in mass (compared to conventional probes, such as He atoms) overcome the diffraction effects which degrade the ultimate resolution of atom scattering microscopy. These results open up an interesting possibility of high lateral resolution microscopy by the use of atomic clusters as a probe.
[All collaborators in this work: Geetika Bhardwaj, Pranav R Shirhatti]

- Complex fluid flows-stability and turbulence. (Prasad Perlekar)
  Prasad Perlekar and colleagues investigated stability, turbulence, and energy transfer mechanisms in various complex fluids. Below the researchers present the key research highlights: (1) They study turbulence modulations in the presence of external stirring in buoyancy-driven bubbly flows. They show that Kolmogorov phenomenology is recovered for scales larger than bubble diameter. While for scales smaller than the bubble diameter, the surface tension provides a dominant energy transfer mechanism.
  (2) They show that topological defects control the coarsening dynamics in the dense suspension of dry active matter, (3) They studied polymeric turbulence at extreme Deborah numbers to uncover new regimes. (4) Using experiments and numerical modeling, they investigate the role of temperature on the spreading of bacterial colonies.
  [All collaborators in this work: Prasad Perlekar, Dhrubaditya Mitra, Marco Rosti, Debjani Pal's group, IIT Bombay, Navdeep Rana, Vikash Pandey]

- Quantifying Intramolecular Ion-Pair Interactions in Biomolecules. (Raghunathan Ramakrishnan)
  Intramolecular ion-pair interactions play a crucial role in shaping the structure and functionality of numerous molecules. By overcoming steric hindrances through appropriate orientation, these interactions contribute to the compact conformation of various peptides. In this research, Raghunathan Ramakrishnan and colleagues introduce a thermodynamic cycle that relies on isoelectronic and alchemical mutation techniques to estimate the energy associated with intramolecular ion-pair interactions. They evaluate these energies for a set of 26 benchmark molecules featuring common ion-pair combinations and compare their findings with results obtained using intramolecular symmetry-adapted perturbation theory. In the case of systems incorporating long linkers, both approaches yield ion-pair energies that deviate by less than 2.5% in the absence of solvent. Their thermodynamic cycle, based on density functional theory, enables the calculation of salt-bridge interactions in model tripeptides using continuum/microsolvation modeling. Furthermore, the researchers apply this methodology to four larger peptides: 1EJG (crambin), 1BDK (bradykinin), 1L2Y (a mini-protein with a tryptophan cage), and 1SCO (a toxin from scorpion venom).
  [All collaborators in this work: Sabyasachi Chakraborty, Kalyaneswar Mandal, Raghunathan Ramakrishnan]

- Deciphering the Molecular-/Atomic-level Details of Mitochondrial Cristae Architecture. (Anand Teertha Vaidya)
  Mitochondria are usually referred to as the 'powerhouses of the cell' as they generate most of the usable energy in cells. The energy-generating machines are located in the

inner membrane folds of mitochondrial, which are called as cristae. The architecture of cristae is critical to the functioning of mitochondria and disorganized cristae are a hallmark of diseases. In the current project, the protein complexes involved in the formation and maintaining the cristae architecture have been purified and several proteins such as Mic10, Mic12 and Mic60 have been crystalized for x-ray diffraction studies. Also, a key regulator of redox-control of the cristae architecture via the protein Mic19 has been identified.

- A lipid-based synthetic “eat-me” signal for neuronal circuit remodelling. (Aneesh Tazhe Veetil)
  Aneesh T Veetil and colleagues have developed a novel synthetic photo-activatable lipid molecule to induce neuronal circuit editing by immune cells in a user-controlled manner. This new method can be used to sculpt user-instructed neuronal circuits.
  [All collaborators in this work: Dhrisya Sathyan, Aneesh T Veetil]

- Study of biomolecular condensation. (Kanchan Garai)
  Biomolecular condensation is ubiquitous and involved in multitude of functions in living cells. Typically, it involves macromolecules such as proteins, nucleic acids and lipids. However, under certain pathological conditions the condensates can transition to solid-like amyloid fibrils. However, little is understood about the molecular mechanism of the phase transitions of the bio-macromolecules. Kanchan Garai and colleagues have used various biophysical approaches, especially single molecule techniques to study phase transition of several amyloid proteins such as amyloid beta, alpha-synuclein and tau. These proteins are involved in various neurodegenerative diseases.
  [All collaborators in this work: Kanchan Garai, Saroj Nandi, Tuomas Knowles (University of Cambridge, UK), Michele Vendruscolo (University of Cambridge, UK)]

- Epitaxial Thin film grown of Mn_3Pt kagome antiferromagnet. (Karthik V Raman)
  Thin film synthesis of new quantum materials are immensely contributing to the recent developments in condensed matter physics, as they offer fundamentally distinct and technologically superior opportunities in tailoring novel device functionalities. One of the promising and under explored materials in this category is the thin-films of kagome materials. In a kagome spin-network, the coexistence of triangular and hexagonal motifs have long known to introduce geometric frustrations displaying several exotic quantum electronic and magnetic ground-states that may be broadly described as frustrated, correlated and topological. In this project, Karthik Raman and colleagues have optimized the growth recipe of epitaxial growth of Mn_3Pt films using co-sputtering technique and confirmed using in-situ RHEED, XRD and reciprocal space mapping.
  [All collaborators in this work: Satyaki Sasmal, Karthik V. Raman]

- High energy electron collimation from laser produced plasmas. (M. Krishnamurthy)
  One of the outstanding problems of intense laser produced plasma is to generate a collimated beam of electrons from the hot dense plasma. This problem was addressed in the context of microdroplet plasma generated from short pulse high repetition rate pulses that generate about 10^16 Wcm^-2 of focused laser intensity. M. Krishnamurthy and colleagues find that a simple idea of using a dielectric capillary like glass in such systems generated a very well collimated beam of electrons. Since the laser plasmas are high repetition rate, the low energy elctrons charge the capillary to suitably guide the

electrons and one can collimate electrons up to 500 keV with beam size ranging from 50 to 200 microns. The detailed mechanisms of the underlying physics is currently under investigation.
[All collaborators in this work: Sonali Khanna, Sourabh Singh, Prashant Singh, Ram Gopal, M. Krishnamurthy]

- Understanding the mechanism of helicase activation and its spatiotemporal regulation during mammalian replication. (Mrinal Srivastava)
  In order to transmit and preserve genetic information, cells must duplicate DNA with very high fidelity. Large metazoan genome duplication is accomplished by assigning thousands of potential origins of replication, a fraction of which are utilized. The remaining sites remain flexibly dormant unless required, as in the case of replication stress. Besides, the start of replication from the utilized origin is also spatiotemporally regulated in S-phase. Arguably, one of the key events during replication initiation is regulated conformational changes in the MCM helicase complex. The MCM complex is loaded onto the DNA in the G1 phase of the cell cycle, in an inactive form. At the selected origins, the MCM complex transitions into an active translocating helicase in the S-phase. However, (a) how this transition is achieved and (b) is regulated in a spatiotemporal fashion is not known. Here, we comprehensively address the dynamics of helicase activation by generating individual cellular model systems with mitigated regulation of replication by introducing strategic mutations or oncogene-induction. Mrinal Srivastava and colleagues will perform biochemical, and cellular characterizations along with comparative proteomics and genomics while evaluating the spatiotemporal progression of replication in order to decipher molecular regulators for genome duplication time and pattern.

- Study of the Conformational Dynamics of Proteins in Solution. (Pramodh Vallurupalli)
  Proteins are not rigid but populate a range of conformational states in solution. Conformational exchange often occurs between a dominant (low energy) ‘major’ state and different sparsely populated ‘minor’ states that are ‘invisible’ to traditional structural tools. Consequently, very little is known about these alternate conformers even though they have implications for health and disease as they are involved in several process like catalysis, aggregation, folding, ligand binding etc. The free energy surface (FES) of model proteins (T4 Lysozyme and the FF domain) is being mapped out at atomic resolution using novel CEST NMR techniques. The thermodynamic (H, S) of the different states and the transition states are also being determined. An important component of the work is the development of new NMR methods particularly to study multistate exchange over a range of timescales (0.1 to 100 ms) and populations (as low as ~0.1%). This will result in an unprecedented atomic resolution picture of the FES of the model proteins, with atomic structures of multiple sparsely populated states.
  [All collaborators in this work: Flemming Hansen (UCL), Ashok Sekhar (IISc Bangalore), Lewis Kay (Toronto)]

- Development of electron and X-ray radiography capabilities with high-repetition rate laser plasma interactions. (Prashant Kumar Singh)
  The robustness of intense laser-driven MeV X-ray for imaging purposes, should be carried out with ‘Industrial’ grade lasers, as they offer an alignment-free system with little to no facility requirements in terms of high-class clean room, temperature and humidity

controlled environment. Experimental works carried out by Prashant K Singh and colleagues have proven the possibility of scaling the laser-plasma interaction mechanism from a scientific grade Ti: Sapphire laser system to an Industrial grade laser showing that it is possible to scale the underlying mechanism. This transition requires confirmation of testing the electron beam generation performance against two parameters: a) Wavelength scaling from 800nm to 1030nm, b) Laser bandwidth going down from 60nm to 10 nm, and Pulse duration increased from 30 fs to 200 fs. The development of bright x-ray source in the MeV energy range would scale up the existing conventional 450 keV NDT testing machine capability to the next level. Although Linac electron accelerator based MeV xray machine are available, this proposal, based on compact laser-driven electron acceleration can offer order of magnitude better spatial resolution (< 100 µm). Furthermore, due to short pulse duration (subpicoseconds), the laser-based x-rays sources would also provide platforms to carry out dynamic or flash X-ray radiographic imaging.
[All collaborators in this work: M. Krishnamurthy, G. Ravindra Kumar, Chaitanya Suddapalli, Ram Gopal]

- Laser matter interaction with orbital angular momentum laser beams. (Ram Gopal)
  Light-matter interaction with laser pulses endowed with orbital angular momentum (OAM) raises a fundamental question on the nature of the transfer of this property of light to matter. When moderately intense (1013-1014 W/cm2), OAM carrying laser pulses interact with a cold jet of Argon atoms, no evidence of angular momentum transfer to the electrons from light is observed. These investigations were carried out through angle and energy-resolved photoelectron spectra obtained in a high-resolution momentum spectrometer, "Reaction Microscope".
  [All collaborators in this work: Arnab Sen (IISER Pune), Abhishek Sinha (IIT H), Sanket Sen (IIT H), Vandana Sharma (IIT-H), Ram Gopal]

- Molecular diffusion in porous metal-organic framework thin films. (Ritesh Haldar)
  Chemical separation can be performed using membrane based technology, which is much more energy efficient compared to the state of the art methods. Metal-organic frameworks are promising molecular sieving materials, which can be used for membrane technology. Recently, Ritesh Haldar and colleagues have evaluated the molecular diffusion mechanism in this porous material. To study those experimentally, they have developed novel MOF thin films, and examined the mass uptake rate under chemical concentration gradient. They report that orientation of the nanochannels along the transport direction is an important parameter, and molecules can diffuse orthogonal to the concentration gradient in heterogeneous pore system.
  [All collaborators in this work: Pratibha Malik, Tanmoy Maity, Sumit Bawari, Soumya Ghosh, Jagannath Mondal, Ritesh Haldar]

- On the origin of universal cell shape variability in confluent epithelial monolayers. (Saroj Kumar Nandi)
  Cell shape is fundamental, both in health and disease. Average cell shape affects crucial biological functions such as division, differentiation, cell death, etc. However, cell to cell shape varies and recent experiments show a remarkably regularity in this cell shape variability. In this work, Saroj Kumar Nandi and colleagues provide a theoretical understanding of the nearly universal distribution of cell shape, characterized via the

aspect ratio, in an epithelial monolayer. They analytically obtain the distribution of aspect ratio in a monolayer and show that the analytical results agree remarkably well with simulations and existing experiments.

- Photochargeable cathodes in Li-ion batteries. (Soumya Ghosh and T N Narayanan)
  In recent years, photochargeable batteries have generated a lot of attention. Soumya Ghosh, T N Narayanan and colleagues investigated one such system, MoS_2/MoO_3, that has been previously shown to function as a photocathode in Li-ion batteries. During the discharge of the battery, Li-ions intercalate MoS_2 layers that should render the system metallic and hence, incapable of photoexcitation. The computational studies by this group show that, in the presence of MoO_3, electron density is extracted from MoS_2, making the system amenable to solar light excitation. This feature is found to disappear for higher concentration of Li-ions, in contrast to an analogous system where the Li-ion induced changes are minimal.
  [All collaborators in this work: Raheel Hammad, Amar Kumar, T. N. Narayanan, Soumya Ghosh]

- Annealing effects of multidirectional oscillatory shear in model glass formers. (Smarajit Karmakar)
  Smarajit Karmakar and colleagues studied effect of cyclic shear on the mechanical properties of amorphous solids at zero temperature and very small strain rate. It was known that unidirectional cyclic shear in these conditions leads to absorbing steady states which are suitable for storing memories in these materials. In this work, the researchers extended some of these ideas and found that if the material is sheared cyclically in all the three shear planes available to a 3d solid, then one attains an interesting steady state which remembers the number of shear directions. For example, if they shear the sample in two orthogonal shear planes, then the steady state absorbing state will have a limit cycle of two, and similar for 3 shear planes there will be a limit cycle with periodicity 3. The researchers then subsequently showed that multi-directional oscillatory shear can lead to much better annealing of the material. They also show that the memory stored using multi-directional shear will be much more robust and stable during reading operations.
  [All collaborators in this work: V.V. Krishnan, Kabir Ramola and Smarajit Karmakar]

- Intracellular reorganization during collective cell migration. (Tamal Das)
  Collectively migrating epithelial cells exhibit complex intracellular dynamics involving the reorganization of cellular organelles such as the Golgi apparatus, lysosomes, and endoplasmic reticulum. This reorganization plays a crucial role in directing cell movement. However, the changes in organelle shape and localization during collective cell migration remain poorly understood. To this end, the cellular organelles in stationary and migrating epithelial cells were mapped by Tamal Das's group to uncover their specific contributions to migration. A fascinating process was discovered in which the Golgi apparatus was found to be actively dispersed around the cell nucleus at the onset of migration. Furthermore, investigations were conducted on how leader cell formation was contributed to by force-responsive alterations in lysosome positioning. Lastly, changes in the structure of the Endoplasmic Reticulum in response to wound curvature were uncovered. These findings deepened the understanding of the intricate interplay between cellular forces and intracellular structures during collective cell migration.

[All collaborators in this work: Purnati Khuntia, Rituraj Marwaha, Simran Rawal, and Tamal Das]

- Specific labeling of proteins for NMR studies. (Sreejith Raran-Kurussi)
  Last year's work highlight was the use of different labeling strategies for preparing specifically labeled proteins. Specific amino acid labeling of α-synuclein was performed for NMR and DNP studies. Apart from the routine laboratory administration and mentoring of students, Sreejith Raran-Kurussi is independently involved in technology development to promote better expression and purification of recombinant proteins. Sreejith's fusion protein technology and other molecular biology tools, like proteases for tag removal, are used by numerous research groups at TIFRH and elsewhere.
  [All collaborators in this work: Ahlawat S, Mopidevi SMV, Mote KR, Agarwal V, Sreejith Raran-Kurussi]

- Enhanced room-temperature spin-valley coupling in V-doped MoS_2
  Achieving room-temperature valley polarization in two-dimensional (2D) atomic layers (2D materials) by substitutional doping opens new avenues of applications. Such layers with valley splitting can find applications in valleytronics, which is considered as the next possibilities for information storage. In a recent work, monolayer MoS_2 when doped with vanadium at low (0.1 atomic %) concentrations, is shown to exhibit high spin-valley coupling, and hence a high degree of valley polarization at room-temperature. Moreover, the researchers have shown that dopant can also introduce valley splitting resulting to a time reversal symmetry breaking and hence a material which can be used for valleytronics at room temperature.This study opens possibilities of room-temperature opto-spintronics using stable 2D materials.
  [All collaborators in this work: Krishna Rani Sahoo, Janmey Jay Panda, Sumit Bawari, Rahul Sharma, Dipak Maity, Ashique Lal, Raul Arenal (Universidad de Zaragoza, Spain), G. Rajalaksmi, and T. N. Narayanan]

- Assignment of aromatic side-chain resonances and characterization of their distance restraints at fast MAS (Vipin Agarwal)
  The assignment of aromatic side-chain spins has always been more challenging than assigning backbone and aliphatic spins. Selective labeling combined with mutagenesis has been the approach for assigning aromatic spins. This study reports a method for assigning aromatic spins in a fully protonated protein by connecting them to the backbone atoms using a low-power TOBSY sequence. The pulse sequence employs residual polarization and sequential acquisitions techniques to record H^N- and H^C-detected spectra in a single experiment. The unambiguous assignment of aromatic spins also enables the characterization of ^1H-^1H distance restraints involving aromatic spins. Broadband (RFDR) and selective (BASS-SD) recoupling sequences were used to generate H^N-H^C, H^C-H^N and H^C-H^C restraints involving the side-chain proton spins of aromatic residues. This approach has been demonstrated on a fully protonated U-[^{13}C,^{15}N] labeled GB1 sample at 95-100 kHz MAS.
  [All collaborators in this work: Sahil Ahlawat, Subbarao Mohana Venkata Mopidevi, Pravin P. Taware, Sreejith Raran-Kurussi, Kaustubh R. Mote and Vipin Agarwal]

- Molecular Materials and Main-group Catalysts (V Chandrasekhar)
  Molecular materials, such as Molecular Magnets, were assembled by using homometallic and heterometallic architectures involving lanthanide or transition metal ions. It has been also possible to prepare compounds containing a single metal ion, viz., single-ion magnets. In another variation of the molecular materials mixed-valence compounds containing Co(II)-Co(III) were shown to be effective reagents for water oxidation reactions. In main-group chemistry use of an unsymmetrical N-P-N ligand for preparing interesting complexes such as with the Y(III) derivative was accomplished. This complex was found to be an excellent catalyst for the hydroboration of ketones and aldehydes at room temperature. Similarly aluminum complexes were prepared which could used for catalytic guanylation of carbodimides.
  [All collaborators in this work: Acharya, J (IIT Kanpur).; Swain, A (IIT Bombay).; Chakraborty, A.; Kumar, V (IIT Kanpur).; Kumar, P (IIT Kanpur).; Gonzalez, J. F (Univ Rennes).; Cador, O (Univ Rennes).; Pointillart, F(Univ Rennes).; Rajaraman, G (IIT Bombay); Krishnan, V (NISER Bhubaneswar).; Chandrasekhar, V.]

Other information:

- Apart from the regular LC MS spectra recordings and other biophysical instruments assistance (for different research groups), Deepa S has contributed to Kanchan Garai lab's research works by purifying different proteins, labelling and assisting in optics lab.
- Kalyan Kumar N and Suman Saurav have been managing the existing (High Performance Computing) HPC data center facility which includes maintenance of Data Center cooling infrastructure, server racks, hardware, software stack, user application management and system administration. They have also been overseeing the management of existing Information Technology Infrastructure (IT-IS) facility which includes maintenance of existing wired and wireless networking switches, IP Telephony, Video conferencing, AV management of Auditorium, classrooms and conference meeting rooms, CCTV surveillance, web management, virtualization server and storage management, etc.,
- Krishnarao Doddapuneni is actively working towards the upkeep of NMR facility. He has been involved in the addition of new 600 MHz NMR spectrometer to the National high-field NMR facility at TIFR Hyderabad.
- Gopalakrishna R has been overseeing animal house facility management according to required standards, implementing disease prevention and control protocols.

New faculty members

- Darshan G Joshi (Date of joining: Feb 03, 2023)
  Research Areas: Theoretical condensed matter physics: Strongly-correlated systems, frustrated magnetism, topological phases, and disordered systems

- Harish Krishnamoorthy (Date of joining: Feb 23, 2022)
  Research Areas: Metaphotonics, Topological and Phase Change Photonics, Hyperbolic metamaterials and metasurfaces, Light-matter interaction, Photonic and Quantum materials

- Vishal Ranjan (Date of joining: Mar 01, 2023)
  Research Areas: Superconducting Circuits, Microwave Quantum Memory, High-sensitivity Electron Spin Resonance

B. Staff Strength:

Faculty :	34 + 3 (Emeritus -1, Visiting Faculty-2)
Research Scholars :	156
Junior Research Fellows :	35
Senior Research Fellows :	19
Post-doctoral Fellows :	52
Research Associates :	04
Project Associates :	05 (External Project_EPIC)
EPIC Consultants :	04 (External Project_EPIC)
Visiting Students :	09 (05 out of 09 are EPIC Project)
Scientific Staff :	24 (07 EPIC Project & 01 outsourced out of 24)
Technical Staff :	14 (03 out of 14 outsourced)
Admin Staff :	25 (01 EPIC Project & 03 outsourced out of 25)
Part Time Legal Consultant :	01
Part Time Medical Officer :	01
Auxiliary Staff :	90 (90 outsourced out of 90 (Security-23 , HK-16 ,Work Assistant-03, Lab Assistant-01, Canteen-15, HVAC-07, Gardener-03, Electrical & Fire safety-09, Plumbing Staff: 05, STP operator-01, Carpenter-01, Driver-06)

C. Awards and Distinctions:

No.	Name of the Awardee	Scope (National/ International)	Name of the Award	Awarding / Electing Body	Date
1.	Pranav R. Shirhatti	National	S. N. Seshadri Memorial Instrumentation Award in Physical Sciences 2022	Indian Physics Association	
2.	Aneesh T Veetil	National	Intermediate Fellow, DBT-Wellcome Trust	DBT-Wellcome Trust	2023 January
3.	Karthik V. Raman	National	S. N. Seshadri Memorial Instrumentation Award	IPA	2022
4.	Karthik V. Raman	International	2022 ACMM Rising Star award	ACMM	2022
5.	Ritesh Haldar	National	Starting research grant	SERB, Govt of India	September 2022
6.	Ritesh Haldar	National	Infosys-TIFR leading edge research grant	Infosys-TIFR	May 2022

7.	Tamal Das	National	Young Scientist Medal	Indian National Science Academy	January 2023
8.	Shilpa Phani Pothapragada	International	Schmidt Science Fellowship	Schmidt Futures Foundation	March 2023
9.	T N Narayanan	International	Alexander von Humboldt Experienced Researcher Fellowship	AvH Foundation	November 2022
10.	T N Narayanan	National	MRSI Medal – 2022, Materials Research Society of India.	Materials Research Society of India	December 2022
11.	T N Narayanan	National	DST-SIRE Fellowship 2022-2023	Department of Science and Technology	May 2022
12.	Vipin Agarwal	International	Executive Member of the NMR/MRI advisory committee to the National High-Field Magnetic Lab	National High-Field Magnetic Lab, University of Florida, USA	January 2023
13.	Vipin Agarwal	International	Time-sensitive award: "New Voices in Magnetic Resonance"	International Society of Magnetic Resonance	June 2022
14.	Vipin Agarwal	National	S. Subramanian's 60^{th} Birthday Lecture Award	National Magnetic Resonance Society of India	February 2023
15.	Sahil Ahlawat	National	Annual NMRS Medal for Young Scientist	National Magnetic Resonance Society of India	February, 2023
16.	Vipin Agarwal	National	Executive council member	National Magnetic Resonance Society of India	2020-2023

D. Publications:

1. Jana, S., Elvers, B. J., Pätsch, S., Sarkar, P., Krummenacher, I., Nayak, M. K., ... & Jana, A. (2023). Air and Moisture Stable para-and ortho-Quinodimethane Derivatives Derived from bis-N-Heterocyclic Olefins. *Organic Letters (highlighted in ChemistryViews: The Magazine of Chemistry Europe).*
2. Nayak, M. K., Sarkar, P., Elvers, B. J., Mehta, S., Zhang, F., Chrysochos, N., ... & Jana, A. (2022). A bis-NHC–CAAC dimer derived dicationic diradical. *Chemical Science*, *13*(42), 12533-12539. *(highlighted in ChemistryViews: The Magazine of Chemistry Europe).*
3. Dolai, R., Kumar, R., Elvers, B. J., Pal, P. K., Joseph, B., Sikari, R., ... & Jana, A. (2023). Carbodicarbenes and striking redox transitions of their conjugate acids: influence of NHC versus CAAC as donor substituents. *Chemistry–A European Journal*, *29*(2), e202202888.
4. Gimferrer, M., Danés, S., Vos, E., Yildiz, C. B., Corral, I., Jana, A., ... & Andrada, D. M. (2023). Reply to the 'Comment on "The oxidation state in low-valent beryllium and magnesium compounds"'by S. Pan and G. Frenking, Chem. Sci., 2022, 13. *Chemical Science*, *14*(2), 384-392.
   For the comment on these artile please see: Chem. Sci. 2023, 14, 379–383 and for our reply please see: Chem. Sci. 2023, 14, 384–392.
5. Das, A., Elvers, B. J., Nayak, M. K., Chrysochos, N., Anga, S., Kumar, A., ... & Jana, A. (2022). Realizing 1, 1-Dehydration of Secondary Alcohols to Carbenes: Pyrrolidin-2-ols as a Source of Cyclic (Alkyl)(Amino) Carbenes. *Angewandte Chemie International Edition*, *61*(28), e202202637.
6. Maiti, A., Elvers, B. J., Bera, S., Lindl, F., Krummenacher, I., Ghosh, P., ... & Jana, A. (2022). Disclosing Cyclic (Alkyl)(Amino) Carbenes as One-Electron Reductants: Synthesis of Acyclic (Amino)(Aryl) Carbene-Based Kekulé Diradicaloids. *Chemistry–A European Journal*, *28*(28), e202104567.
7. Pasnuri, N., Jaiswal, M., Ray, K., & Mazumder, A. (2023). Buffered EGFR signaling regulated by spitz-to-argos expression ratio is a critical factor for patterning the Drosophila eye. *PLoS Genetics*, *19*(2), e1010622.
8. Nandy, B., Kumar, S. C., & Ebrahim-Zadeh, M. (2022). Yb-fiber-pumped high-average-power picosecond optical parametric oscillator tunable across 1.3− 1.5 µm. *Optics Express*, *30*(10), 16340-16350.
9. Kumar, V., Sharma, V., Singh, S., Kumar, S. C., Forbes, A., Ebrahim-Zadeh, M., & Samanta, G. K. (2022). Imaging inspired characterization of single photons carrying orbital angular momentum. *AVS Quantum Science*, *4*(1), 015001.
10. Varun Sharma, S. Chaitanya Kumar, G. K. Samanta, M. Ebrahim-Zadeh, "Tunable, highpower, high-order optical vortex beam generation in the mid-infrared," Opt. Express 30, 1195 (2022)
11. Sanchez, A. D., Kumar, S. C., & Ebrahim-Zadeh, M. (2022). Ultrashort Pulse Generation From Continuous-Wave Driven Degenerate Optical Parametric Oscillators. *IEEE Journal of Selected Topics in Quantum Electronics*, *29*(1: Nonlinear Integrated Photonics), 1-8.
12. Kurian, K. G., Sahoo, S. S., Madhu, P. K., & Rajalakshmi, G. (2023). Single-beam room-temperature atomic magnetometer with large bandwidth and dynamic range. *Physical Review Applied*, *19*(5), 054040.
13. Panda, J. J., Sahoo, K. R., Praturi, A., Lal, A., Viswanathan, N. K., Narayanan, T. N., & Rajalakshmi, G. (2022). High-sensitivity characterization of ultra-thin atomic layers using spin-Hall effect of light. *Journal of Applied Physics*, *132*(7), 075302.
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17. Mondal, A., Save, S. N., Sarkar, S., Mondal, D., Mondal, J., Sharma, S., & Talukdar, P. (2023). A Benzohydrazide-Based Artificial Ion Channel that Modulates Chloride Ion Concentration in Cancer Cells and Induces Apoptosis by Disruption of Autophagy. *Journal of the American Chemical Society*, *145*(17), 9737-9745.
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19. Jamuna, N. A., Kamalakshan, A., Dandekar, B. R., Chittilappilly Devassy, A. M., Mondal, J., & Mandal, S. (2023). Mechanistic Insight into the Amyloid Fibrillation Inhibition of Hen Egg White Lysozyme by Three Different Bile Acids. *The Journal of Physical Chemistry B*, *127*(10), 2198-2213.
20. Bawari, S., Narayanan, T. N., & Mondal, J. (2023). Insights into the reaction pathways of platinum dissolution and oxidation during electrochemical processes. *Electrochemistry Communications*, *147*, 107440.
21. Wasim, A., Gupta, A., Bera, P., & Mondal, J. (2023). Interpretation of organizational role of proteins on E. coli nucleoid via Hi-C integrated model. *Biophysical Journal*, *122*(1), 63-81.
22. Bawari, S., Guha, A., Narayanan, T. N., & Mondal, J. (2022). Understanding water structure and hydrogen association on platinum–electrolyte interface. *Oxford Open Materials Science*, *2*(1), itac014.
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25. Krishnan, V. V., Ramola, K., & Karmakar, S. (2023). Annealing effects of multidirectional oscillatory shear in model glass formers. *Physical Review Applied*, *19*(2), 024004.
26. Nampoothiri, J. N., D'Eon, M., Ramola, K., Chakraborty, B., & Bhattacharjee, S. (2022). Tensor electromagnetism and emergent elasticity in jammed solids. *Physical Review E*, *106*(6), 065004.
27. Maharana, R., Nampoothiri, J. N., & Ramola, K. (2022). First-contact-breaking distributions in strained disordered crystals. *Physical Review E*, *106*(6), 064901.
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44. Taware, P. P., Jain, M. G., Raran-Kurussi, S., Agarwal, V., Madhu, P. K., & Mote, K. R. (2023). Measuring Dipolar Order Parameters in Nondeuterated Proteins Using Solid-State NMR at the Magic-Angle-Spinning Frequency of 100 kHz. *The Journal of Physical Chemistry Letters*, *14*(15), 3627-3635.

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95. Book chapter: P. Malik, T. Maity, and R. Haldar,* Structural Characterization of Porous Organic Materials (RSC Book chapter) 2023.
96. Book chapter: Hang, H. C., Pratt, M. R., & Prescher, J. A. (Eds.). (2023). *Advanced Chemical Biology: Chemical Dissection and Reprogramming of Biological Systems*. John Wiley & Sons.
97. Conference Proceedings: A lipid-based synthetic “eat-me” signal for neuronal circuit remodeling. Dhrisya Sathyan and Aneesh T Veetil
98. Conference Proceedings: Sukeert, S. Pizzurro, A. Esteban-Martin, R. Gotti, L. Carra, G. Piccionno, A. Agnesi, F. Pirzio, S. Chaitanya Kumar, M. Ebrahim-Zadeh, “Efficient femtosecond optical parametric generation in group-velocity-matched MgO:PPLN at 10 MHz,” Advanced Solid-State Lasers Conference, Barcelona, Spain, Paper: ATh3A.5, December 2022

E. Conferences organised:

- Chaitanya Kumar Suddapalli, Served on the Nonlinear Frequency Generation and Conversion: Materials and Devices committee, SPIE Photonics West-2022, San Francisco, USA, January 2022.

- Jagannath Mondal, Organiser, 'Molecular Simulation: Focus on Method', TIFR Hyderabad, December 2022
- Kaustubh R Mote, Co-organizer: NMR Meets Biology, Hospet/Hampi, Karnataka, India, 5-11 December 2022 (www.tifrh.res.in/!nmr/nmr-meets-biology)
- Pranav R Shirhatti, Spectroscopy and Dynamics of Molecules and Clusters - 2022, Malpe, Karnataka, November 2022
- Saroj Kumar Nandi, jointly organized a conference: Frontiers in Active and Soft Matter 2023, February 2023
- Smarajit Karmakar, Compflu-2022, IIT Kharagpur, Session Organized 'Soft Condensed Matter', Kolkata, December 2022
- T N Narayanan, Organizer, International Conference on Advances in Renewable Energy (CARE-2023), jointly Organised by HRI, Prayagraj, India and TIFR-Hyderabad, India, at HRI Campus, February 2023.
- T N Narayanan, Convener, International Workshop on Nano-Engineered Materials which also includes an exclusive workshop on advanced materials for post graduate students, Jointly Organised with IISER Thiruvananthapuram, TIFR-Hyderabad, and IIT Kharagpur, January 2023
- Vipin Agarwal, Organizer, 3rd India-Japan Bilateral meeting on Magnetic Resonance, University of Hokkaido, Hokkaido, Japan February 2023

F. Invited lectures given:

- Adish Dani, Seminar at International Conference on Advanced Biomedical Imaging, IIT-Madras, Chennai, India, January 2023.
- Adish Dani, Title: 'Single molecule imaging of cochlear ribbon synapse protein architecture', No Garland Neuroscience conference, IISER Pune, India, March 2023.
- Chaitanya Kumar Suddapalli, Title: 'Mid-infrared optical parametric oscillators: challenges and advantages, SCOP, Physical Research Laboratory, Ahmedabad, India, September 2022
- Kabir Ramola, IMSc Diamond Jubilee Colloquium, IMSc Chennai, India, May 2022
- Kabir Ramola, Statistical Physics and Complex Systems, IIT Kharagpur, India, July 2022
- Kabir Ramola, Soft and Active Matter Seminar, IIT Hyderabad, India, November 2022
- Kabir Ramola, Statistical Physics of Complex Systems, ICTS, Bengaluru, India, December 2022
- Kabir Ramola, National Conference on Frontiers in Physics, University of Hyderabad, India, March 2023
- Kabir Ramola, Steady state phenomena in soft matter, active and biological systems, SNCBS, Kolkata, India, March 2023
- Kabir Ramola, Aditi Simha Memorial Symposium, IIT Chennai, India, March 2023
- Kalyaneswar Mandal, 'Reciprocally chiral recognition to block malaria parasite entry into red blood cells', Institute Colloquium, Indian Institute of Chemical Technology Hyderabad, India, March 2023.
- Kalyaneswar Mandal, 'Chemical protein synthesis', ARUMDA Symposium, TIFR Hyderabad, India, March 2023.
- Kalyaneswar Mandal, 'Chemically synthesised proteins to stop malaria parasite entry into red blood cells', Frontiers in Chemical Sciences - 2022, Department of Chemistry, IIT Guwahati, India, December 2022
- Kalyaneswar Mandal, 'Reciprocally chiral recognition to stop malaria parasite entry into red blood cells', TIFRH In-house Symposium, TIFR Hyderabad, India, September 2022.

- Kalyaneswar Mandal, ‘Mirror-image proteins to block red blood cell invasion by malaria parasites’, Visva-Bharati Chemistry Alumni Lecture Series, Department of Chemistry, Siksha Bhavana, Visva Bharati, Santiniketan, India, June 2022
- Kalyaneswar Mandal, ‘Mirror-image protein as a potential antimalarial therapeutic’, Future Oriented Research Conferences and Exhibitions (FORCE) – Interdisciplinary Initiative in Chemical Sciences (IICS), Agra, India, July 2022
- Kaustubh R Mote, ‘REDOR at 100 kHz MAS’, India-Japan NMR Meeting, Hokkaido University, Hokkaido, Japan, February 2023
- Kaustubh R Mote, ‘Organic chemistry and NMR: An inseparable pair’, National Initiative for Undergraduate Sciences, Chemistry XVIII, via Zoom, December 2022
- Kaustubh R Mote, ‘Accessing dipolar order parameters in non-deuterated proteins at the MAS frequency of 100 kHz’, NMR Meets Biology, Hospet/Hampi, Karnataka, India December 2022
- Kaustubh R Mote, ‘Protein dynamics at 100 kHz MAS’ (TIFR Hyderabad in-house symposium, Hyderabad, India, September 2022.
- Manish Jaiswal, ‘Tales of the fly and the human: Understanding biology and diseases’, Departmental seminar series, Dr. D. Y. Patil Biotechnology & Bioinformatics Institute, Tathawade, Pune, April 2022.
- Manish Jaiswal, ‘Genetic screens: targeting mitochondrial shape, size, and numbers’ Invited speaker for the month of May 22, University of Hyderabad, Biochemistry-Research Talk, May 2022
- Manish Jaiswal, ‘Genetic Screening: Mitochondrial Shape, size and number’ India Investigator Network Webinar series, May 2022
- Manish Jaiswal, ‘Genetic screens: targeting mitochondrial shape, size and numbers’, Invited talk, University of Kashmir, September 2022
- Manish Jaiswal, ‘Adaptive/maladaptive metabolic signaling in responses to mitochondrial stress in development and disease’, In house Symposium, TIFRH, September 2022
- Manish Jaiswal, ‘Bendless is required for PINK1 activity to regulate mitochondrial quality control in a Leigh Syndrome model’ Departmental talk, Kasturba Medical College, MAHE, Manipal, September 2022
- Manish Jaiswal, ‘My journey as a PI: Challenges and achievements. Grant Cell Workshop’, Kasturba Medical College, MAHE, Manipal, September 2022
- Manish Jaiswal, Keynote lecture: ‘Novel insight into retinal degeneration caused by mitochondrial dysfunction using Drosophila’, Annual meeting of Association for Research in Vision and Ophthalmology (ARVO) India, Indian Eye Research Group, (IERG), September 2022.
- Manish Jaiswal, Mitochondria are not kidney shaped organelles. Outreach event 'Advances in Life Science Research', October 2022.
- Manish Jaiswal, ‘Identification of novel regulators of mitochondrial fusion through genetic screens in Drosophila’, UCL IHA Virtual Symposium: Neurodegeneration in Flies. November 2022
- Rajit Naraynan, Tarana Anand, Priyanka Pandey, Sonal N Jaiswal, Manish Jaiswal, ‘Elucidation of the regulatory mechanism of mitochondrial dynamics under stress’, Ramalingaswami Fellowship & MK Bhan-Young Researcher Fellowship Joint Conclave 2022-23. Dr. MR Das Convention Centre, Rajiv Gandhi Centre for Biotechnology, Thiruvanthanapuram, 30th November – 3rd December, 2022.
- Manish Jaiswal, ‘Regulation of mitochondrial shape, size and number’, Departmental talk, Biological sciences, Rani Durgavati Vishwavidyalaya, Jabalpur, Madhya Pradesh, December, 2022.
- Manish Jaiswal, ‘Genetic screens: targeting mitochondrial shape size and numbers. inStem scientific seminar series’, InStem Bangalore, January 2023

- Manish Jaiswal, ‘Genetic screens: targeting mitochondrial shape size and number’, SYNAPSIS is an effort by the Dept of Biological Sciences, Birla Institute of Technology and Science-Pilani (BITS-Pilani), Hyderabad, January 2023
- Manish Jaiswal, ‘Adaptive/maladaptive responses to mitochondrial stress in development and disease’ The Mito-Metab meeting series, IISER-Pune, February 2023
- Manish Jaiswal, ‘E2 ubiquitin ligase Bendless is required for PINK1 stability’, Autophagy India Network (AIN) meeting, CSIR-Institute of Microbial Technology (IMTECH), Chandigarh, February 2023
- P K Madhu, ‘Basics of solid-state NMR’, NMR Meets Biology, Hampi, Karnataka, India, December 2022
- P K Madhu, ‘NMR methods for biomolecular applications’, STUTI, BITS Pilani, October 2022
- P K Madhu, ‘Recoupling and faster acquisition schemes in solid-state NMR’, Rocky mountain conference on magnetic resonance, Denver, USA, July 2022
- P K Madhu, ‘Site-specific probes for biomolecules: Recoupling and faster acquisition’, ENS Paris, France, March 2022
- Pranav R Shirhatti, Lorentz Center workshop, Energy Dissipation at Interfaces: From Catalysis to Astrochemistry 2022, May 2022
- Pranav R Shirhatti, Fifth International Workshop on Scattering of Atoms and Molecules from Surfaces, Cambridge, UK, September 2022
- Pranav R Shirhatti, National conference on atomic and molecular physics 2023, IIST Trivandrum, February 2023
- Anand T Vaidya, ‘Towards the Atomic Details of Mitochondrial Cristae Architecture’, Mitochondria and Metabolism Meeting, IISER Pune, February 2023
- Anand T Vaidya, ‘Deciphering the Molecular Details of Mitochondrial Cristae Architecture’, Inhouse Symposium, Tata Institute of Fundamental Research (TIFR), Hyderabad, September 2022
- Anand T Vaidya, ‘Unravelling the Molecular Basis of Mitochondrial Cristae Organization: Synthesis and Purification of Mic10 and it’s Binding Partners’, Science and Engineering Research Board (SERB) Meeting, Indian Institute of Technology, Indore, July 2022
- Aneesh T Veetil, One Day Symposium on Interdisciplinary Approaches Addressing Augmentation of Livestock Reproduction, NIAB, Hyderabad, September 2022
- Kanchan Garai, ‘Investigation of protein aggregation using single molecule fluorescence techniques’, Workshop - Liquid, soft, alive: Identifying the biological questions in the physics of cells, Centre Européen de Calcul Atomique et Moléculaire, Ecole Polytechnique Fédérale de Lausanne (EPFL), Lausanne, February 2023
- Kanchan Garai, ‘Single molecule investigation of amyloid aggregation of proteins’, IICB, Kolkata, June 2022
- Mrinal Srivastava, ‘Mechanisms of maintaining replication integrity’, Centre for BioSystems Science and Engineering (BSSE) Seminar series, Indian Institute of Science, Bangalore, India, January 2022
- Mrinal Srivastava, ‘Molecular programming of replication fork to ensure genome fidelity’, GATI-webinar, CSIR- Indian Institute of Chemical Technology, Hyderabad, India, April 2022
- Mrinal Srivastava, ‘Molecular programming of replication dynamics, timing, and patterns’, Soft Matter Young Investigators Meet, Jal Mahal Resorts, Mysore, India, June 2022
- Mrinal Srivastava, ‘Molecular programming of replication dynamics, timing, and patterns’, In-house Symposium, Tata Institute of Fundamental Research Hyderabad, Hyderabad, India, September 2022

- Mrinal Srivastava, ‘When and where of mammalian replication’, SERB Scientific Social Responsibility- Advances in Life Science Research Seminar, School of Life Sciences, University of Hyderabad, Hyderabad, India, October 2022
- Mrinal Srivastava, ‘Molecular programming of replication dynamics, timing, and patterns’, Statistical Biological Physics: from Single Molecule to Cell, TIFR-International Centre for Theoretical Sciences, Bangalore, India, October 2022
- Mrinal Srivastava, ‘DNA damage response sub-library genetic screen to identify cross-talk between repair pathways’, New England Biolabs Seminar Series, November 2022.
- Pramodh Vallurupalli, ‘Exploring the free energy surface of proteins using CEST NMR experiments’, MBU@50, IISc Bangalore, January 2023.
- Pramodh Vallurupalli, ‘Exploring the free energy surface of proteins using CEST NMR experiments’, 3rd Indo-Japan NMR Meeting, Sapporo, Japan, February 2023
- Prashant Kumar Singh, 48th European Conference on Plasma Physics (EPS-2022), June 27 to July 1, 2022
- Prashant Kumar Singh, ‘Particle acceleration and fusion neutrons with few-cycle relativistic intense laser pulses’, AAPPS-DPP 2022 Annual Conference, October 2022
- Saroj Kumar Nandi, ‘On the origin of universal cell shape variability in confluent epithelial monolayers’, SMYIM, June 2022.
- Saroj Kumar Nandi, ‘Are glasses Fickian yet non-Gaussian? Various time-scales of glasses’, Compflu 2022, IIT Kharagpur, December 2022
- Saroj Kumar Nandi, ‘Non-trivial effects of activity on the glassy dynamics of self-propelled particules’, Indian statistical physics community meeting, ICTS Bangalore, February 2023
- Saroj Kumar Nandi, Invited visit, IIT Bombay, ‘On the origin of universal cell shape variability in confluent epithelial monolayers’, IIT Bombay, February 2023
- Saroj Kumar Nandi, ‘Glassy dynamics in living systems’, Summer school on soft condensed matter, BHU, March 2023
- Smarajit Karmakar, Frontiers in Non-equilibrium Physics, IMSc Chennai, January 2023
- Smarajit Karmakar, Lorentz Center, Leiden, The Netherlands, July 2022.’
- Tamal Das, ‘Mechanobiology of Collective Cell Dynamics: An Interdisciplinary Inquiry’, CeNSE DBT Nano-Biotechnology Alliance (CDNA) Conference, Centre for Nano Science and Engineering, IISc, Bengaluru, June 2022
- Tamal Das, ‘Mechanobiology of Collective Cell Dynamics’, 19th Horizons in Molecular Biology Symposium, Göttingen, Germany, September 2022
- Tamal Das, ‘Mechanobiology of Collective Cellular Systems: Cell Migration, Cancer, and Development’, HFSP Symposium, CDFD, Hyderabad, February 2023
- Tamal Das, ‘Mentor Talk - Unravelling the Mechanobiology of Collective Cell Dynamics: An Interdisciplinary Journey’, YIM 2023, IIT Gandhinagar, Gandhinagar, February 2023
- Tamal Das, ‘Mechanobiology of Collective Cell Dynamics’, 67th Annual Meeting of the Biophysical Society (Mechanobiology sub-group), San Diego, USA, February 2023
- Tamal Das, ‘Unravelling the mechanobiology of cell competition during cancer initiation: Biophysical view of oncogenesis’, Indian Biophysical Society Meeting 2023, NCBS-TIFR, Bengaluru, March 2023
- T N Narayanan, ‘Next Generation Batteries: Air-Batteries to Solar Batteries’, International Conference on Nanomaterials for Electro-Catalysis Technology (I-CONNECT), IIT Delhi, March 2023

- T N Narayanan, ‘Engineering Atomic Layer Interfaces for Energy Applications’, VIT University, Chennai, January 2023
- T N Narayanan, ‘Next Generation Batteries: Air-Batteries to Solar Batteries’, International Conference on Energy Conversion and Storage (IECS- 2023), January 2023, IIT Chennai Research Park [Keynote Lecture]
- T N Narayanan, ‘Inspired to do Materials Research’, talk during the post graduate students workshop conducted as a part of International Workshop on Nanoengineered Materials, IISER Thiruvananthapuram, January 2023
- T N Narayanan, ‘Engineering Atomic Layer Interfaces for Applications’,International Workshop on Nanoengineered Materials, IISER Thiruvananthapuram, January 2023 [Invited Talk]
- T N Narayanan, ‘Engineering Atomic Layer Interfaces for Applications’, International Conference on Functional Materials for Advanced Technology organised by Central University Kerala India, January 2023 [Keynote Lecture]
- T N Narayanan, ‘Atomic Layer Interfaces for Energy Applications, IUMRS-ICA 2022, IIT Jodhpur, December 2023 [MRSI Medal Lecture]
- T N Narayanan, ‘Our Recent Efforts Towards Two Electrode Solar Batteries: Possibilities & Challenges, 6th IEEE International Conference on Emerging Electronics (ICEE), December 2023 [Invited Talk]
- T N Narayanan, ‘Atomic Layers in Catalysis: Hydrogen Generation with TMDs, Institute of Physical Chemistry’, FSU, Jena, November 2022 [Invited Lecture Series]
- T N Narayanan, ‘Engineering Interface and Morphology of Nanostructures for Energy Devices, International Conference on Frontiers in Materials for Technological Applications (FIMTA-2022), CSIR-IMMT Bhubaneswar, India, August 2022 [Invited Talk]
- T N Narayanan, ‘Engineering Interface and Morphology of Two-Dimensional Materials for Energy Devices’, Conference on Physics of Nano Materials -II (PNM-II), Institute of Nanosciene and Technology (INST), Mohali, India, July 2022 [Invited Talk]
- Vipin Agarwal, Analytic and Research Development Science Fair 2023, Novartis, Online Presentation, March 2023
- Vipin Agarwal, 3rd India-Japan NMR workshop, Hokkaido University, Hokkaido, February 2023
- Vipin Agarwal, S. Subramanian’s 60th Birthday Lecture Award, XXVIIIth Annual Symposium of National Magnetic Resonance Society of India and Conference on Magnetic Resonance in Biomolecules and Biomedicine, IISER Berhampur, February, 2023
- Vipin Agarwal, ‘Mapping interatomic 1H-1H distances at fast Magic Angle Spinning (MAS)’, TIFR in-house symposium, TIFR, Hyderabad, September 2022
- Vipin Agarwal, NMR user workshop, National High-Field NMR facility, TIFR, Hyderabad, August 2022
- Vipin Agarwal, ‘Mechanism of polarization exchange amongst chemically similar and distinct protons during weak rf irradiation at fast magic angle spinning’, JMR/JMRO/ISMAR symposium “New Voices in Magnetic Resonance, online meeting June 2022 (JMR New Voices issue Award Talk)
- V. Chandrasekhar, ‘Mono- and Tetranuclear Lanthanide Complexes: Synthesis, Structure and Magnetism’, TIFR Hyderabad In-House Symposium, September 2022
- V. Chandrasekhar, ‘Single-molecule and Single-ion Magnets Containing Transition and Lanthanide Metal Ions’, Institute for Inorganic Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany, September 2022

- V. Chandrasekhar, ‘Reactivity of an NHC-coordinated Diphosphene and an Unsymmetrical N-P-N Ligand’, Institute fur Inorganic Chemistry, Technische Universität Braunschweig, Germany, September 2022
- V. Chandrasekhar, ‘Reactivity of an NHC-coordinated Diphosphene and an Unsymmetrical N-P-N Ligand’, Institute of Inorganic Chemistry, University of Heidelberg, Heidelberg, Germany, October 2022
- V. Chandrasekhar, ‘Reactivity of an NHC-coordinated Diphosphene and an Unsymmetrical N-P-N Ligand’, Institute of Inorganic Chemistry, Karlsruhe Institute of Technology, October 2022
- V. Chandrasekhar, ‘Phosphorus-based Ligands in Magnetism and Catalysis International Conference on Main Group Synthesis and Catalysis (ICMGSC), IISER Trivandrum February 2023
- V. Chandrasekhar, ‘Phosphorus-based Ligands in Magnetism and Catalysis’, Department of Chemistry, IIT Hyderabad, April 2023

G. Major ongoing and future projects:

- Single cell transcriptome of the mouse vomeronasal neuroepithelium indicates a specialized endoplasmic reticulum environment in neuronal subsets. (Devakinandan G V S and Adish Dani)
  The vertebrate vomeronasal (VNO) system is an important model to understand how sensory information leads to innate and social behaviors. With the expression of several evolutionarily and functionally distinct genes, VNO neurons offer an intricate system to understand the cellular and molecular biology associated with sensory signaling. Adish Dani and colleagues performed single cell RNA sequencing of the mouse VNO neuroepithelium to understand the diversity, gene co-expression patterns, and functional differences amongst neuronal subtypes. In addition to the known major neuronal subtypes, the analysis reveals a diversity of cell types comprising glia, immune and sustentacular cells, with genes specific to each. Pseudo-time developmental analysis indicates; neurons originating from common progenitors diverge in gene expression during maturation, with transient and persistent transcription factor expression at critical branch points. Within mature sensory neurons, the researchers find significantly higher expression of endoplasmic reticulum genes in a neuronal subtype, indicative of a putative functional requirement for protein maturation.

- Resolving cochlear ribbon synapse protein organization with single molecule fluorescence nanoscopy. (Gayatri Chandran, Devakinandan G V S, Adish Dani (TIFRH), Mark Rutherford (Washington University in St Louis, USA)
  The ribbon synapse is a macromolecular complex specialized for rapid and graded transmission of auditory signals to the brain. In order to understanding the structure, function, and diversity of ribbon synapses, Adish Dani and colleagues developed single molecule 3D-STORM to resolve the protein organization of cochlear inner ear hair cell (IHC) ribbon synapses in the mouse organ of Corti whole mount preparations. Imaging the presynaptic ribbon protein Ribeye along with postsynaptic scaffolding protein Homer1 and AMPA type Glutamate receptors, we measured the size, diversity,

distribution of pre, post-synaptic proteins from wild-type mice across postnatal developmental ages and compared these with synapses from Vglut3 deficient mice that are congenitally deaf and defective in IHC glutamatergic synaptic transmission. The researchers observe that in several synapses, localizations of postsynaptic proteins Homer1 and GluA2 undergo a pancake to doughnut shape transition during postnatal development. This transition is not observed in synapses from Vglut3-/- mice and is accompanied by a significant increase in the size of the postsynaptic receptor distribution. These data indicate that glutamate release actively shapes the distribution of post-synapse glutamate receptors as well as their underlying scaffolding proteins. The researchers further demonstrate the existence of glutamate receptor nano-clusters within the postsynapse. These methods and data lay the foundation for further structure-function studies to investigate IHC ribbon synapse plasticity during development and in loud noise-induced synaptopathy.

- Role of Stx1 in Store-Operated Calcium Entry (Adish Dani and Monika Vig)
  Store-operated calcium entry (SOCE) is necessary for sustained calcium signaling in several cell types. Orai1, the pore subunit of store-operated CRAC (Calcium Release Activated Calcium) channels along with Stim1, the ER-membrane resident calcium sensor involved in Orai1 activation were believed to form the essential elements of SOCE. Point mutations in Orai1 and Stim1 have been found to result in immunodeficiency and autoimmunity in human patients and mice. Previous studies from the lab have shown that ɑ-SNAP (alpha-soluble NSF associated protein) directly associates with Orai1 and Stim1 and is required for the functional assembly of the CRAC channel complex. It is also shown that ɑ-SNAP's role in SOCE is independent of its function of SNARE-complex disassembly, following synaptic vesicle fusion. With the hypothesis that additional SNARE family proteins might regulate SOCE, RNAi screens from the lab have further identified a target-SNARE, Stx1 as one of the potential SNARE family proteins to have a functional role in CRAC channel activation. This research team's goal is to understand the molecular mechanism of regulation of CRAC channels by Stx1.

- Nucleolar DDR, and live cell biophyscial measurements of DDR. (Sinjini Ghosh, Shantam Yagnik, Aprotim Mazumder)
  The researchers are studying the roles of the nucleolus in mediating DDR and how repair can take place when rDNA itself is damaged; and also how DDR couples with nuclear mechanics using sensors that either report on forces across the nuclear envelope or on the recruitment of specific proteins to sites of damage. They find that the expansion of nucleoli upon DNA damage is ATP-dependent, and is also dependent on cytoskeletal elements like actin. Using methods of super-resolution microscopy the group is investigating how the compartmentalization of the nucleolus changes under conditions of DNA damage. FRET and lifetime based sensing of tension across the nuclear envelope is now standardized. An expulsion of the critical transcription factor YAP1 under laser-induced DNA damage that may be related to changes in nuclear mechanics is being investigated in greater detail.

- Studying responses to UV, oxidative damage, and the roles of A-type lamins in DDR. (Karan Bansal, Shravasti Misra, Souvik Sen, Aprotim Mazumder)
  Apart from the more converged directions described above, other projects are underway, which will further the understanding of DDR in terms of cell to cell

heterogeneity and live cell dynamics. Newer approaches are being developed for investigating ultraviolet damage response dynamics in living cells. Rather than a linear cascade of factors, such responses may be fine-tuned by multiple feedback loops. Further, Aprotim Mazumder and colleagues have also just begun to investigate how cells deal with oxidative stress and how 8-oxoguanine may be used as an epigenetic mark, and how A-type lamins may be involved in DDR. These studies are likely to be more advanced in the coming days.

- Chaitanya Kumar Suddapalli's research group is working towards the development of novel ultrafast mid-infrared sources. They aim to generate high average power, high repetition rate mid-infrared radiation using second order nonlinear interactions, while the low repetition rates in combination with short pulse duration will provide access to high intensities, critical to understand various fundamental phenomena.

- Functional dynamics in actins. (Kaustubh R Mote)
  Kaustubh R Mote and colleagues are working towards understanding actin dynamics using NMR spectroscopy with a focus on the following questions: (1) How do actins respond to changes in nucleotide state and how does this result in change of the actin from a filamentous state to a soluble state, and vice versa. (2) Can the transition state between the two nucletide forms (ADP and ATP) give hints to how the coupling of conformational changes is achieved. (3) Can we map the active site dynamics by using 31P NMR experiments? (4) Does nucleotide dynamics have any role in modulating actin structure and function? (5) How does the actin MreB respond to the presence of lipids? How does polymerization depend on lipid binding? What is the binding interface for lipid?

- Membrane Transport. (Kaustubh R Mote)
  Researchers are using two membrane transports: a) the mitochondrial pyruvate carrier (MPC) and b) the SemiSWEET carrier to answer the following questions in the field of active transport: (1) Are there intermediate, asymmetric SemiSWEET conformations that allow the transport of the asymmetric substrate glucose? (2) What is the structure of the MPC in the fully functional heterodimeric form? (3) Can we design a high throughput assay based on fluorescence to screen MPC inhibitors and more importantly, activators? (4) Where do the different classes of inihibitors (cinnamate based and thiazoldienedione based) bind MPC?

- NMR Methods (Kaustubh R Mote)
  The following new NMR methods with direct application for proteins are being worked on: (1) A double-frequency-selective REDOR that will allow multiple long-range distances in proteins to be determined, (2) Homonculear decoupling at fast MAS frequencies > 50 kHz, and upto 100 kHz to extend 1H coherence lifetimes to measure dynamics, (3) A simple method to identify beta-sheets, loops, and alpha-helices in proteins.

- Mito-Nuclear communication - The dMyc mediated mitochondrial biogenesis and mitochondrial stress: (Aravind H, Manish Jaiswal)
  Mitochondrial biogenesis is a tightly regulated cellular process that profoundly affects development, cellular homeostasis, and stress adaptation. However, how mitochondrial

biogenesis is regulated during various developmental, cellular, or physiological contexts is unknown. Recently Manish Jaiswal and colleagues found that mutations in many genes essential for mitochondrial function in flies cause stress-induced mitochondrial biogenesis. Using these mutants, they have identified that increased mitochondrial biogenesis due to mitochondrial dysfunction requires a nuclear factor Myc. They are currently investigating how mitochondria dysfunction activates Myc. The researchers are also investigating if a similar phenomenon exists in human mitochondrial diseases, which are also characterised by increased mitochondrial content.

- Polyphosphates (PolyP) in metazoan: method development, biology and mitochondria (Sunayana Sarkar, Manish Jaiswal)
  Polyphosphate (polyP) is a linear polymer of inorganic phosphate, which exists in all life forms, its function in multicellular organisms has been enigmatic. Due to the lack of a genetically tractable metazoan model organism to manipulate polyP *in vivo*, the systematic study of polyP function in multicellular organisms remains challenging. Thus, in my lab, the researchers initiated polyP research using *Drosophila*, the best-suited multicellular model for genetic manipulation, with the idea that it can accelerate the discovery of polyP function in multicellular organisms. Towards this, they are currently developing biochemical, genetic and microscopic technologies to isolate, quantify, manipulate and image polyP in Drosophila tissues. The researchers are also developing a FRET-based sensor to detect polyP to facilitate the quantification and localisation of polyP in live organisms and cell lines. To interrogate the organismal function of polyP, they are also developing transgenic fly lines to facilitate polyP depletion in a tissue-specific and cellular compartment-specific manner.

- Determine the mechanism of induction of HLH disease in human patients with Stx mutations and Stx knockout mice. (Monika Vig)
  Syntaxin, along with other genes identified in a screen conducted by Monika Vig and colleagues, regulate a rare immunological disease called Familial Hemophagocytic Lymphohistiocytosis (FHLH) in humans. This is a heterogeneous disease that likely results from immunodeficiency in certain immune cell types and a resultant autoimmunity that likely results from propensity for infections. Point mutations in molecular components that are necessary for SOCE also result in immunodeficiency. In this project the researchers will aim to assess the mechanism underlying immunodeficiency induced by the deficiency of Stx and assess whether this is related to regulation of SOCE by Stx. Primary lymphocytes isolated from healthy humans and potentially HLH patients as well as a knockout mouse model of Stx will be used for this study.

- Test the hypothesis that store-operated Orai channels display flexible stoichiometry in response to different stimuli. (Monika Vig)
  It is well accepted that Orai multimers form the pore of CRAC channels. However, the stoichiometry of Orai1 homomers and hetero-multimers formed, along with Orai2 and Orai3, remains debated. A number of different approaches have been used to address this question, but a unifying model has not yet emerged. Earlier approaches have used varying numbers of covalently linked Orai1 concatamers and showed that tetrameric Orai1 concatamers reconstitute currents. Other groups have used a combination of fluorescence resonance energy transfer (FRET), single-molecule tracking, and brightness analysis to determine the stoichiometry of resting Orai1 as a tetramer. Chemical crosslinking followed by gel electrophoresis has also been used to determine the number

of Orai1 subunits, but the conclusions have varied. More recently, x-ray crystallography of purified *Drosophila* Orai found that pure hexameric assemblies of Orai form the pore of CRACs, whereas others showed that hexamers of Orai1 were non-selective. Therefore, Orai1 stoichiometry remains unestablished and necessitates using approaches that allow direct visualization of Orai multimers in their native environment. Studies (by Monika Vig and colleagues) using step-photobleaching of fluorescently labelled Orai1 have suggested variable stoichiometry of Orai1 in resting versus stimulated live cells (Li et al., 2016). The researchers will build on these studies by generating and performing step-photobleaching analysis on a series of Orai1, Orai2, Orai3, single, double or triple knockout and knock-in cell lines generated in the lab. These studies will help address the potential contribution and stoichiometries of Orai heteromers in resting and store-depleted conditions and also assess the contribution of SNAREs in this process.

- ZULF NMR (P K Madhu)
  Zero-to-ultra-low-field nuclear magnetic resonance (ZULF NMR) is a way to perform NMR experiments under conditions dominated by internal spin interactions, when the truncating effect of Zeeman interaction is absent. But, the low spin-precession frequencies in such small external fields necessitate the use of special techniques for detecting the signals. Optical detection of NMR signals using an atomic magnetometer can be a good choice here. An alkali atom magnetometer that detects pico-Tesla magnetic fields in 1-25 kHz frequency range has been developed by the researchers. This will be used to study NMR signals in ZULF regime in both solution and solid samples. The researchers plan to combine this optical detection with cycling of magnetic field to create initial polarisation in the sample. Such experiments on solution samples detect the J-coupling between the sample nuclei and, with special encoding, the chemical-shift signature through field cycling. In solids such experiments will be dominated by dipole interaction and could provide distance constraints between the nuclei in the sample. The researchers propose to devise methods of initial spin-state preparation to tune the interaction under study. These would involve techniques to influence the interactions using external magnetic fields. In the later stages, hyperpolarisation techniques to increase sensitivity will be explored.

- Radio-frequency atomic magnetometry (P K Madhu)
  The atomic coherences created by the mixing of magnetic and electric fields in atomic vapour are interesting systems for magnetic spectroscopy. The nonlinear magneto-electric (ME) effect in the atomic system generates optical fields. This process will be studied theoretically and experimentally to understand the coherence generation and evolution. The sensitivity of the system to measure radio-frequency magnetic fields has been demonstrated in the lab by the researchers. This work will be continued to further explore the viability of this phenomenon in the understanding of spin exchange process in atomic systems.
  In mixtures of alkali vapours and noble gases like Rb-Xe, optical pumping of the alkali and spin exchange interaction between Xe and Rb can efficiently polarise the noble-gas nuclei. The spin exchange interaction is effected by the ambient condition and this can also be tuned to modify the interaction. The researchers propose to use the radio-frequency magnetometry technique for understanding the interactions between the metal electron and the noble gas nuclei that lead to this spin exchange. Theoretical studies that look at the effect of the spin interactions on the alkali energy structure and

spin evolution will be complemented by experimental studies that use polarimetry and ME effect based measurements of spectroscopic effect of the interactions.

- Spin-noise spectroscopy (P K Madhu)
  The Faraday-rotation noise spectrum of transmitted light through a spin system can be correlated with magnetic resonance of the system. Recently, the applications of this experimental approach have emerged in studying magnetic resonance and spin dynamics in atomic and solid-state magnetic systems. The precision polarimetry techniques that have been perfected in the lab will be combined with high-frequency (GHz) spectral analysis to establish spin-noise spectroscopy. This will allow the researchers to study stochastic noise in spin systems of various density. Spatio-temporal analysis will be added to the experimental set up to enable studies of the spin dynamics in such systems.

- Unification of spin decoupling and recoupling (P K Madhu)
  P K Madhu and colleagues have developed state-of-the-art methods for both heteronuclear and homonuclear spin decoupling in the last ten years. Currently, they have a good theoretical understanding of both the processes and factors limiting the line width. In the heteronuclear spin decoupling front, the major emphasis will be on the unification of several of the decoupling schemes in vogue. Such an attempt will help the researchers in demystifying and setting up a coherent methodology to understand the decoupling process. This will be attempted both from an internal spin interaction point of view and numerical and experimental analysis of the scheme as a function of phase and pulse duration of the decoupling schemes in practice, as most of the schemes can be treated as a pulse- and phase-modulated methods. The analysis will also include magic-angle spinning frequency and radio-frequency dependence to cover most of the experimental conditions. The researchers expect to find resonance conditions with such a comprehensive analysis which may correspond to good and bad decoupling conditions. This can then lead to refined decoupling schemes that will be also robust to various experimental parameters and covering a wide range of MAS and RF frequencies. The bad decoupling conditions will be further explored in the direction of recoupling (retrieving spin interactions that are otherwise lost due to MAS) of spin interactions. Such areas may lead to RF and MAS conditions for efficient recovery of various spin interactions that can give information on geometry more efficiently than the existing schemes. The philosophy here will be to place under one umbrella the seemingly conflicting two issues, namely, decoupling and recoupling.

- Spin locking half-integer spin quadrupolar nuclei (P K Madhu)
  Cross-polarisation to and from half-integer spin quadrupolar nuclei is rendered difficult under magic-angle spinning due to the time dependence of the quadrupolar spin interaction. The problem essentially reduces to the inefficiency of spin locking of such spins under MAS. Cross-polarisation is hence possible only under extreme conditions of low radiofrequency amplitudes or high MAS. P K Madhu and colleagues will be looking into the design of efficient pulse schemes that achieve spin lock of such spins under all experimental conditions. Phase-modulated pulses will be an option to begin with in this case which may be extended, if successful, to more sophisticated schemes.

- Off-magic-angle-spinning experiments (P K Madhu)

Experiments are being planned in both rare and abundant spin systems to measure internuclear distances under off-MAS conditions without making use of radio-frequency driven dipolar recoupling schemes. These experiments may have the further advantage of measuring long-range distances in the presence of short-range distances thus paving the way to obtain more structural constraints in various molecules.

- Pranav R Shirhatti and colleagues aim to explore and evaluate 2D materials as suitable candidates for atomic mirrors as focussing elements in high lateral resolution atom scattering microscopy. The ultimate goal would be to produce to produce high intensity and tightly focused atomic beams, overcoming the limits imposed by the size and pumping rates of vacuum pumps.

- MolDis project (https://moldis.tifrh.res.in) (Raghunathan Ramakrishnan)
  Over the past 5+ years, Raghunathan Ramakrishnan and colleagues have diligently generated a wealth of data through various studies, and they have now made this data available to the public through MolDis. Their aim is to not only share this data with researchers, but also to continually improve the analytics platform to make it even more effective and useful. The researchers aim to expand the scope of MolDis and equip it with advanced analytical tools that will allow scientists to quickly and easily re-use the datasets in their own research. This will not only promote new scientific discoveries, but also facilitate the integration of these datasets into pedagogical settings to complement the educational experience for students. In summary, the MolDis platform is a valuable resource for researchers and educators alike. In the next round of the development of the MolDis platform, the researchers will develop workflows to enable querying pre-trained ML models of molecular and materials properties to generate data dynamically. These pre-trained models will also be made accessible to the public as modules that can be imported in a Python code.

- Indo-South Africa Collaborative Project on Computational Studies on Atmospherically Relevant Molecules (Raghunathan Ramakrishnan)
  Raghunathan Ramakrishnan and colleagues have identified several scopes of applying the large molecular datasets and the relevant modeling tools to understand the kinetics and mechanisms of gas phase processes relevant to atmosphere and combustion chemistry. Recently, they have investigated the structural factors influencing the thermodynamic and kinetic stability of free-radical intermediates, especially the hydroperoxyalkyl radical (also known as QOOH). This collaborative work undertaken with Lyudmila Moskaleva (University of the Free State, South Africa), is under consideration for publication (https://arxiv.org/abs/2305.12706). In this work they have systematically explored the influence of inductive and resonance effects on governing the energetic preferences of key species in hydrocarbon combustion. The researchers plan to undertake projects of more general scope to understand the stability of radicals across larger datasets covering captodative effects. These investigations are likely to suggest reactions to study in experimental conditions to trap long-lived free radical intermediates that can be characterized through spectroscopy. Further, the datasets that they have planned to develop will cover interesting species such as the Criegee intermediates interacting with solvent molecules, and other radicals such as hydroxyl and hydroperoxyl radicals. These large datasets will facilitate the microkinetic modeling of

elementary processes such as the formation of aerosols, brown carbon responsible for photo-induced fog, and soot-formation.

- Development of a AI/ML model for characterizing the spectrum of melanin. (Raghunathan Ramakrishnan)
  Raghunathan Ramakrishnan and colleagues have investigated data-driven modelling of electronic excited state spectra for large molecular datasets. They have collaboratively (with Debashree Ghosh of IACS) explored such modelling for BODIPY dyes and have published the findings in the past. Currently they are working towards applying the data-driven strategies to model biologically relevant molecules such as the melanin pigment and design a framework for rapid estimation of their UV/visible spectra. In this long-time collaborative project, the researchers aim to develop ML models for excited state potential energy surfaces relevant for non-adiabatic dynamics. Their preliminary findings have been communicated for publication: https://doi.org/10.26434/chemrxiv-2023-tpw0p.

- Deciphering the molecular-/atomic-level details of mitochondrial cristae architecture (Anand T Vaidya)
  The ongoing project on mitochondrial cristae architecture needs detailed structure of the proteins, and their complexes, involved in maintaining the precise architecture. In this project the current crystals of Mic10, Mic12 and Mic60 will be analyzed for x-ray diffraction quality and the structures will be determined. Next, the complexes of these proteins and others will be purified for structure determination using both x-ray diffraction analysis and cryo-electron microscopy studies. Also, these proteins will be analyzed to understand the confirmational changes that are relevant for their role in redox-sensing and redox-regulation of cristae architecture.

- Aneesh Tazhe Veetil's lab is broadly interested in imaging and modulation of the innate immune cells of the brain called microglia. There are two ongoing projects in the lab that focus on the design and synthesis of new chemical tools for imaging microglia cells in live brains. In addition to the imaging projects, the researchers use cellular engineering and synthetic biology approaches to remotely modulate microglia. Several projects are in progress in the direction of immune modulation in the brain.

- Study of liquid to solid transition in liquid-liquid phase separation (LLPS) of amyloid proteins (Kanchan Garai)
  Transition of LLPS to amyloid is hypothesized to play important roles in the pathology of multiple neurodegenerative diseases. Literature data and recent findings from Kanchan Garai's lab suggests that LLPS of amyloid proteins can facilitate nucleation of soluble monomers to insoluble fibrils. However, systematic studies on such systems are currently rare in the literature. The researchers are developing single molecule techniques to study LLPS and measure nucleation of amyloid fibrils within the LLPS. The goal is provide a quantitative framework for describing liquid to solid transition of amyloid proteins.

- Manipulation of spin-triplet superconductivity using unconventional spin texture systems (Karthik V Raman)
  Thin film heterostructure of superconductors in proximity with non-collinear magnetic textures, such as skyrmions, can prove to be experimentally suitable for engineering

topological superconductivity. Such unconventional magnetic structures can induce spatially inhomogeneous Rashba spin–orbit interactions that offer unprecedented opportunities to introduce spin-triplet correlation and to generate a rich phase diagram of topological superconductivity. Currently, much of the experimental activity in topological superconductivity is limited to the realization of superconductor proximity effect in high spin-orbit 1-D nanowires or 2-D electron gas layers, without the incorporation of the physics of magnetic textures. The former research program has found it difficult to probe topological superconductivity and the hunt for Majorana fermions is actively pursued. Experimentally, the latter scheme utilizing magnetic textures is not realized. Research activity in this direction offers the benefit of external tunability of the topological phase by generating skyrmion states in applied magnetic field. The broken time-reversal symmetry arising from the presence of magnetic moments, the band topology, and the particle–hole symmetry of the superconducting state, together makes the system conceptually rich and experimentally rewarding. In this proposal, Karthik Raman and colleagues shall work with the above scheme that can revolutionize our fundamental understanding of topological superconductors in the quest for Majorana fermions.

- Regulation of interactions of DNA damage clamp, 9-1-1 and its implications in the assembly of repair factories and pathway choice. (Mrinal Srivastava)
  Cells have multiple DNA repair pathways to tackle various kinds of damage. Each repair pathway requires the concerted action of specific sets of DNA damage sensors, signaling pathways, and DNA processing activities at DNA damage sites. In mammalian cells, DNA replication and DNA repair factories have been spatially separated. Perhaps such spatial separation averts illegitimate activation of checkpoint and DNA damage response to single-stranded regions and ends generated during replication, especially in the case of lagging strands. Such separation is thought to be brought about through the evolution of a specialized DNA repair clamp, 9-1-1. However, the exact functions and regulations of 9-1-1 components and their various complexes are not yet deciphered. For this project, using various biochemical, molecular cell biology, and proteomics methods, Mrinal Srivastava and colleagues are exploring crucial questions related to the essential, supposed DNA repair clamp, 9-1-1. To this end, the researchers have successfully purified 9-1-1 protein complex along with paralogs and clamp loaders. Single-molecule studies will be carried out in collaboration with Mahipal Ganji, Indian Institute of Science, Bangalore. The researchers anticipate exciting findings on the translocation speed, DNA context for loading as well as translocation and nuclease boundary during homologous recombination etc. This part of project is anticipated to be finished by end of this year and manuscript will be submitted. Besides, the group is also exploring role of RAD9 and HUS paralogs, RAD9B and HUS1B in DNA repair using cell-based assay systems. Lastly, ability of RAD9A to form phase separated foci at the site of DNA repair is being investigated.

- Understanding the mechanism of polymerase switch during translesion synthesis in mammalian cells and its implications in genetic integrity. (Mrinal Srivastava)
  Mammalian DNA replisome complex are tremendously specialized machineries not only duplicate expansive genome efficiently but also achieves this with high specificity and accuracy. Replicative polymerases cannot traverse lesions that significantly distort geometry of DNA. On the other hand, TLS polymerases synthesize DNA at lower fidelity

due to lack of proof reading activity and owing to their flexible active sites can accommodate and bypass lesions that block replication fork. Human cells encode around 17 polymerases that belong to primarily four families - A, B, Y, X and AEP (archeo-eukaryotic primase) family. Replicative polymerases belong to B-family. Primary TLS polymerases such as POLs h, i, k and REV1 are Y-family polymerases. Whereas POL q and z belongs to A-and B-family, respectively. As translesion synthesis is mutagenic, various elegant studies have pointed that TLS polymerase recruitment to replication fork is highly regulated. How and which TLS polymerase is recruited at the site of DNA damage on replication fork (1st polymerase switch) and how its substituted again by replicative polymerase when damage is bypassed (2nd polymerase switch) is not well understood in vertebrates. Significant progress has been made for this project as all the polymerases are endogenously tagged with proteomics tags with CRISPR-CAS9 mediated knock-in strategy and proteomics studies are underway. Further, the researchers are establishing a SPLIT-FAST based assay system to study kinetics and sequence of polymerase recruitment. The group will also perform a genome-wide analysis of human cancers to predict mutation signatures due to translesion synthesis.

- Understanding molecular regulators of replication origin selection and firing in mammalian cells (Mrinal Srivastava)
  In order to transmit and preserve genetic information, cells must duplicate DNA with very high fidelity. Large metazoan genome duplication is accomplished by assigning thousands of potential origins of replication, a fraction of which are utilized. The remaining sites remain flexibly dormant unless required, as in the case of replication stress. Besides, the start of replication from the utilized origin is also spatiotemporally regulated in S- phase. Arguably, one of the key events during replication initiation is regulated conformational changes in the MCM helicase complex. The MCM complex is loaded onto the DNA in the G1 phase of the cell cycle, in an inactive form. At the selected origins, the MCM complex transitions into an active translocating helicase in the S-phase. However, (a) how this transition is achieved and (b) is regulated in a spatiotemporal fashion is not known. Here, Mrinal Srivastava and colleagues are comprehensively addressing the dynamics of helicase activation by generating individual cellular model systems with mitigated regulation of replication by introducing strategic mutations or oncogene- induction. They are performing biochemical, and cellular characterizations along with comparative proteomics and genomics while evaluating the spatiotemporal progression of replication in order to decipher molecular regulators for genome duplication time and pattern. To this end, key cell-based reagents have been generated and collaborations for acquiring samples from Meier-Gorlin Syndrome patients have been established. The researchers are getting interesting results regarding presence of MCM10 on the replication fork during helicase firing as well as translocation. Further role of B-to A-DNA transition is being explored in order to activate helicase on the licensed origins.

- Inspecting genetic vulnerability and co-dependencies of PCNA to explore functions of novel replication proteins. (Mrinal Srivastava)
  Whole-genome sequencing has revealed hypomorphic mutations in eight genes in MGORS patients so far and all of them are associated with origin licensing and initiation. Recently, DONSON was identified as a novel gene responsible for MGORS. Mrinal Srivastava's analysis on genome wide CRISPR-CAS9 loss of function screen to evaluate

dependencies of PCNA depletion reveals DONSON as one of the top candidates along with CDC45. Role of DONSON in regulation and assembly of pre-RC complex is not yet explored. Srivastava hypothesizes that DONSON has an earlier unknown important role in steps of replication, probably regulating replication licensing and origin firing. Experiments are being performed to determine whether DONSON expression or its chromatin loading is regulated in cell-cycle dependent manner and in presence of CDK inhibitors. Cell cycle profile, growth defects, doubling-time of DONSON depleted cells and their chromosomal aberration frequency is being evaluated. Components of licensing factors and origin firing components levels in whole cell extract and chromatin fraction will be deciphered at different time points in cell-cycle in DONSON deficient cells. Together, these analyses of assembly, disassembly and kinetics of known pre-IC and pre-RC components will enlighten the roles of DONSON in eukaryotic replication. Further, synergy of DONSON with that of PCNA and CDC45 would be analyzed.

- Exploring the Free Energy Surface (FES) of a protein. (Pramodh Vallurupalli)
  Pramodh Vallurupalli and colleagues aim to explore and understand how a protein molecule explores its FES. The researchers are attempting to do this by studying conformational exchange in different molecules as described below.
  ***(a) Structural and biophysical description of the folding mechanism of the FF Domain*:** Recently the researchers showed that the broadening of the minor state dips in ^{15}N CEST profiles can be used to inform on other sparsely populated states that are in intermediate to fast time-scale exchange with it. Their analysis of ^{15}N CEST profiles that exploits the minor unfolded (U) state linewidths of the 71-residue A39G FF domain establishes a folding mechanism that can be described in terms of a four-state exchange process involving exchange between the folded (F) and U state via two intermediates I1 (0.34%) and I2 (0.19%) and two different paths [Figure 1]. U interconverts with I1 on the 0.1 ms timescale while U, I1 and I2 interconvert with each other on the ~1 ms timescale and then interconvert with F on the ~15 ms timescale. The researchers also established that WT FF folds via the same intermediates. In the case of A39G FF folding intermediates had not been discovered so far, while in the case of WT FF only I1 had been described so far highlighting the power of this methodology. The structure of I1 is already known and the researchers are now determining the structure of the I2 state using shifts obtained from CEST experiments. They will also obtain the thermodynamic parameters (H, S and m) for all three sparsely populated states in addition to all four transition states. This will provide an unprecedented atomic level description of the folding mechanism. They will then combine this data with computational techniques to understand how the states interconvert with one another. By adding appropriate peptides to the FF sample, Vallurupalli and colleagues will also test using ^{15}N CEST experiments if any of these folding intermediates are involved in function, by determining the mechanism by which the FF domain binds to its recognition sequence on RNAP.

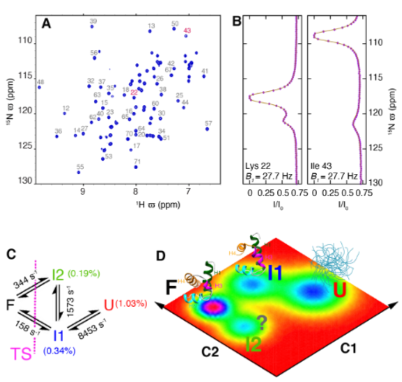

Figure 1: A39G FF folds via two intermediates and two paths. A) 1GHz ^{15}N-^{1}H HSQC at 2.5 °C contains only native state peaks, but ^{15}N CEST (B) clearly detects the minor unfolded state (U), whose dips have varying widths. An analysis of this CEST data that accounts for the varying widths shows (C) that molecule folds via two intermediates I1 and I2 and transition state separates F from the other states. A schematic representation of the FES requires atleast two coordinates and structures of F, I1 (and U) are known but the structure of I2 is unknown.

(b) Folding mechanism of T4 Lysozyme**:** Lysozyme from T4 phage (T4L) has been used as a model system to study protein folding, conformational dynamics and ligand binding etc. Despite intensive investigation over several years, the folding mechanism of this two-domain (164 aa) protein is still unknown. Folding studies using stopped-flow fluorescence techniques suggested that the protein folds via intermediates. However, the structures of these intermediates are still unknown. Pramodh Vallurupalli and colleagues are investigating the folding mechanism using CEST experiments. Preliminary CEST experiments showed that in addition to the native and unfolded forms the protein also populates to ~5% an alternate conformer whose structure differs from the native form in the N terminal domain. Stopped flow data suggested that this alternate conformer is a folding intermediate. The researchers developed a novel double resonance CEST experiment to probe this multi-state exchange process directly and found that the protein folds from the unfolded state to the native state directly without passing through this intermediate termed B. The minor state chemical shifts suggest that this conformation of T4L in the B state is very similar to structure of T4L in the ground state. Nonetheless the interconversion rate is very similar to the folding rate (~5 s^{-1}). The researchers are trying to understand why the interconversion between the two very similar conformers is so slow. They also find that the unfolded state dips are broadened in the CEST profiles just as in the case of A39G FF described above, suggesting that there is a folding intermediate. They are attempting to test if this second intermediate is indeed a folding intermediate.

(c) Understanding how protein molecules surmount activation barriers**:** The above two studies aim to map out the FES of proteins by studying conformational exchange. The researchers are also interested in understanding how protein molecules surmount the activation barriers to interconvert between these different states. They are attempting to obtain information regarding the barrier crossing events for two processes, i) the interconversion between the Phe114 exposed and buried states in the case of T4L cavity mutants and ii) interconversion between the native and B state in the case of WT T4L. The group plans to understand the activation process by studying the exchange processes using as a function of temperature, pressure, viscosity etc. The temperature dependence of the rates will give us the activation enthalpy and entropy, the pressure dependence of the rates will give us the activation volume (ie does the molecule locally unfold) and finally the viscosity dependence of the rates will tell us if collisions with water or collisions between the protein molecules are providing the activation energy. MD simulations will be analyzed to obtain insights into the dynamics and will aid in interpreting the experimental observations and in designing the next set of experiments.

- Development of new NMR methods to study conformational exchange (Pramodh Vallurupalli)

  Despite the success of NMR spectroscopy in detecting and characterizing protein 'invisible' conformers, the methods that are currently available have shortcomings. Pramodh Valurupalli and colleague plan to address some of these shortcomings as described below.

  (a) CEST experiments to study faster (multi-state) exchange processes**:** CEST experiments have largely been used to study minor states that are in slow exchange with a major state. Even in the case of the A39G FF domain described above the U (~1%) state is in slow exchange with the F state, but Vallurupalli and colleagues used the width of the distinct U state dips to detect intermediates I1 (~0.3%) and I2 (~0.2%) that are in rapid exchange (0.1 – 1 ms) with it. Based on their work in the case of the A39G FF domain and building upon recent work from the Al-Hashimi lab, the researchers now plan to use CEST experiments to study multi-state exchange occurring on the millisecond, even when there are no slow processes (no distinct dips). Simulations suggest that this should be possible and that in some cases it is advantageous to use ^{15}N CEST data rather than ^{1}H/^{15}N CPMG data to study exchange occurring in the millisecond time-scale. They will also attempt to carry out a combined analysis of CEST and CPMG data.

***(b) Identifying subtle changes in structure*:** There has almost always been a change in the backbone conformation of the protein when the minor state structure has been determined from relaxation dispersion data. However often the chemical shift differences between the major and minor states are relatively small (State B of T4L) suggesting that there are only small structural differences between the two forms. These small changes in structure are possibly due to changes in the side-chain conformation. The researchers will try to develop methods to obtain the structures of such minor state conformers. Strategies include using CEST experiments to obtain side chain chemical shifts in the minor state and residual dipolar couplings (RDCs) at several side-chain positions to elucidate the subtle differences between the conformation of side-chains in the major and minor states. They will also attempt to detect if the hydrogen bonding in the minor state differs from the major state by measuring hydrogen exchange rates in the minor state.

***(c) Machine learning to analyze CEST data*:** As mentioned above ^{15}N CEST experiments have now emerged as a valuable tool to study multi-state exchange and characterize the FES of a protein. It is however very challenging and cumbersome to analyze this CEST data and tease out the details of the exchange process from it. In collaboration with Flemming Hansen (UCL), the researchers plan to develop machine learning tools trained on synthetic CEST data to assist in the analysis of ^{15}N CEST data. If the machine learning tool can be trained to suggest possible multi-state exchange scenarios (rates, populations and chemical shifts), the researchers can then test these various models to select the appropriate one.

- Optical control of relativistic electrons and VUV-XUV photons by few-cycle ultrashort laser pulses. (Prashant Kumar Singh)

  i) Relativistic electron beam: With addition of deformable mirror system, relativistic intensity can be achieved by focusing the few-cycle, mJ laser pulse to diffraction limit, the so-called lambda-cube regime. The basic idea here would be to achieve maximum field gradients in both spatial and temporal domains, which can result in highest possible laser intensity for a given laser system. By adopting thin plate based bandwidth generation and compression by chirped mirrors, the existing 30 fs kHz laser will be shorten down to 5 femtosecond. These 2-optical cycle (5 fs) pulse, having 1 mJ energy, can be focus down to 1 μm diffraction limited spot. The quiver energy of electron oscillating in the light field can be in relativistic regime. By tailoring the parameters such as laser polarization, preplasma condition and angle of incidence, the different mechanism of electron acceleration will be investigated. The observation of electron angular distribution and kinetic energy spectrum could help us in understanding and controlling the physical scenario of acceleration mechanism.

ii) VUV-XUV high-harmonic photon beam: The nonlinear response of electrons oscillation in the light field leading to high-harmonic-generation (HHG). The resultant broad HHG spectrum, spanning up to 100's of eV in the frequency domain, naturally leads to the possibility of ultrashort attosecond light pulse in temporal domain. Such ultrashort pulses can provide a pathways to probe phenomenon occurring on the time-scale of electrons in atoms, molecules or in solid. For the HHG from solid targets, two distinct theoretical mechanism have been suggested. At the moderate, sub-relativistic laser intensity, HHG process is dominated by the Coherent Wake Emission (CWE) process, where electrons driven inward by the laser electric field drive a coherent wake inside the plasma. Therefore the CWE process demonstrate a high-energy spectral-cut off, limited by the maximum plasma density that target can support. However, in the relativistic laser intensity regime, the HHG is driven by Relativistic Oscillating Mirror (ROM) mechanism, which inherently being a surface phenomenon is independent of target density and directly scalable with laser intensity. In this proposal the understanding of electron acceleration mechanism will be applied towards establishing the underlying HHG process and could be beneficial for the generation of stable, bright high-harmonic pulses. As the plasma density scale-length plays a critical role in governing dynamics of nature of laser-plasma interaction, an independent probe, synchronized to the main pulse will be developed to control the plasma scale-length.

b) Structural dynamics of matter probe with intense laser-driven ultrafast electron diffraction (Prashant Kumar Singh)

The particle-wave duality nature of the electrons is well exploited via electron microscopy and diffraction in revealing atomic structures and detecting local lattice variations from equilibrium with highest spatial resolution. The ultrafast lasers have added a new dimension to this field where besides the static picture, the ultrafast timescales dynamics involving phenomenon such as phase transitions, chemical reaction dynamics, the coupling of electronic and nuclear degrees of freedom in medium can be probe. At present the ultrafast electron diffraction (UED) studies are carried out by generating electrons from photocathode followed by acceleration up to 100 keV. However, due to space charge factor, the temporal resolution what can be achieved from these UED diagnostics are limited to 300 – 500 fs range. Alternatively, the intense laser driven electrons beams can be as short as 10 femtosecond. In this proposal, Prashant Kumar Singh and colleagues are planning to use the kHz, 2mJ laser pulse for accelerating electron beam from liquid jet or gas jet system with expected energy of 300 – 500 keV. The electron beam will be collimated by using ether a solenoid or a tapered glass fibres where electrons beams are confined and transported over several cm distance due to charging of the glass inner wall. The UED capability of the collimated electron beam as a proof-of-principle would be investigated by observing static diffraction from nanometer thin crystalline foils. Subsequently, the UED probing set up will be upgraded to suit the pump-probe configuration where dynamics of the matter can be probe with 10's femtosecond temporal resolution. The laser-driven UED experiments offer an advantage of having jitter-free pump-probe synchronisation in time-domain, as both electron beam and the pump beams are originated from the same laser pulse.

c) Ultrafast dynamics of dense plasmas with femtosecond x-ray phase contrast imaging (Prashant Kumar Singh)

Conventional X-ray radiography, based on attenuation of X-ray photons as the beam travels through a medium, has been very effective for studying high-energy-density physics, medical and biophysics. However most often, the object, such as soft biological medium or a dynamic shock wave may not have sufficient opacity contrast and therefore X-ray absorption radiography fails to provide a clear picture. Fortunately, these limitations can be overcome by X-ray Phase Contrast Imaging, which is sensitive to variation of phase (or density gradient) of the transmitted x-ray beam. Despite having a poor chromatic coherence, the laser-driven x-ray source can have very large spatial coherence ($d = \lambda l/\sigma$, where λ: x-ray wavelength, l: source to image distance, σ: x-ray source size) due to small x-ray source size (10's μm) and therefore are well suited for in-line x-ray phase contrast imaging. In this proposal, Prashant Kumar Singh and colleagues are planning to irradiate high-repetition rate targets such as liquid jets or droplets with few-cycle, mJ laser pulse at relativistic intensity to generated bright x-ray photon flux. In the first phase, static phase-contrast images will be optimized based on the balance between the x-ray photon flux and source size by tuning the laser-plasma interaction conditions. For the dynamic phase-imaging, infrared laser will be used as a pump beam, which will be probe by a time-delayed x-ray pulse.

- Photophysical properties of metal-organic semiconductor thin films for sensing applications. (Ritesh Haldar, Pratibha Malik)
  Metal-organic framework semiconductors have unique features, such as tunable and predictable chemical space, well-defined spatial geometry of the organic and inorganic nodes, and very high functional porosity. However, the materials are difficult to utilize in device based applications due to the processibility issues. Ritesh Haldar and colleagues are developing novel methodologies to fabricate thin films of these porous semiconductors and explore those for sensing applications (e.g. gas, ion and volatile organic sensing).

- Mixed-matrix membranes for gas separation. (Ritesh Haldar, Susmita Kundu, Tanmoy Maity)
  High selectivity and high flux gas separation is a grand challenge. Using mixed-matrix membranes, i.e. a composite of two gas permeable materials, it is feasible to purify gases efficiently and economically. Ritesh Haldar and colleagues are devising new matrix components to achieve efficient separation of H_2/CO_2, H_2/N_2 and N_2/CO_2 gas mixtures.

- Porous organic membranes for ion separation. (Ritesh Haldar, Ramya A R)
  Ion selective membranes are very important for cathode materials (water electrolyser) and osmotic energy harvesting. The chemical functionality of the membrane and the porosity, both act as the controlling parameters. Achieving high ion selectivity requires chemical precision. Ritesh Haldar and colleagues are exploring these possibilities by using conjugated porous polymer thin films, which are grown at the liquid-liquid interface.

- Diffusion controlled continuous flow catalysis. (Ritesh Haldar, Suvendu Panda, Tanmoy Maity)
  Catalysis rate depends on the substrate reactivity and diffusion rate. In case of porous heterogeneous catalyst, substrate diffusion is controlled by the pore size and pore surface-substrate interaction. By tuning those parameters, it is possible to utilize

diffusivity as the rate determining step. Ritesh Haldar and colleagues are exploring such possibilities by using metal-organic framework as catalyst.

- The Theory of Glassy Dynamics. (Saroj Kumar Nandi)
  A liquid crystallizes when cooled below its melting point. However, crystallization is a time-consuming process. First, a tiny volume of the crystalline phase nucleates and if its volume is larger than a specific value, it grows and spans the entire system. If the crystallization process is avoided, e.g., via fast cooling or introducing polydispersity, then the relaxation time and viscosity of the liquid increase quite rapidly with decreasing temperature, and the system becomes solid for all practical purposes. This state of the system is known as glass. The precise mechanism behind this dramatic change in dynamics without much change in the static properties continues to be debated. The problem also has applications in several fields such as dynamics in various biological systems, computer optimization, earthquake pattern, etc. Thus, it is a fascinating problem with profound theoretical and practical importance. All the existing theories fail in some regime or the other. This illustrates the difficulty of the problem. Even some of the basic characteristics of a glassy system continue to be debated to date. In this work, the researchers first want to understand the system properties without embracing any particular theory. Specifically, they will analyze the glassy characteristics to understand their origin and if they are related or distinct facets of the dynamics. Metastability plays a crucial role in glassy dynamics; they will study the nature of metastability in such systems. They will then develop the theoretical framework from these understandings.

- Glassy dynamics in biological systems (Saroj Kumar Nandi)
  Recent experiments show glassiness is crucial for many biological processes, such as wound healing, embryogenesis, bronchial asthma, cancer, development, etc. Most of these systems can be conveniently modeled as active systems of self-propelled particles. Apart from self-propulsion, biological systems contain many other types of activity, such as changing protein conformations, gradient sensing, division, differentiation, apoptosis, etc. Moreover, many of the cellular systems are confluent. Therefore, developing a coherent theoretical framework for such systems is a daunting task. The researchers have extended theories of equilibrium glasses for active and confluent systems. They are currently including these other forms of activity. The long-term goal in this direction will be to understand the specific need for slow dynamics in different biological processes and reveal the system-specific parameters to control the dynamics. Such a program requires close collaboration of theory, simulations, and experiments. At different stages of the work, Saroj Kumar Nandi's group will collaborate with colleagues from TIFRH, Smarajit Karmakar, and Tamal Das.

- Yielding behaviour in confluent tissues (Saroj Kumar Nandi)
  The physics of yielding in particulate glassy systems seems to be controlled by a random critical point that separates a ductile, continuous yielding from brittle, sudden yielding. The parameter that controls the yielding behavior is the nature of the disorder that comes from the preparation history. A well-annealed glass shows brittle yielding whereas a poorly annealed glass is ductile. The preparation history will strongly depend on the initial concentration. In contrast, in confluent cellular monolayers, the concentration always remains unity. These systems are known to show glassy behavior. The question that Saroj Kumar Nandi and colleagues will explore in this work is what is their yielding

behavior? Is the physics of yielding different in these systems? This question is also relevant from the biological point of view. During development, cancer progression, wound healing, etc. collective cellular movement results from compression or stretching. Also, shear-like perturbation is abundant where a certain number of cells start moving due to biological signaling.
The researchers will first explore the yielding behavior in different model confluent systems, such as the Vertex model or the Voronoi model; they will also develop an analytical theory to corroborate the simulation results. Eventually, the researchers will test these findings in experimental systems. This work will be in collaboration with Peter Sollich, Tamal Das, and Manish Jaiswal.

- Fibrillar aggregation kinetics in Amyloid beta proteins (Saroj Kumar Nandi)
  Fibrillar aggregation of Amyloid-beta proteins leads to different neurodegenerative diseases, such as Alzheimer's or Huntington's disease. There seem to have three possible distinct stages in the aggregation process: the conformational changes of the individual proteins, the change in form in the oligomer, and finally the aggregation kinetics leading to the fibrillar structure. Most research works, at present, are focused on understanding the third stage via kinetic equations. Crucially, the first two stages can be included within this framework in the form of kinetic rates. Then a reliable estimate of the rate constants in the aggregation process becomes key to understanding the growth process. Kanchan Garai investigates this process experimentally, via modified home-built fluorescence spectroscopy. Currently, Saroj Kumar Nandi's group is collaborating with Kanchan Garai's group in analyzing some aspects of the data and how understanding the aggregation process via the rate constants. They aim to understand the first two stages of the problem in further detail, namely the conformational changes in the protein and the change of form in the oligomer that allows the growth process.

- Length and Time scales in Active and Passive glass Forming Liquids. (Smarajit Karmakar)
  Recent findings of glass-like dynamical behaviour in various biologically relevant systems lead to development of a new field called "active matter" in which the constituent particles experience thermal as well as other non-equilibrium fluctuations (self-propulsion) and these materials in the dense limit produces a new type of glasses known in the literature as active glasses. Emergence of glassiness in these active glasses are of immediate importance because of their possible implications in various biological processes. Some of the recent work by Smarajit Karmakar and colleagues suggest that the growth of dynamical and static length scales in these glasses may be enhanced by many factors leading to the possibility of better understanding the physics of glass formation in a diverse set of physically relevant contexts.

- Yielding of Amorphous Solids at Bulk and Nano Scale. (Smarajit Karmakar) Understanding the failure mechanisms of glassy materials is of great practical importance. Using highly parallelized in-house molecular dynamics simulations code, the researchers perform simulations of tensile testing on the "active glasses". They have found evidence that in certain regimes, introducing activity can decrease the ductility of such systems, which goes counter to intuition. Understanding the mechanism which leads to this, and whether activity can drive a ductile-to-brittle transition, would have implications in understanding and even designing various bio-materials.

- Understanding the physics of failure mechanisms in amorphous solids at mesoscale. (Smarajit Karmakar)
  In this part of the project, Smarajit Karmakar and colleagues want to study the plasticity in amorphous solids using continuum simulations. They want to develop a FE model of amorphous plasticity with information taken from extensive microscopic simulations so that they can mimic the metallic glass closer. This study will help develop a mesoscale model of amorphous solids which will take into account the effect of fragility in failure behaviour of these materials. [Collaborators: Pinaki Chaudhuri (IMSc, Chennai) and Vishwas Venkatesh (IIT-Palakkad)]

- Origin of Ferroelectric nematic phase. (Smarajit Karmakar)
  The researchers aim to develop an understanding of this ferroelectric nematic phase using MD simulation to study the rheological properties ferroelectric nematic liquid crystals in the presence of an electric field. They want to study the system's response with increasing shear rate in the presence of the electric field and to confirm whether shear can give rise to flexo-electric polarization, which was observed very recently in experiments. [Collaborator: Surajit Dhara, (University of Hyderabad)]

- Tuning Brittle Yielding transition in ultra-stable amorphous solids with rod-like inclusion - Micro-alloying. (Smarajit Karmakar)
  In this proposed work, the researchers aim to study the effect of rod-like inclusions as possible "soft pinning" sites to tune the brittle yielding in ultra-stable glasses and thereby understand possibly the origin of the shear-banding instability in systems with a high degree of annealing.

- Anomalous Low Frequency Vibrational Modes in Amorphous solids. (Smarajit Karmakar)
  In this project Smarajit Karmakar and colleagues aim to develop a theoretical understanding of the emergence of universal ▯5 vibrational density of states in stable amorphous solids with zero bulk and shear stress rather in competition with the usual Debye like density of states. They also aim to study the role of these modes which are believed to be quasi-localized spatially on the mechanical properties of these solids. [Collaborator: Kabir Ramola (TIFR-H)]

- Active micro-rheology of soft deformable objects. (Smarajit Karmakar)
  In recent experimental work, the active micro-rheology is used to distinguish healthy red blood cell from sick cells (Langmuir 37, 289-296 (2021)). Besides the potential application in many biological and real-life system, the active micro-rheology of the deformable objects is not fully explored. Therefore, to have a better understanding of the micro-rheology and deformable system, Smarajit Karmakar and colleagues aim to analyse the local dynamics of such deformable complex system by analysing the probe dynamics, and try to explore how the deformability of particles influence the dynamics of system.

- Probing the Role of Mechanics and Geometry in Tissue Development and Cancer Initiation (Praver Gupta, Simran Rawal, Sanak Banerjee, Aaheli Shee Burman, Padmashree D, Tamal Das, Dapeng Bi (Northeastern University, USA), Friedhelm Serwane (LMU, Germany))

Previously, Tamal Das and colleagues used cultured epithelial monolayers as a model system to study collective migration and cell competition. This system yielded fundamental discoveries and allowed us to dissect molecular mechanisms. Now, the researchers aim to investigate collective cell dynamics in a 3D tissue environment using mouse models and organoids, focusing on tissue development and cancer initiation. The objectives include developing tools for 3D force measurements, understanding how forces influence tissue development and oncogenesis, and studying the impact of tissue geometry on these processes. Specifically, the researchers will explore skin epidermis development and cell competition-based defence in the lung and intestinal epithelial tissue. They are also trying to uncover how cells sense tissue curvatures at a multicellular level. With this interdisciplinary approach, Tamal Das's group aims to address unresolved questions regarding tissue mechanics and cancer biophysics.

- Solar Battery. (T N Narayanan)
  T N Narayanan and colleagues are exploring an energy harvesting cum storage system known as solar batteries. Initial studies could demonstrate the working of a proto type device. However, a lot remains understood in terms of the functioning of such a solar battery. A two electrode battery, similar to that we use in our daily use, is modified with a photoactive cathode and a light entering window function as a light chargeable battery. The mechanism of charging is experimentally demonstrated. It has been shown that the band structure changes in materials with heterostructure is different from what they do individually.

- α-synculein is an intrinsically disordered protein (IDP) having tendency to form fibrillar aggregates causing group of neurodegenerative diseases known as synucleinopathies. It includes Parkinson's disease (PD), Dementia with Lewy bodies (DLB), multiple systems atrophy (MSA) and pure autonomic failure (PAF). All these diseases have deposition of α-synculein but have different symptoms and pathology and accumulation at different parts of the brain. PD and DLB have accumulation of α-synculein in Lewy bodies while in MSA it is in cytosol of oligodendrocytes. The different patients suffering single disease have differences in pathology and aggressive behavior of disease. The exact mechanism and residue-specific interactions that result in the structural evolution of monomer to the phase-separated droplet, form droplets to oligomers and subsequently to fibrils are still not known. Vipin Agarwal and colleagues are using solid-state NMR spectroscopy to decipher the structure and the types of intra- and inter-molecular interactions at the atomic/molecular level that enable these structural transitions. This information will help answer the question how the same protein can enable different diseases.

- Vipin Agarwal and colleagues are interested in the structural characterization and structural differentiation of amyloids formed by the wt- and the mutant p53 DNA binding domain (DBD). p53 is a transcription factor that inhibits genes required for cell cycle progression and activates genes leading to apoptosis. The function of p53 is to prevent the cell from becoming cancerous by controlling its cell division. Hence, it is called the "guardian of the genome." Thus, mutations in p53 can lead to loss of function and the progress of cancer in about 50% of reported human cancers. The aggregates of p53 have been observed in malignant cancers.

- India is the global pharmacy of the world, providing cheap medicines to the globe. The generic Indian medicine provides an avenue for health care, especially to the economically weaker people in the world. Several reports have shown that generic medicines with chemically identical molecules have failed to provide identical pharmacological properties compared to the original drugs. The three-dimensional structure of molecules is an important missing link in resolving this problem. Solid-state NMR provides a complementary view to decipher and characterize the structure of pharmaceutical molecules in the solid-form. Vipin Agarwal and colleagues have been developing new solid-state NMR experiments to decipher structural information. Most notably amongst them being the ability to directly measure 1H-1H distances.

H. Science Communication and Public Outreach:

Reported by Anusheela Chatterjee: The science communication efforts at the TIFR Hyderabad Science Media Centre have taken the form of talks (including Sawaal-Jawaab: Conversations on Science), articles, videos, illustrations, press releases and social media engagement. Research highlights tailored for a non-expert audience have been reported. In addition to research communication, a range of community outreach events were organised to promote an appreciation of fundamental sciences among the public. Highlights have been mentioned below:

- TIFR Hyderabad Science Fair: On 19 September, 2022 TIFR Hyderabad (TIFRH) organized a science fair for school students to commemorate the foundation day of the institute. The science fair included games, a science theatre, an exhibition of science themed art and guided tours of labs. Around 250 students and teachers from schools in Hyderabad attended the event. TIFRH members arranged a host of fun games and activities - a demonstration of the properties of liquid nitrogen, introduction to the concept of pH through a riddle based game, a science pictionary, explanation of surface tension through a paper boat race where liquid soap is used to steer the boats due to surface tension, explanation of the periodic properties of elements through a puzzle based game and demonstration of the properties of non-Newtonian fluids. In the activity about non-Newtonian fluids, the students had a lot of fun walking, running, and jumping on cornflour slurry to understand what a non-Newtonian fluid is. The students visited TIFRH labs. A science art exhibition was also organized with art works contributed by TIFRH members. The visitors saw fruit flies and crystals under the microscope as well. The programme ended with ‘Spikes Up’, a science play about how vaccines work. Research scholars dressed up as different organs, objects, virus particles and immune cells and put on a fun show with references to popular culture.
- India Science Festival: TIFR Hyderabad was a knowledge partner of the India Science Fest 2023 that was being held at the Hyderabad Public School. This edition of the festival began with a pre-fest event at the TIFR Hyderabad campus ‘Be a Scientist for a Day’ on January 07, 2023. During this pre-fest event, we welcomed school students from Jawahar Navodaya Vidyalayas in Medak, Vizianagaram, Yanam, Rangareddy and Karimnagar. Members of the public also attended this event. The visitors were assigned mentors in TIFR Hyderabad and they spent the entire day getting introduced to the research at TIFRH and conducting experiments such as sorting fruit flies, building a spectrometer and running gels.

On January 21 and 22, 2023, TIFR Hyderabad put up a booth at the festival venue Hyderabad Public School) and interacted with science enthusiasts from all across the city. The booth included exhibits and games explaining fundamental science concepts and a microscopy station to look at fruit flies. The institute had put up a booth on both days of the festival conducting science themed games and demos, conveying basic concepts as well as highlighting the research from the institute. In addition to the institute's participation in the science booths, Pranav R Shirhatti conducted a session at the India Science Festival to demonstrate spectroscopy and its basic concepts.

Apart from the above, faculty members at TIFR Hyderabad have participated in the following outreach programmes:

Pranav R Shirhatti**:**

- Delivered a popular science lecture for undergraduate students at the NIUS workshop conducted by HBCSE, Mumbai

Chaitanya Kumar Suddapalli:

- Contributing toward optics-themed outreach activities through initiation and support of ongoing efforts to start a student chapter at TIFR Hyderabad

Kabir Ramola:

- Mentor and Speaker for National Initiative on Undergraduate Science - 19th Batch, HBCSE (2022-2023)

Manish Jaiswal:

- Radio & TV Programs: Youtube: https://www.youtube.com/watch?v=BsmbnIjwa1E

Neurodegeneration and mitochondrial dysfunction by Dr. Manish Jaiswal
Video made by: Longevity India

- Invited to give a lecture in an induction course for newly recruited PGT-Biology teachers training program at Navodaya Leadership Institute, Jawahar Navodaya Vidyalaya Nallagandla, Hyderabad. 06.06.2022 to 17.06.2022.
- Invited to conduct a workshop for school teachers by Vigyan Pratibha teachers workshop, University of Calicut, 21–23 September 2022, Co-organized by: Department of Mathematics, University of Calicut and The Institute of Mathematical Sciences (IMSc), Chennai. https://www.imsc.res.in/outreach/vpchennai/TWKer2022.html

Anand Vaidya:

- Resource Person at the Vigyan Pratibha Teachers Workshop, Institute of Mathematical Sciences (IMS), Chennai, August 2022.
- Resource Person at the Vigyan Pratibha Teachers Workshop, University of Calicut, Kozhikode, October 2022.
- Resouce Generation Camp for the Vigyan Pratibha Program, Homi Bhabha Centre for Science Education (HBCSE), Mumbai, Novemebr 2022

(Teachers groups worked with were mainly from Kendriya Vidyala Sangathan system and the Jawahar Navodaya Vidyalaya)

Vipin Agarwal:

- Basic Introduction to Solid-State NMR Spectroscopy, India EMBO Lecture course: Structure, dynamics and interactions in biomolecular systems using NMR spectroscopy, 12-16 December, IISER Behrampur, Orissa (2022). This is a workshop organized by the European molecular Biology lab for encouraging the use of NMR technique amongst biology and life-science students in India.
- A tutorial was delivered at a national workshop highlighting the basics NMR spectroscopy in deciphering structures of small molecules and proteins. A part of the lecture also focused on how NMR could be used, as quantitative tool is study protein-ligand and protein-protein interactions at an atomic level.
- National Workshop on NMR Spectroscopy, Organised by Kerala NMR Society, 16th-18th September, Kottayam, Kerala (2022) (Talk)