1. Research Highlights

- Assaying DNA damage responses and gene expression at a single cell level with tools of microscopy: (Aprotim Mazumder)
  Chromatin packaging can affect DNA damage responses (DDR), and the group investigates this in living and fixed cells. Very different dynamics of heterochromatin proteins HP1α and HP1β at sites of laser induced double strand breaks was observed. HP1α is enhanced at sites of DNA damage, compared to HP1β, which is found on expanding chromatin away from the damage spot. Further, in a collaborative study with the Notani lab at NCBS, Aprotim Mazumder's group is investigating the cell-to-cell variability of enhancer-mediated gene expression. In a developmental context, they used single molecule RNA detection to investigate the links between EGFR signaling and cell differentiation/proliferation. They 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.
  [All collaborators in the work: Krishanu Ray, Manish Jaiswal, Dimple Notani, Aprotim Mazumder]

- Molecular organization of auditory ribbon synapses: (Adish Dani)
  Adish Dani's group has investigated the ultrastructure of Inner ear hair cell ribbon synapses in the mouse cochlea using single molecule fluorescence nanoscopy. Their results indicate that glutamate receptor organization on the post-synaptic membrane is influenced by the release or non-release of glutamate neurotransmitter. Glutamate receptor ion channels seems to undergo a postnatal developmental transition from a planar distribution to a doughnut shaped structure around the onset of hearing. This developmental transition is abolished in a mouse model of congenital deafness that lacks glutamate in synaptic vesicles of cochlear cells. Furthermore, the group has observed receptor nano-domains within the post-synaptic membrane. These experiments provide the framework to further investigate synaptopathy associated with loud-noise induced deafness.
  [All collaborators in the work: Gayatri Chandran, Devakinandan GVS, Vishnu Krishnan, Mark Rutherford (Washington University School of Medicine, St Louis, USA) and Adish Dani]

- Unravelling the molecular basis of mitochondrial cristae dynamics (Anand T. Vaidya)
  Mitochondria are small sacs or organelles in almost all of our cells, which generate the energy for the cells. In many of these diseases, the internal structure of mitochondria, called

the cristae, is altered. Mitochondrial cristae are formed and maintained by the MICOS complex, which is made up of several proteins. Many of these proteins have been purified and key regions of these proteins that control their interactions have been identified. These interactions are central to the efficient functioning of the MICOS complex and the mitochondria. The molecular and details of these interactions will be discovered soon.

- Synthesis and reactivity of NHC-coordinated phosphinidene oxide: (Anukul Jana)
  Anukul Jana and colleagues reported the synthesis of an N-heterocyclic carbene (NHC)-stabilised phosphinidene oxide by the controlled oxygenation of a phosphinidene at ambient conditions. NHC-Stabilised phosphinidene oxide further oxygenated to a phosphinidene dioxide. The stoichiometric reduction of a phosphinidene oxide with KC8 resembles the pinacol coupling reaction – the reduction of a carbonyl compound. Notably, 160 years after the pinacol coupling reaction was discovered, this research demonstrates that phosphinidene oxide can also be coupled reductively in a similar manner. The convenient synthesis of the NHC-stabilised phosphinidene oxide and its utilisation as a novel synthon for different phosphorus compounds with a wide range of oxidation states facilitates, opens up a new landscape in phosphorus chemistry.
  [All collaborators in the work: Debabrata Dhara, Ramapada Dolai, Hemant Rawat, Anukul Jana ; Pradeep Kumar Pal, U. Deva Priyakumar (International Institute of Information Technology, Hyderabad) ; Nicolas Chrysochos, Benedict J. Elvers, Carola Schulzke (Universität Greifswald, Greifswald, Germany) ; Ivo Krummenacher, Holger Braunschweig (Institute of Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron (ICB), Julius-Maximilians-Universität Würzburg, Germany) ; Vadapalli Chandrasekhar (Indian Institute of Technology Kanpur)]

- Chemical imaging and therapeutic modulation of microglial cells in the brain: (Aneesh T. Veetil)
  Aneesh T. Veetil's group will develop small-molecule-based fluorescent imaging probes that are targetable to specific types of cells in the brain (e.g. microglia). They will employ such newly synthesized probes to image microglial cells in health and disease conditions. In a separate research direction, the group will chemically synthesize and screen biologically active molecules to modulate functionally aberrant microglial cells.

- Direct simulation of oligosaccharide recognition by Galectin: (Jagannath Mondal)
  The recognition of carbohydrates by lectins plays key roles in diverse cellular processes such as cellular adhesion, proliferation, and apoptosis, which makes it a therapeutic target of significance against cancers. One of the most functionally active lectins, galectin-3 is distinctively known for its specific binding affinity toward β-galactoside. However, despite the prevalence of high-resolution crystallographic structures, the mechanistic basis and more significantly, the dynamic process underlying carbohydrate recognition by galectin-3 are currently elusive. Jagannath Mondal's group has used computer to simulate the full carbohydrate recognition pathway by the galectin-3. The recognition pathway catches the carbohydrate in its act of binding the designated binding site and identifies the key intermediates en route the pathways.
  [All collaborators in the group: Jaya Krishna Koneru, Suman Sinha and Jagannath Mondal]

- Theoretical Characterization of Athermal Materials: (Kabir Ramola)

Kabir Ramola's group has been developing theoretical techniques to characterize amorphous solids such as granular materials and structural glasses: materials that simultaneously exhibit properties of liquids as well as solids. Recently, they developed a perturbation expansion for athermal systems that allows an exact determination of displacement fields away from the crystalline state as a response to microscopic disorder. They also derived exact results for correlations in the displacement fields in near-crystalline athermal systems in two dimensions. Additionally, they showed that the low-frequency regime of the density of states of structural glass formers is crucially sensitive to the stress-ensemble from which the configurations are sampled. These studies pave the way for a more microscopic characterization of ubiquitous amorphous materials.

- Pf-AMA1 expression, refolding and functional characterization: (Kalyaneswar Mandal)
  A simple yet effective protocol for the expression of an essential *P. falciparum* protein, apical membrane antigen 1 (AMA1), from *E. coli* had been developed. The PfAMA1 is a potential vaccine candidate and an essential target for the development of novel peptide or protein therapeutics. Presence of multiple cysteine residues in the AMA1 protein sequence makes the refolding of the protein with correct disulfide combinations after expression in bacteria extremely challenging. The modified refolding method using step-wise dialysis technique reported by Kalyaneswar Mandal and colleagues was scalable and highly reproducible. The functional activity of the refolded protein was evaluated by the binding of the PfAMA1 protein with a known inhibitory peptide PfRON2 ectodomain using surface plasmon resonance (SPR) and isothermal titration calorimetry (ITC).
  [All collaborators in this work: A Biswas, S Raran-Kurussi, A Narayan, A Kar, PC Mashurabad (UoH), MK Bhattacharyya (UoH) and K Mandal]

- Study of protein aggregation using single molecule techniques: (Kanchan Garai)
  Amyloid aggregation of proteins is involved in the pathology of several diseases including Alzheimer's and Parkinson's disease. Kanchan Garai's group has built a superresolution microscope to monitor the growth of the protein amyloids in real time. The technique enables the measurement of rates of elongation and secondary nucleation of the growth of the fibrils of amyloid beta peptide. Furthermore, it has helped observe the effect of various important factors such as lipids and apolipoprotein E on the growth of the amyloids. For example, the researchers find that apoE is a strong inhibitor of aggregation of amyloid beta. On the other hand, lipids do not appear to affect the elongation of the fibrils but it could alter the pathway of aggregation by promoting morphologically different protein-lipid condensates. The amyloid-lipid condensates may play important roles in the pathology of Alzheimer's disease.
  [All collaborators in this work: Kanchan Garai, Tuomas Knowles (University of Cambridge, United kingdom) and Sara Linse (Lund University, Sweden)]

- In-depth analysis of anisotropic magnetoconductance in Bi_2Se_3 thin films with electron–electron interaction corrections: (Karthik V. Raman)
  A combination of out-of-plane (OOP) and in-plane (IP) magnetoconductance (MC) study in topological insulators (TI) is often used as an experimental technique to probe weak anti-localization (WAL) response of the topological surface states (TSSs). However, in addition to the above WAL response, weak localization (WL) contribution from conducting bulk states are also known to coexist and contribute to the overall MC; a study that has so far received

limited attention. Karthik V. Raman's group has performed experiments to accurately extract the above WL contribution by systematically analyzing the temperature and magnetic field dependency of conductivity in Bi2Se3 films. For accurate analysis, they quantify the contribution of electron–electron interactions to the measured MC which is often ignored in the WAL studies. Moreover, their work show that the WAL effect arising from the TSSs with finite penetration depth, for OOP and IP magnetic field can together explain the anisotropic magnetoconductance (AMC) and, thus, the investigated AMC study can serve as a useful technique to probe the parameters like phase coherence length and penetration depth that characterise the TSSs in 3D TIs.
[All collaborators in this work: Satyaki Sasmal, Joynarayan Mukherjee, Dhavala Suri and Karthik V. Raman]

- Correlations using recycle delays (CURD): (Kaustubh R. Mote)
  Pulse sequences used to record multidimensional datasets consist of 2 major sections: (I) the section where tailored pulse seqeunces are applied to obtain the desired spectra and (ii) the section where one waits for the magnetization to re-equilibrate so that the experiment can be repeated to increase the signal. Typically, the second part is 1-2 orders of magnitude longer, taking up the bulk of the experimental time. With CURD (Correlations using recycle delays), Kaustubh R. Mote's group has devised a method to use this waiting period as a part of coherent spin dynamics and record multiple experiments that will be directly beneficial to speed up data collection in proteins.
  [All collaborators in this work: Pravin P. Taware, Sreejith Raran-Kurussi, Kaustubh R. Mote]

- Regulation of mitochondrial dynamics and biogenesis: (Manish Jaiswal)
  A genetic screen was performed to identify the regulators of mitochondrial dynamics and biogenesis in *Drosophila*. The screen revealed that mitochondrial stress induces mitochondrial biogenesis and degradation of Mitofusin, a mitochondrial fusion protein. It was predicted that the reduced levels of Mitofusin can suppress fusion of defective mitochondria to maintain healthy mitochondrial pool. Similarly, induction of mitochondrial biogenesis was predicted to be a compensatory response to meet cellular metabolic needs under stress. Further, it was found that the Mitofusin degradation under stress is achieved by the coordinated activates of PINK, PARK and Ben proteins. Mutation in any of these was found to suppress stress induced Mitofusin degradation, which resulted in altered mitochondrial size and subsequently retinal degeneration.
  [All collaborators in this work: Rajit Naraynan, Tarana Anand, Aravind H, Manish Jaiswal
  Priyanka Pande (CCMB), Sonal N Jaiswal (CCMB)]

- Chirp dependence in Electron acceleration from micro-droplets (M. Krishnamurthy)
  M. Krishnamurthy's group explored the role of pulse width on the Two plasmon decay mechanism of electron acceleration from liquid droplets. Increasing the pulse duration to ps for the laser pulses of same energy decreased the ability of accelerate electrons in droplets. But importantly going from 40fs to about 200fs, has very marginal change in electron acceleration. Furthermore, there is no dramatic chirp dependence in electron acceleration in this regime.
  [All collaborators in this work: Sonali Khanna, Ram Gopal, M. Krishnamurthy]

- Role of SNARE family genes in store-operated calcium influx: (Monika Vig)

Identification and characterization of the genes involved in activating store-operated calcium entry (SOCE) via calcium release activated calcium (CRAC) ion channels has been a major goal of Monika Vig's lab. It was hypothesized that SNAP receptor (SNARE) family proteins play an unconventional, direct role in SOCE. Building on earlier collaborative work with Adish Dani's lab (eLife 2013, MBoC 2016, eLife 2017), a genetic screen was performed to identify the specific SNARE family genes involved in regulating SOCE. The screen was highly successful and several genes were identified that significantly regulate SOCE. Interestingly, most of the genes identified in this screen regulate a rare immunological disease called Familial Hemophagocytic Lymphohistiocytosis (FHLH) in human patients, the mechanistic basis of which remains unestablished. Characterization of each of these genes and their specific mutations found in human FHLH patients has been planned, which will also benefit human patients with immunodeficiency and autoimmunity.
[All collaborators in this work: Monika Vig and Adish Dani]

- Phase transitions in magnets in random fields: (Mustansir Barma)
  Random disorder has interesting effects on phase transitions in cooperative magnetic systems comprised of a fully-coupled set of spins, each of which points along a circle. Spins tend to align in the same direction, but fixed fields with random orientations for each spin tend to destroy alignment. The resulting phase boundary was determined exactly. With random magnetic fields, the boundary was shown to include a multi-critical point, separating a part with continuous transitions from one with first order transitions. By contrast, with random crystal fields, the transition stayed continuous throughout. In general, the shape of the boundary depends on the distribution of random fields, but was shown not to change for a family of distributions of disorder which reduce the symmetry of the circle to four-fold symmetry.
  [All collaborators in this work: Sumedha (NISER, Bhubaneswar) and Mustansir Barma]

- Doping of soft semiconductors: (Pabitra K. Nayak)
  Organic semiconductors are an emerging class of semiconductors. It is essential to increase their charge carrying capacity for their usage in highly efficient optoelectronic devices. Inexpensive and commercially available chemicals like dimethyl sulfoxide (DMSO) and Hydrobromic acid (HBr) which form an adduct were used as effective p-dopants for a range of organic semiconductors. These adduct-based dopants are compatible with both solution and vapour-phase processing. The use of the dopants in metal halide perovskite solar cells, organic thin-film transistors, and organic light-emitting diodes resulted in improved performances in devices. This new type of dopant opens up new ways of doping of organic semiconductors.
  [All collaborators in this work: Nobuya Sakai (University of Oxford), Ross Warren (University of Oxford), Fengyu Zhang (Princeton University), Simantini Nayak (CSIR_IMMT, Bhubaneswar),Junliang Liu (University of Oxford),Sameer V. Kesava (University of Oxford), Yen-Hung Lin, (University of Oxford), Himansu S. Biswal, (NISER-Bhubaneswar), Xin Lin (Princeton University), Chris Grovenor, (University of Oxford), Tadas Malinauskas, (Kaunas University of Technology), Aniruddha Basu (KAUST, Saudi Arabia), Thomas D. Anthopoulos (KAUST, Saudi Arabia), Vytautas Getautis (Kaunas University of Technology), Antoine Kahn (Princeton University), Moritz Riede (University of Oxford), Pabitra K. Nayak (TIFR Hyderabad), Henry J. Snaith (University of Oxford)]

- Neutral atom scattering based mapping of atomically thin layers: (Pranav R. Shirhatti)
  Atom scattering from surfaces is known to be extremely sensitive to the structure and the nature of interaction among them. Taking advantage of this high sensitivity, Pranav R. Shirhatti and colleagues have demonstrated that up to single atomic thin layers (MoS_2 on SiO_2) can be imaged using atom scattering based microscopy methods. By varying the incidence energy of the incident He and Kr atoms, the contrast of the images change, providing deeper insight into the atom surface scattering processes responsible for contrast generation.
  [All collaborators in this work: Pranav R. Shirhatti, T. N. Narayanan, Geetika Bhardwaj]

- Solid-state NMR: Principles and applications: (P. K. Madhu)
  P. K. Madhu and colleagues has been advancing the feasibility of solid-state NMR spectroscopy method to a wide range of materials of high relevance. These are battery-related materials comprising electrodes and electrolytes and perovskites for efficient and stable solar cells. Spectroscopic tools, hence, would be put into applications in energy harvesting and storage. Solid-state NMR methods have been refined for better sensitivity and resolution. This translates into obtaining spectra with narrower line-widths and elucidating structure and dynamics in materials.
  [All collaborators in this work: P. K. Madhu, P. K. Nayak, T. N. Narayanan, V. Arunachalam]

- Zero-Ultra Low field NMR with Atomic Magnetometers: (G. Rajalakshmi)
  Zero-to-ultra-low-field nuclear magnetic resonance (ZULF NMR) is an emerging technique to study samples under conditions dominated by internal spin interactions. In the absence of the truncating effects of Zeeman interaction, the NMR signal is determined by local internal interactions alone. G. Rajalakshmi and P. K. Madhu have led a research effort to develop an atomic magnetometer to detect these low frequency NMR signals. Spin evolution in ultra-low-field regime for various systems is studied theoretically and the expected NMR signals are evaluated for solid samples. A system to measure these signals is being built in the lab.
  [All collaborators in this work: G. Rajalakshmi, P. K. Madhu, George Kurian K. K.]

- Turbulence in active matter: (Prasad Perlekar)
  The theory of active matter — systems whose constituents convert a sustained supply of fuel into movement—is the framework of choice for understanding the collective behavior of motile particles. Like condensed matter in general, active systems display many types of order and operate in a variety of dynamical regimes. Prasad Perlekar's group is interested to investigate how groups of motile organisms in a bulk fluid medium, spontaneously organize into a flock in which their tail-to-head vectors on average point in a common direction. In now-standard terminology, the researchers consider polar, wet active matter, described by a vector order parameter characterizing the degree and direction of common orientation and movement. In a recent paper, the group has shown that in such system inertia can stabilize aligned states against small perturbations. Their investigation revealed that the interplay of activity and inertia leads to a novel non-equilibrium transition from defect-ridden turbulence to noisy but aligned flocks. The group will continue the ongoing investigations in this direction.

- Developing methods to explore the free energy surface of proteins and capturing structures of minor folding intermediates: (Pramodh Vallurupalli)

Despite the critical role that protein conformational dynamics plays in protein function, folding, misfolding and aggregation, studying the different conformational states that the protein molecule samples as it crisscrosses its free energy surface (FES) remains a challenge. Pramodh Vallurupalli's group is developing CEST based NMR methods to explore the free energy surface of the protein by detecting processes with rates varying from 10 s-1 to 10,000 s-1 and populations as low as 0.1%. In a recent study, the group showed that the FF domain from HYPA/FBP11 folds on a rugged free energy surface with multiple folding intermediates and multiple folding paths. They are attempting to obtain the structures of some of these sparsely populated intermediates to obtain an unprecedented view of protein folding.

- Digital chemistry: (Raghunathan Ramakrishnan)
  Raghunathan Ramakrishnan's group works on several aspects of digital chemistry, an emerging discipline focussing on data-driven discoveries. The group has developed machine learning models to predict UV/Vis and 1H and 13C NMR spectra of organic molecules. To develop these models, some of the large datasets ever reported have been generated ab initio. All the data generated for these projects have been made publicly available to enhance the visibility of the works.

- Photophysical properties of metal-organic framework thin film: (Ritesh Haldar)
  Metal-organic frameworks (MOFs) are extensively studied for gas storage, separation and catalytic applications, because MOFs feature high surface area with easily tunable structure. With regard to advanced applications, e.g. in area of optoelectronics, drug delivery, hierarchical structure of MOFs (MOF-on-MOF) are important to realize. Structural complexity in the hierarchical MOFs is high and hence methodologies that can allow straight forward fabrication of complex structures are important. In this context, Ritesh Haldar and colleagues have shown that it is possible to fabricate multilayer heteroepitaxial MOF structures and carry out spatioselective photoreaction at the MOF-MOF interface. Using this spatioselective photoreaction, it was possible to delaminate 2D MOF layers with well-defined thickness.

- Theory and simulation for equilibrium glassy dynamics in cellular Potts model of confluent biological tissue: (Saroj K. Nandi)
  Glassy dynamics in a confluent cellular monolayer is fundamental in morphogenesis, wound healing, bronchial asthma, and many others. Therefore, a detailed theoretical framework for such a system is essential. Saroj K. Nandi's group combined analytical theory and simulations of a simple confluent model, where cells are treated as polygons and have developed a comprehensive theoretical framework. Their study elucidates the crucial role of geometric constraints in bringing about two distinct regimes in the dynamics, as the target perimeter varies. The distinctive interaction potential arising from the perimeter constraint in such systems leads to the unusual sub-Arrhenius relaxation. Comparison with existing experiments shows that this theory captures the basic phenomenology of glassy dynamics in a biological system.
  [All collaborators in this work: Souvik Sadhukhan and Saroj Kumar Nandi]

- Physics of active glasses - new frameworks to understand its properties: (Smarajit Karmakar)
  Activity-driven glassy dynamics, while ubiquitous in collective cell migration, intracellular transport, dynamics in bacterial and ant colonies, etc, also extends the scope and extent of

the as-yet mysterious physics of glass transition. Smarajit Karmakar's group's recent studies on active glasses lead to a new discovery that active glasses are very different from their equilibrium counterparts and the physics cannot be described by simple effective temperature like quasi-equilibrium scenario. The group proved this by computing, for the first time, the static and dynamic length scale in these systems and tested some of the extensions of the equilibrium theories for active glasses. This also created a platform which allowed them to study various other dynamical and mechanical properties of these systems. One such is the discovery of an additional peak in four-point dynamic susceptibility which is uniquely related to the total degree of activity in these systems. This helped the researchers to propose a new method to measure the degree of activity in active glassy systems especially in experiments where measurement of activity may not be directly available as it is generated in the system via various chemical and biological processes like ATP consumptions etc. Finally, in another recent work, this group was able to show that activity leads to brittle-like failure in these systems which is completely counterintuitive and mysterious from the existing concepts of equilibrium systems.

- Defects in graphene oxide and Au: (Soumya Ghosh)
  Different physical and chemical properties are enhanced upon introducing defects. Oxidation of graphene to graphene oxide (GO) constitutes an important step in functionalization of graphene. The oxidation process, however, introduces several non-6-membered rings in the structure making it non-planar that can be considered as defects. The extent of defects has been characterized by the percentage of non-sp2 carbon (pnsc) atoms in the structure. In this study, the Soumya Ghosh's group considered the defect polygons as 3D polygons and computed their area. Although both pnsc and the relative area of the defect polygons show similar trend during the simulated evolution of graphene to GO, the non-sp2 carbons atoms are not exclusive to the defect sites. The researchers are currently investigating how the relative area of the defect sites can be correlated with other experimental markers for identifying defects, e.g. signature Raman shifts. In a second project simulation models for grain boundaries between single crystalline Au planes are being generated in order to find the correlation between grain boundary energies and different macroscopic and microscopic structural parameters.
  [All collaborators in this work: Sownyak Mondal, Nandana Pal Chowdhury and Soumya Ghosh]

- Comparison of fusion Tags for protein expression: (Sreejith Raran-Kurussi, Deepa B., Kaustubh R. Mote)
  This study reports large-scale protein production driven by a kanamycin-resistant Gateway expression vector based on a spider protein. Sreejith Raran-Kurussi is working towards technology development to promote better expression and purification of recombinant proteins.

- Atomic layer heterostructures and their interactions with light: (T. N. Narayanan)
  Atomic layers (two dimensional layers) such as MoS_2 are known for their high surface area and intriguing properties such as high light matter interaction volume. However, one of the issues with these layers is their ambient stability. Recent work from T. N. Narayanan's group shows that this can be addressed by encapsulating MoS_2 with a fluorographene (FG) layer, where the synergistic interactions of MoS_2 and FG can expand the photosensitivity wavelength range of the heterostructure based photodetector. This also provides

extraordinary stability to the device. Similar heterostructures are also shown for their applicability in Solar Batteries, a battery which can be directly charged by sunlight, where they form a type II band structure. The researchers from this group constructed a solar battery with the type II like heterostructure of MoS_2 and MoO_3. This work also reports an enhanced performance in light assisted charging and discharging for longer cycles.
[All collaborators in this work: Amar Kumar, Pallavi Thakur, Rahul Sharma, Krishna Rani Sahoo, T. N. Narayanan, Soumya Sankar, V.P.S. Awana (NPL, New Delhi), Mahesh Kumar (NPL, New Delhi), Prince Sharma (NPL, New Delhi), Anand P. B. (Rice University, USA), and P M Ajayan (Rice University, USA).]

- Mechanobiology of Collective Cellular Dynamics: An Interdisciplinary Inquiry: (Tamal Das)
  An interdisciplinary approach to biological research was taken in Tamal Das's group, combining biophysics with cell biology. With this approach, both general principles and the molecular mechanisms underlying the cellular ability to maintain the tissue integrity, synchronize cell motions, and organize intracellular structures were elucidated. It was revealed that cell and tissue mechanics played critical roles in these processes. For example, it was discovered that a mechanical mismatch between normal and cancer cells caused a competitive elimination of the latter from the epithelium. Interestingly, pathological stiffening of extracellular matrix abrogated this fundamental epithelial defense against cancer, explaining the strong susceptibility of fibrotic tissue to cancer. In addition, how cell and tissue mechanics regulated the large-scale coherent organization of intracellular structures during collective cell dynamics was elucidated. To this end, a new process of actin cytoskeleton-mediated Golgi dispersion was discovered, and this process was found exclusive to collective cell migration.
  [All collaborators in this work: Shilpa P. Pothapragada, Purnati Khuntia, Praver Gupta, Rituraj Marwaha, Simran Rawal, and Tamal Das]

- Molecular Magnets: (V. Chandrasekhar)
  V. Chandrasekhar's group has been working on molecular systems that can function as magnets. These include polynuclear complexes containing transition metal ions or lanthanide metal ions or heterometallic complexes containing 3d/4f metal ions. They have also been focusing on systems that contain a single metal ion either, lanthanide or transition metal ion. These are called as mononuclear single molecule magnets.
  [All collaborators in this work: J. Acharya (IIT Kanpur), Saurabh Singh (IIT Hyderabad), A. Swain (IIT Bombay), A. Chakraborty, V. Kumar (IIT Kanpur), P. Kumar (IIT Kanpur), J. F. Gonzalez, (Univ Rennes), O. Cador (Univ Rennes), F. Pointillart (Univ Rennes), G. Rajaraman, (IIT Bombay), V. Chandrasekhar]

- Solid state NMR method developments to address problems in structural biology: (Vipin Agarwal)
  Vipin Agarwal's group has been involved in the following research efforts: (a) Designing symmetry sequence for selective proton-proton recoupling with experimental polarization transfer efficiencies on the order of 50-60%. (b) Design of an experiment that increase the density of structural restraints by a factor of 3 and improve protein structure determination by solid-state NMR. (c) Design of multiple quantum and recoupling experiments that provide better recoupling and improved characterization of small molecules at slow and fast MAS. (d) Expressing segmentally labelled a-synuclein protein samples and preparing liquid-liquid phase separated samples and oligomers.

- Effect of ficoll crowder on the structure and stability of Chemotaxis Y protein in the presence and absence of magnesium: (Krishnarao Doddapuneni)

Macromolecular crowding has been studied widely on different proteins. However, the interaction between the crowder and proteins at a molecular level has not been defined. In collaboration with V. Ramakrishna lab at BITS Hyderabad, Krishnarao Doddapuneni is probing the molecular interactions of Chemotaxis Y (CheY) (a bacterial regulatory protein) with a ficoll crowder. CheY changes its conformation in the presence of magnesium. The structural conformations and stability of CheY protein-ficoll crowder complex was studied in the presence of magnesium and absence of magnesium. These studies were done using different biophysical methods like circular dichroism, florescence, and nuclear magnetic resonance spectroscopy. This results shows that while the structure and thermal stability of CheY remain largely unperturbed in the presence of ficoll, the presence of magnesium alters the confirmation of the protein. The results from biophysical approaches, when combined with 2D NMR data, reveal that the rearranged conformation prompted by magnesium provides an altered surface for the crowder to interact differently and destabilize the protein.

Other highlights:

- Sreejith Raran-Kurussi has actively participated in the research design and execution of the NMR group's entire protein production efforts. He has prepared over 100 new plasmids and re-engineered many existing protein expression constructs in the laboratory to suit large-scale protein production. The fusion proteins and other molecular biology tools like proteases for tag removal developed by Sreejith Raran-Kurussi are used by several research groups around the globe.
- In addition to regular LC MS spectra recordings and other biophysical instruments assistance (for different research groups), Deepa S. has been involved in the following research activities in Kanchan Garai's research group: (a) Purification of recombinant Abeta 42 WT/ abeta 42 Cys and labeling with Atto 425/TMR dye. (b) Purification of Apo E3 WT protein. (c) Optimization trials to prevent Abeta 42 aggregation during purification and to improve yield. (d) Guiding research scholars for labelled(15N 13C Abeta40, 15N labelled Apo E) /unlabelled protein purification (TEV protease, Alpha synuclein WT, Tau cysless fusion protein)
- High Performance Computing facility is managed by Kalyan Kumar N. In this reporting period, he upgraded the existing HPC Data center for accommodating new HPC clusters (2 GPU based HPC Clusters for Jagannath Mondal). Suman Saurav is overseeing web and network administration, some of which include upgradation of firewall and ISP bandwidths. The IT services in the institute are jointly handled by Kalyan Kumar N. and Suman Saurav. They have been addressing specific computing and IT requirements for existing and upcoming research labs and facilities on campus.
- In addition to maintaining the TIFRH Animal facility, Gopalakrishna R. has been working towards standardising the mouse *(Mus musculus)* sperm cryopreservation procedure in the facility. IAEC approvals were secured for the establishment of sperm cryopreservation protocol.
- Aathif Ahmed Odam is involved in reverse engineering and customized design, development and documentation of ultra high vacuum systems and cryogenic systems.
- Krishnarao Doddapuneni is maintaining the National Facility for High-Field NMR facility at TIFRH. He is also involved in the efforts to upgrade the facility.

1. Staff Strength: (Academic, Students/PDF/JRF, Scientific & Technical, Admin. & Aux)

Faculty	: 28 + 3 (Emeritus -1, Visiting Faculty-2)
Research Scholars	: 123
Junior Research Fellows	: 17
Senior Research Fellows	: 04
Post-doctoral Fellows	: 31
Project Associates	: 08 (External Project_EPIC)
EPIC Consultants	: 03 (External Project_EPIC)
Visiting Students	: 16
Visiting Fellows	: 04
Short Term Visitors	: 02
Scientific Staff	: 17
Technical Staff	: 14 (03 out sourced out of 14)
Admin Staff	: 25 (01 outsourced out of 25)
Part Time Legal Consultant	: 01
Part Time Medical Officer	: 01
Auxiliary Staff	:75 (74 outsourced out of 75 (Security-16, HK-13, Work Assistant-01, Lab Assistant-01, Canteen-12, HVAC-06, Gardener-02, Electrical & Fire safety-09, Plumbing Staff: 04, STP operator-01, Carpenter-02, Driver-07)

3. Awards/Distinctions:

No.	Name of the Awardee	Scope (National/ International)	Name of the Award	Awarding / Electing Body	Date
1.	Aneesh T. Veetil	International	DBT-Wellcome Trust Intermediate Fellowship (3.5 crore INR for 5 years)	India Alliance (DBT-Wellcome Trust)	January 2022
2.	Kabir Ramola	National	INSA Award for Young Scientists	INSA	October 2021
3.	Pabitra K. Nayak	National	Swarna Jayanti Fellowship	Department of Science and Technology	May 2021

4.	Pabitra K. Nayak	National	Editorial Board Member	Indian Journal of pure and applied Physics	December 2021
5.	Mrinal Srivastava	National	Ramalingaswami Fellowship	DBT	August 2021
6.	Smarajit Karmakar	International	Humboldt Fellowship for experienced Researcher	Alexander von Humboldt Foundation, Germany	August 2021
7.	T. N. Narayanan	National	Infosys-TIFR Fellowship (2021).	Infosys-TIFR	September 2021
8.	Vipin Agarwal	National	Executive council member	National Magnetic Resonance Society of India	2020-2023

4. Number of students graduated: (Ph.D. / M.Sc.)

PhD - 12
MSc - 5 (as part of Integrated MSc - PhD)

5. Publications:

1) Torabi, S.F., Chen, Y.L., Zhang, K., Wang, J., DeGregorio, S.J., Vaidya, A.T., Su, Z., Pabit, S.A., Chiu, W., Pollack, L. and Steitz, J.A., 2021. Structural analyses of an RNA stability element interacting with poly (A). *Proceedings of the National Academy of Sciences*, 118(14), p.e2026656118.
2) Dwivedi, A., Padala, C., Kumari, A., Khumukcham, S.S., Penugurti, V., Ghosh, S., Mazumder, A., Goffin, V. and Manavathi, B., 2022. Hematopoietic PBX-interacting protein is a novel regulator of mammary epithelial cell differentiation. *The FEBS Journal*, 289(6), pp.1575-1590.
3) Pasnuri, N., Jaiswal, M., Ray, K. and Mazumder, A., 2021. Buffered EGFR signaling regulated by spitz to argos expression ratio is critical for patterning the Drosophila eye. *bioRxiv*.
4) Kumar, R., Richter, S., Maity, S., Sarkar, P., Chrysochos, N., Pati, S.K., Ghosh, P., Schulzke, C. and Jana, A., 2022. Activation of O 2 across a C (sp 3)–C (sp 3) bond. *Chemical Communications*, 58(19), pp.3122-3125.
5) Maiti, A., Sobottka, S., Chandra, S., Jana, D., Ravat, P., Sarkar, B. and Jana, A., 2021. Diamidocarbene-Based Thiele and Tschitschibabin Hydrocarbons: Carbonyl Functionalized Kekulé Diradicaloids. *The Journal of Organic Chemistry*, *86*(23), pp.16464-16472.
6) Kumar, R., Chandra, S., Nayak, M.K., Singha Hazari, A., Elvers, B.J., Schulzke, C., Sarkar, B. and Jana, A., 2021. An Air-Stable Alkene-Derived Organic Radical Cation. *ACS omega*, *7*(1), pp.837-843.
7) Kundu, A., Chandra, S., Mandal, D., Neuman, N.I., Mahata, A., Anga, S., Rawat, H., Pal, S., Schulzke, C., Sarkar, B. and Chandrasekhar, V., 2021. Twisted Push–Pull Alkenes Bearing

Geminal Cyclicdiamino and Difluoroaryl Substituents. *The Journal of Organic Chemistry*, *86*(18), pp.12683-12692.

8) Dhara, D., Pal, P.K., Dolai, R., Chrysochos, N., Rawat, H., Elvers, B.J., Krummenacher, I., Braunschweig, H., Schulzke, C., Chandrasekhar, V. and Priyakumar, U.D., 2021. Synthesis and reactivity of NHC-coordinated phosphinidene oxide. *Chemical Communications*, *57*(75), pp.9546-9549.
9) Mahata, A., Chrysochos, N., Krummenacher, I., Chandra, S., Braunschweig, H., Schulzke, C., Sarkar, B., Yildiz, C.B. and Jana, A., 2021. α, α′-Diamino-p-tetrafluoroquinodimethane: Stability of One-and Two-Electron Oxidized Species and Fixation of Molecular Oxygen. *The Journal of Organic Chemistry*, *86*(15), pp.10467-10473.
10) Veetil. A. T., and Krishnan, Y., 'Chemical Dissection and Reprogramming of Biological Systems, (H. Hang, M. Pratt, J. Prescher, eds., Wiley-VCH). DNA function, synthesis, and engineering. *Advanced Chemical Biology*. (*in print*, 2021).
11) Koneru, J.K., Sinha, S. and Mondal, J., 2021. Molecular dynamics simulations elucidate oligosaccharide recognition pathways by galectin-3 at atomic resolution. *Journal of Biological Chemistry*, *297*(5).
12) Mukhopadhyay, S., Bera, S.C. and Ramola, K., 2022. Observation of two-step aggregation kinetics of amyloid-β proteins from fractal analysis. *Physical Biology*, *19*(4), p.046001.
13) Krishnan, V.V., Ramola, K. and Karmakar, S., 2022. Universal non-Debye low-frequency vibrations in sheared amorphous solids. *Soft Matter*, *18*(17), pp.3395-3402.
14) Acharya, P., Das, D. and Ramola, K., 2021. Disorder perturbation expansion for athermal crystals. *Physical Review E*, *104*(3), p.034608.
15) Das, D., Acharya, P. and Ramola, K., 2021. Long-range correlations in pinned athermal networks. *Physical Review E*, *104*(1), p.014503.
16) Biswas A, Raran-Kurussi S, Narayan A, Kar A, Mashurabad PC, Bhattacharyya, MK and Mandal K* (2021) Efficient refolding and functional characterization of PfAMA1(DI+DII) expressed in E. coli. *Biochemistry and Biophysics Reports* 26:100950.
17) Sarkar, A. and Mandal, K., 2021. Repurposing an antiviral drug against SARS-CoV-2 main protease. *Angewandte Chemie International Edition*, *60*(44), pp.23492-23494
18) Das A, Yadav A, Gupta M, Purushotham R, Terse VL, Vishvakarma V, Singh S, Nandi T, Banerjee A, Mandal K, Gosavi S, Das R, Ainavarapu SRK* and Maiti S* (2021) Rational design of protein- specific folding modifiers. *Journal of the American Chemical Society* 143: 18766-18776.
19) Thakur, P., Mannuthodikayil, J., Kalita, G., Mandal, K. and Narayanan, T.N., 2021. In situ surface modification of bulk or nano materials by cytochrome-c for active hydrogen evolution catalysis. *Materials Chemistry Frontiers*, *5*(3), pp.1295-1300.
20) Zimmermann, M.R., Bera, S.C., Meisl, G., Dasadhikari, S., Ghosh, S., Linse, S., Garai, K. and Knowles, T.P., 2021. Mechanism of secondary nucleation at the single fibril level from direct observations of Aβ42 aggregation. Journal of the American Chemical Society, 143(40), pp.16621-16629.
21) Bhardwaj, A., Prasad P, S., Raman, K.V. and Suri, D., 2021. Observation of planar Hall effect in topological insulator—Bi2Te3. *Applied Physics Letters*, 118(24), p.241901.
22) Sasmal, S., Mukherjee, J., Suri, D. and Raman, K.V., 2021. In-depth analysis of anisotropic magnetoconductance in Bi2Se3 thin films with electron–electron interaction corrections. *Journal of Physics: Condensed Matter,* 33(46), p.465601.
23) Jha, A., Mote, K.R., Chandra, S., Madhu, P.K. and Dasgupta, J., 2021. Photoactive Anthraquinone-Based Host–Guest Assembly for Long-Lived Charge Separation. *The Journal of Physical Chemistry C*, *125*(20), pp.10891-10900.

24) Raran-Kurussi, S., Sharwanlal, S.B., Balasubramanian, D. and Mote, K.R., 2022. A comparison between MBP-and NT* as N-terminal fusion partner for recombinant protein production in E. coli. *Protein Expression and Purification*, *189*, p.105991.
25) Taware, P.P., Raran-Kurussi, S., Mote, K.R., 2022. CURD: a Single-Shot Strategy to Obtain Assignments and Distance Restraints for Proteins Using Solid-State MAS NMR Spectroscopy. J. Phys. Chem. B 126, 3269–3275.
26) Ahlawat, S., Mote, K.R., Lakomek, N.A. and Agarwal, V., 2022. Solid-State NMR: Methods for Biological Solids. *Chemical Reviews*, *122*(10), pp.9643-9737.
27) Datta, S. and Jaiswal, M., 2021. Mitochondrial calcium at the synapse. *Mitochondrion*, *59*, pp.135-153.
28) Jha, J., Rajeev, R., Trivikram, T.M., Gopal, R. and Krishnamurthy, M., 2021. A non-uniform charging scheme to decipher charge state propensities measured in nano-cluster ionization. *The European Physical Journal Special Topics*, *230*(23), pp.3997-4009.
29) Ramanagoudr-Bhojappa, R., Miao, Y. and Vig, M., 2021. High affinity associations with α-SNAP enable calcium entry via Orai1 channels. *Plos one*, *16*(10), p.e0258670.
30) Sumedha and Barma, M., 2022. Solution of the random field XY magnet on a fully connected graph. Journal of Physics A: Mathematical and Theoretical, 55(9), p.095001.
31) Sumedha and Barma, M., 2022. Phase transitions in X Y models with randomly oriented crystal fields. *Physical Review E*, *105*(2), p.024111.
32) Kotak, J.D. and Barma, M., 2022. Bias induced drift and trapping on random combs and the Bethe lattice: Fluctuation regime and first order phase transitions. *Physica A: Statistical Mechanics and its Applications*, *597*, p.127311.s
33) Sakai, N., Warren, R., Zhang, F., Nayak, S., Liu, J., Kesava, S.V., Lin, Y.H., Biswal, H.S., Lin, X., Grovenor, C. and Malinauskas, T., 2021. Adduct-based p-doping of organic semiconductors. *Nature Materials*, *20*(9), pp.1248-1254.
34) Sterling, C.M., Kamal, C., Man, G.J., Nayak, P.K., Simonov, K.A., Svanstrom, S., García-Fernández, A., Huthwelker, T., Cappel, U.B., Butorin, S.M. and Rensmo, H., 2021. Sensitivity of Nitrogen K-Edge X-ray Absorption to Halide Substitution and Thermal Fluctuations in Methylammonium Lead-Halide Perovskites. *The Journal of Physical Chemistry C*, *125*(15), pp.8360-8368.
35) Nayak, P.K., 2021. RESEARCH HIGHLIGHTS: Perovskites.
36) Man, G.J., Sterling, C.M., Kamal, C., Simonov, K.A., Svanström, S., Acharya, J., Johansson, F.O., Giangrisostomi, E., Ovsyannikov, R., Huthwelker, T. and Butorin, S.M., 2021. Electronic coupling between the unoccupied states of the organic and inorganic sublattices of methylammonium lead iodide: A hybrid organic-inorganic perovskite single crystal. *Physical Review B*, *104*(4), p.L041302.
37) Zohar, A., Kulbak, M., Turren-Cruz, S.H., Nayak, P.K., Kama, A., Hagfeldt, A., Snaith, H.J., Hodes, G. and Cahen, D., 2021. In Operando, Photovoltaic, and Microscopic Evaluation of Recombination Centers in Halide Perovskite-Based Solar Cells. *ACS applied materials & interfaces*.
38) Ganesh, N., Schutt, K., Nayak, P.K., Snaith, H.J. and Narayan, K.S., 2021. 2D position-sensitive hybrid-perovskite detectors. *ACS Applied Materials & Interfaces*, *13*(45), pp.54527-54535.
39) Cohen, A., Brenner, T.M., Klarbring, J., Sharma, R., Fabini, D.H., Korobko, R., Nayak, P.K., Hellman, O. and Yaffe, O., 2022. Diverging Expressions of Anharmonicity in Halide Perovskites. *Advanced Materials*, *34*(14), p.2107932.
40) Bhardwaj, G., Sahoo, K.R., Sharma, R., Nath, P. and Shirhatti, P.R., 2022. Neutral-atom-scattering-based mapping of atomically thin layers. Physical Review A, 105(2), p.022828.

41) Singh, S.K., Kumar, A. and Shirhatti, P.R., 2022. A simple and low-cost setup for part per billion level frequency stabilization and characterization of red He-Ne laser. arXiv preprint arXiv:2202.09577.
42) Taur, A., Singh, S.K. and Shirhatti, P.R., 2021. Identifying signatures of thermal and non-thermal reaction pathways in plasmon induced H2+ D2 exchange reaction.
43) Kurian, K.G., Madhu, P.K. and Rajalakshmi, G., 2022. Solid-state NMR signals at zero-to-ultra-low-field. *Journal of Magnetic Resonance Open*, *10*, p.100049.
44) Fritzsch, J., Korn, A., Surendran, D., Krueger, M., Scheidt, H.A., Mote, K.R., Madhu, P.K., Maiti, S. and Huster, D., 2021. Probing the Influence of Single-Site Mutations in the Central Cross-β Region of Amyloid β (1–40) Peptides. *Biomolecules*, *11*(12), p.1848.
45) Ivanov, K.L., Mote, K.R., Ernst, M., Equbal, A. and Madhu, P.K., 2021. Floquet theory in magnetic resonance: Formalism and applications. *Progress in Nuclear Magnetic Resonance Spectroscopy*, *126*, pp.17-58.
46) Kupče, Ē., Mote, K.R., Webb, A., Madhu, P.K. and Claridge, T.D., 2021. Multiplexing experiments in NMR and multi-nuclear MRI. *Progress in Nuclear Magnetic Resonance Spectroscopy*, *124*, pp.1-56.
47) Rana, N. and Perlekar, P., 2022. Phase ordering, topological defects, and turbulence in the three-dimensional incompressible Toner-Tu equation. *Physical Review E*, *105*(3), p.L032603.
48) Ramadugu, R., Perlekar, P. and Govindarajan, R., 2022. Surface tension as the destabiliser of a vortical interface. *Journal of Fluid Mechanics*, *936*.
49) Pandey, V., Mitra, D. and Perlekar, P., 2022. Turbulence modulation in buoyancy-driven bubbly flows. *Journal of Fluid Mechanics*, *932*.
50) Bhatnagar, A., Pandey, V., Perlekar, P. and Mitra, D., 2022. Rate of formation of caustics in heavy particles advected by turbulence. *Philosophical Transactions of the Royal Society A*, *380*(2219), p.20210086.
51) Popli, P., Perlekar, P. and Sengupta, S., 2021. Pattern stabilization in swarms of programmable active matter: A probe for turbulence at large length scales. *Physical Review E*, *104*(3), p.L032601.
52) Chatterjee, R., Rana, N., Simha, R.A., Perlekar, P. and Ramaswamy, S., 2021. Inertia drives a flocking phase transition in viscous active fluids. *Physical Review X*, *11*(3), p.031063.
53) Meibohm, J., Pandey, V., Bhatnagar, A., Gustavsson, K., Mitra, D., Perlekar, P. and Mehlig, B., 2021. Paths to caustic formation in turbulent aerosols. *Physical Review Fluids*, *6*(6), p.L062302.
54) Tiwari, V.P., Toyama, Y., De, D., Kay, L.E. and Vallurupalli, P., 2021. The A39G FF domain folds on a volcano-shaped free energy surface via separate pathways. *Proceedings of the National Academy of Sciences*, *118*(46), p.e2115113118.
55) Gupta, A., Chakraborty, S., Ghosh, D. and Ramakrishnan, R., 2021. Data-driven modeling of S0⟶ S1 excitation energy in the BODIPY chemical space: High-throughput computation, quantum machine learning, and inverse design. *The Journal of Chemical Physics*, *155*(24), p.244102.
56) Gupta, A., Chakraborty, S. and Ramakrishnan, R., 2021. Revving up 13C NMR shielding predictions across chemical space: Benchmarks for atoms-in-molecules kernel machine learning with new data for 134 kilo molecules. Machine Learning: Science and Technology, 2(3), p.035010.
57) Hassan, Z.M., Weidler, P.G., Nefedov, A., Luo, Y., Heißler, S., Tsotsalas, M., Haldar, R. and Wöll, C., 2022. Spectroscopic Investigation of Bianthryl-Based Metal–Organic Framework Thin Films and Their Photoinduced Topotactic Transformation. *Advanced Materials Interfaces*, *9*(13), p.2102441.

58) Mostaghimi, M., Rêgo, C.R., Haldar, R., Wöll, C., Wenzel, W. and Kozlowska, M., 2022. Automated Virtual Design of Organic Semiconductors Based on Metal-Organic Frameworks. Front. Mater. 9: 840644. doi: 10.3389/fmats.
59) Liu, X., Mazel, A., Marschner, S., Fu, Z., Muth, M., Kirschhöfer, F., Brenner-Weiss, G., Bräse, S., Diring, S., Odobel, F. and Haldar, R., 2021. Photoinduced Delamination of Metal–Organic Framework Thin Films by Spatioselective Generation of Reactive Oxygen Species. *ACS Applied Materials & Interfaces*, *13*(48), pp.57768-57773.
60) Karmakar, S., Ghosh, A., Prasad, K., Rahimi, F.A., Rambabu, D., Haldar, R. and Maji, T.K., 2021. Multicolour lanthanide (III) porous 1D coordination polymers: tunable wide spectrum emission and efficient Cu II sensing. *Dalton Transactions*, *50*(37), pp.13002-13011.
61) Nefedov, A., Haldar, R., Xu, Z., Kühner, H., Hofmann, D., Goll, D., Sapotta, B., Hecht, S., Krstić, M., Rockstuhl, C. and Wenzel, W., 2021. Avoiding the Center-Symmetry Trap: Programmed Assembly of Dipolar Precursors into Porous, Crystalline Molecular Thin Films. *Advanced Materials*, *33*(35), p.2103287.
62) Laha, S., Haldar, R., Dwarkanath, N., Bonakala, S., Sharma, A., Hazra, A., Balasubramanian, S. and Maji, T.K., 2021. A Dynamic Chemical Clip in Supramolecular Framework for Sorting Alkylaromatic Isomers using Thermodynamic and Kinetic Preferences. *Angewandte Chemie International Edition*, *60*(36), pp.19921-19927.
63) Nandi, S.K., Karmakar, S., Interplay of Disorder and Fluctuations in Physical Systems – Celebrating the Science of Giorgio Parisi, Physics Nobel Laureate 2021, *Physics News*, 54, 4 (2021).
64) Sadhukhan, S. and Nandi, S.K., 2021. Theory and simulation for equilibrium glassy dynamics in cellular Potts model of confluent biological tissue. *Physical Review E*, *103*(6), p.062403.
65) Nandi, S.K., Heidenreich, M., Levy, E.D. and Safran, S.A., 2019. Interacting multivalent molecules: affinity and valence impact the extent and symmetry of phase separation. *arXiv preprint arXiv:1910.11193*.
66) Paul, K., Nandi, S.K. and Karmakar, S., 2021. Non-trivial activity dependence of static length scale and critical tests of active random first-order transition theory. *arXiv preprint arXiv:2111.09829*.
67) Sadhukhan, S. and Nandi, S.K., 2021. The origin of universal cell shape variability in a confluent epithelial monolayer. *arXiv preprint arXiv:2108.03884*.
68) Paul, K., Nandi, S.K. and Karmakar, S., 2021. Dynamic heterogeneity in active glass-forming liquids is qualitatively different compared to its equilibrium behaviour. *arXiv preprint arXiv:2105.12702*.
69) Mandal, R., Nandi, S.K., Dasgupta, C., Sollich, P. and Gov, N.S., 2021. The random first-order transition theory of active glass in the high-activity regime. *arXiv preprint arXiv:2102.07519*.
70) Tah, I., Mutneja, A. and Karmakar, S., 2021. Understanding slow and heterogeneous dynamics in model supercooled glass-forming liquids. *ACS omega*, *6*(11), pp.7229-7239.
71) Mutneja, A. and Karmakar, S., 2021. Translational dynamics of a rod-like probe in supercooled liquids: an experimentally realizable method to study Stokes–Einstein breakdown, dynamic heterogeneity, and amorphous order. *Soft Matter*, *17*(23), pp.5738-5746.
72) Adhikari, M., Karmakar, S. and Sastry, S., 2021. Spatial Dimensionality Dependence of Heterogeneity, Breakdown of the Stokes–Einstein Relation, and Fragility of a Model Glass-Forming Liquid. *The Journal of Physical Chemistry B*, *125*(36), pp.10232-10239.
73) Mutneja, A. and Karmakar, S., 2021. Probing Dynamic Heterogeneity and Amorphous Order Using Rotational Dynamics of Rodlike Particles in Supercooled Liquids. *Physical Review Applied*, *16*(3), p.034022.

74) Nandi, U.K., Patel, P., Moid, M., Nandi, M.K., Sengupta, S., Karmakar, S., Maiti, P.K., Dasgupta, C. and Maitra Bhattacharyya, S., 2022. Thermodynamics and its correlation with dynamics in a mean-field model and pinned systems: A comparative study using two different methods of entropy calculation. *The Journal of Chemical Physics*, *156*(1), p.014503.
75) Karmakar, S., 2022. Physics of Disordered Systems. *Resonance*, *27*(1), pp.19-38.
76) Tah, I. and Karmakar, S., 2022. Kinetic fragility directly correlates with the many-body static amorphous order in glass-forming liquids. *Physical Review Materials*, *6*(3), p.035601.
77) Adhikari, M., Karmakar, S. and Sastry, S., 2022. Dependence of the glass transition and jamming densities on spatial dimension. *arXiv preprint arXiv:2204.02936*.
78) Dey, S., Mutneja, A. and Karmakar, S., 2021. Enhanced Phonon Peak in Four-point Dynamic Susceptibility in the Supercooled Active Glass-forming Liquids. *arXiv preprint arXiv:2112.15574*.
79) Krishnan, V.V., Ramola, K. and Karmakar, S., 2021. Annealing effects of multidirectional oscillatory shear in model glass formers. *arXiv preprint arXiv:2112.07412*.
80) Dattani, U.A., Karmakar, S. and Chaudhuri, P., 2021. Universal mechanical instabilities in the energy landscape of amorphous solids: evidence from athermal quasistatic expansion. *arXiv preprint arXiv:2109.06902*.
81) Das, R., Bhowmik, B.P., Puthirath, A.B., Narayanan, T.N. and Karmakar, S., 2021. Soft-Pinning: Experimental Validation of Static Correlations in Supercooled Molecular Glass-forming Liquids. *arXiv preprint arXiv:2106.06325*.
82) Kumar, S., Bawari, S., Narayanaru, S., Narayanan, T.N. and Satpati, A.K., 2021. Enhanced Electron Transfer Kinetics of Covalent Carbon Nanotube Junctions. *The Journal of Physical Chemistry C*, *126*(1), pp.239-245.
83) Biroju, R.K., Harrison, P., Theis, W., Rees, N.V., Sharma, R., Narayanan, T.N. and Hahm, M.G., 2021. Pt147 nanoclusters soft-landed on WS2 nanosheets for catalysis and energy harvesting. *ACS Applied Nano Materials*, *4*(12), pp.13140-13148. [Cover Page]
84) Bawari, S., Nair, M.N., Mondal, J. and Narayanan, T.N., 2021. Elucidating the Mechanism of Nitrogen Doping in Graphene Oxide: Structural Evolution of Dopants and the Role of Oxygen. *The Journal of Physical Chemistry C*, *125*(41), pp.22547-22553.
85) Guha, A., Sharma, R., Sahoo, K.R., Puthirath, A.B., Shyaga, N., Ajayan, P.M. and Narayanan, T.N., 2021. One-Dimensional Hollow Structures of 2 O-PdS2 Decorated Carbon for Water Electrolysis. *ACS Applied Energy Materials*, *4*(9), pp.8715-8720.
86) Stavrou, M., Papadakis, I., Bawari, S., Narayanan, T.N. and Couris, S., 2021. Giant broadband (450–2300 nm) optical limiting and enhancement of the nonlinear optical response of some Graphenes by defect engineering. *The Journal of Physical Chemistry C*, *125*(29), pp.16075-16085.
87) Sahoo, K.R., Sharma, R., Bawari, S., Vivek, S., Rastogi, P.K., Nair, S.S., Grage, S.L. and Narayanan, T.N., 2021. Room-temperature ferromagnetic wide bandgap semiconducting fluorinated Graphene-hBN vertical heterostructures. *Materials Today Physics*, *21*, p.100547.
88) Facile Water Oxidation by Dinuclear Mixed-Valent CoIII/CoII Complexes: Role of Coordinated Water, Atanu Dey,* Anku Guha, Vierandra Kumar, Sumit Bawari, **T. N.Narayanan***, and V Chandrasekhar*, **Dalton Transactions** 50, 14257-14263 (2021).
89) Sharma, P., Sharma, R., Awana, V.P.S., Narayanan, T.N., Gupta, B.K., Vashistha, N., Tyagi, L. and Kumar, M., 2021. Low-temperature ultrafast optical probing of topological bismuth selenide. *Journal of Alloys and Compounds*, *886*, p.161235.
90) Kumar, A., Thakur, P., Sharma, R., Puthirath, A.B., Ajayan, P.M. and Narayanan, T.N., 2021. Photo Rechargeable Li-Ion Batteries Using Nanorod Heterostructure Electrodes. *Small*, *17*(51), p.2105029.

91) Sharma, R., Sharma, P., Sahoo, K.R., Sankar, S., Awana, V.P.S., Kumar, M. and Narayanan, T.N., 2021. Giant photoresponsivity of transfer free grown fluorographene–MoS2 heterostructured ultra-stable transistors. *Materials Today*, *50*, pp.69-78. [Cover Page]
92) Thakur, P., Alam, K., Roy, A., Downing, C., Nicolosi, V., Sen, P. and Narayanan, T.N., 2021. Extending the Cyclability of Alkaline Zinc–Air Batteries: Synergistic Roles of Li+ and K+ Ions in Electrodics. *ACS Applied Materials & Interfaces*, *13*(28), pp.33112-33122.
93) Pothapragada, S.P., Gupta, P., Mukherjee, S. and Das, T., 2022. Matrix mechanics regulates epithelial defence against cancer by tuning dynamic localization of filamin. *Nature communications*, *13*(1), pp.1-12.
94) Khuntia, P., Rawal, S., Marwaha, R. and **Das**,T., Actin-driven Golgi apparatus dispersal during collective migration of epithelial cells, *PNAS,* 2022. (In Press)
95) Ahlawat, S., Mote, K.R., Raran-Kurussi, S. and Agarwal, V., 2022. Mechanism of selective polarization exchange amongst chemically similar and distinct protons during weak rf irradiation at fast magic angle spinning. Journal of Magnetic Resonance, p.107236.
96) Duong, N.T., Agarwal, V. and Nishiyama, Y., 2022. Separating an overlapped 1H peak and identifying its 1H-1H correlations with the use of single-channel 1H solid-state NMR at fast MAS. *Solid State Nuclear Magnetic Resonance*, *117*, p.101774.
97) Zhang, R., Agarwal, V. and Nishiyama, Y., 2021. Proton triple-quantum solid-state NMR spectroscopy at slow MAS~ 10 kHz. *Journal of Magnetic Resonance Open*, *8*, p.100020.
98) Nishiyama, Y., Agarwal, V. and Zhang, R., 2021. Efficient symmetry-based γ-encoded DQ recoupling sequences for suppression of t1-noise in solid-state NMR spectroscopy at fast MAS. *Solid State Nuclear Magnetic Resonance*, *114*, p.101734.
99) Potnuru, L.R., Duong, N.T., Sasank, B., Raran-Kurussi, S., Nishiyama, Y. and Agarwal, V., 2021. Selective 1H–1H recoupling via symmetry sequences in fully protonated samples at fast magic angle spinning. *Journal of Magnetic Resonance*, *328*, p.107004.
100) Chandrasekhar, V., Thirumoorthi, R., Dhanwant, K. and Saini, A., 2021. Photophysical studies of organostannoxane supported hexafluorophore assemblies. *Inorganica Chimica Acta*, *522*, p.120378.
101) Biswal, P., Samser, S., Nayak, P., Chandrasekhar, V. and Venkatasubbaiah, K., 2021. Cobalt (II) porphyrin-Mediated Selective Synthesis of 1, 5-Diketones via an Interrupted-Borrowing Hydrogen Strategy Using Methanol as a C1 Source. *The Journal of Organic Chemistry*, *86*(9), pp.6744-6754.
102) Kumar, P., Biswas, S., Swain, A., Acharya, J., Kumar, V., Kalita, P., Gonzalez, J.F., Cador, O., Pointillart, F., Rajaraman, G. and Chandrasekhar, V., 2021. Azide-Coordination in Homometallic Dinuclear Lanthanide (III) Complexes Containing Nonequivalent Lanthanide Metal Ions: Zero-Field SMM Behavior in the Dysprosium Analogue. *Inorganic Chemistry*, *60*(12), pp.8530-8545.
103) Kalita, P., Goura, J., Nayak, P., Colacio, E. and Chandrasekhar, V., 2021. Octanuclear {Ln8} complexes: magneto-caloric effect in the {Gd8} analogue. *Journal of Chemical Sciences*, *133*(3), pp.1-11.
104) Karmakar, H., Anga, S., Panda, T.K. and Chandrasekhar, V., 2022. Aluminium alkyl complexes supported by imino-phosphanamide ligand as precursors for catalytic guanylation reactions of carbodiimides. *RSC advances*, *12*(8), pp.4501-4509.
105) Chandrasekhar, V., 2022. Lanthanide and transition metal complexes as molecular magnets. *Dalton Transactions*, *51*(11), pp.4199-4201.
106) Biswal, P., Samser, S., Meher, S.K., Chandrasekhar, V. and Venkatasubbaiah, K., 2022. Palladium-Catalyzed Synthesis of α-Methyl Ketones from Allylic Alcohols and Methanol. *Advanced Synthesis & Catalysis*, *364*(2), pp.413-419.

6. Conferences organized:

- Feb 09 – 11, 2022 - ICONS4 meeting on hyperpolarisation and solution-state NMR (Online)

7. Invited lectures given:

- Aprotim Mazumder, Scientific seminar at the DBS Annual Talks, TIFR Mumbai (December, 2021)

- Kalyaneswar Mandal, 'HTS in drug discover and engineering', AICTE-ATAL Sponsored National FDP on "Artificial Intelligence in Drug Design and Development: Current and Future Perspectives" (virtual mode), Acharya & BM Reddy College of Pharmacy, Bengaluru, (November 22- 26, 2021) [Invited Talk as Resource Person]

- Kalyaneswar Mandal, Invited Talk:'Blocking red blood cell invasion by malaria parasites using D-proteins', 6th Annual Conference and Symposium on the Challenges in Chemical Biology (SCCB-2021) organized by Chemical Biology Society, India (virtual mode), Indian Institute of Chemical Biology, Kolkata, (September 16-17, 2021)

- Kanchan Garai, FCS 2021 organized by IISER Thiruvananthapuram and RGCB Thiruvananthapuram, (November 29 - December 04, 2021)

- Manish Jaiswal, 'Recent Advances in Neurodegenerative disease Research', CSIR-Indian Institute of Chemical Biology in connection with the 39th Annual Conference of the Indian Academy of Neurosciences (https://www.iiserkol.ac.in/~ian2021/), webinar, (November 16, 2021)

- Manish Jaiswal, 'Regulation of mitochondrial fusion under stress', Celebrating 20 years of establishment of the Department of Biological Sciences and Bioengineering at IIT Kanpur, https://sites.google.com/view/bsbeat20/schedule/day, (September 28, 2021)

- Manish Jaiswal, Invited talk at Glendale International School, Hyderabad to discuss viruses with school students on Virus appreciation day, Webinar, (October 4, 2021)

- Manish Jaiswal, Invited talk: 'Cellular Therapies: An Update, By Department of Transfusion Medicine', Haematology & Central Research Lab, ESIC Medical College Hospital, Hyderabad, (November, 27, 2021)

- Manish Jaiswal, Invited lecture: 'How to perform large scale genetic screens'. Event Course on Methods in Drosophila Biology, organized by C-CAMP, Bangalore, (April 20, 2021)

- Mustansir Barma, 'Dynamics of Extremes', 87th Annual Meeting of the Indian Academy of Sciences Virtual meeting, (November 2021)

- Mustansir Barma, 'Coarsening and Extremes, Current trends in non-equilibrium physics', organized by Jawaharlal Nehru University, New Delhi, Virtual meeting, (November 2021)

- Mustansir Barma, 'Coarsening in Aggregation-Fragmentation Systems: Condensates and Extremes', Statistical Physics: Recent developments and future directions, organized by ICTS-TIFR, Bengaluru, Virtual meeting, (February 2022)

- Pabitra K. Nayak, Invited Talk: 'Abduct-based p-doping of Organic Semiconductors', Emerging Low Dimensional Materials, Jain University, Bangalore, (September 2021)

- Pabitra K. Nayak, Invited Talk: 'Adduct based doping of Organic semiconductor', Asia-Pacific Conference on Condensed Matter Physics 2021, South Korea, (December 2021)

- Pabitra K. Nayak, Invited Talk: 'Doping of organic semiconductor, Recent Trends in Chemical Sciences (RETICS-2021)', Sambalpur University, (December 2021)

- Pabitra K. Nayak, Keynote Lecture: 'Doping of soft semiconductors for optoelectronics, Advances in Energy, Environment for Sustainable Development (AEESD 2022)'- SOA University Bhubaneswar, (January 2022)

- Pranav R. Shirhatti, Invited lecture, Elementary process in surface chemistry, NIUS Workshop, organized by HBCSE, (December 2021)

- P. K. Madhu, 'Heteronuclear spin decoupling for all (commercial) MAS frequencies: Methods and recipes', Experimental NMR Conference (ENC), Virtual, Asilomar, USA, (March 29-31, 2021)

- P. K. Madhu, 'Echo-based schemes in solid-state NMR for resolution and geometry parameters', Leipzig Spin Resonance Colloquium, Virtual, Univ. of Leipzig, Germany, (May 19, 2021)

- P. K. Madhu, 'Echo-based schemes in solid-state NMR for decoupling and recoupling', Magnetic Resonance Seminar, Weizmann Institute of Science, Israel, Virtual, (June 20, 2021).

- P. K. Madhu, 'Recoupling schemes in solid-state NMR in a new light', ISMAR-APNMR-NMRSJ-SEST 2021, Virtual, Osaka, Japan, (August 22-27, 2021).

- P. K. Madhu, 'Molecular structure and dynamics through the NMR looking glass', NMR-HR MS Workshop, NIIT Calicut, Virtual, (September 21-26, 2021)

- P. K. Madhu, 'Molecular structure and dynamics through the NMR looking glass', Spectroscopic Techniques: A Tool in Contemporary Research, Bangalore, (January 10-14, 2022)

- P. K. Madhu, 'Site-specific probes for Biomolecules: Recoupling and faster acquisition', ENS, Paris, (March 24, 2022)

- Prasad Perlekar, 'Turbulence modulation in buoyancy driven bubbly flows, Conference: BIRS Workshop: Stochastic Approaches to Turbulence in Hydrodynamical Equations: New Challenges at the Mathematics-Physics Interface', Canada, (February 28- March 03, 2022)

- Ritesh Haldar, 'Exciton Coupling and Diffusion Anisotropy in Surface-anchored MOF Thin Films', Invited talk in ePorMat-2021, jointly organized by NISER Bhubaneswar, VIT Chennai and IIT Jammu, Online, (August, 2021)

- T. N. Narayanan, 'Engineering Interfaces Towards Catalysis', Indo-US SPARC Workshop on India Mission for Green Hydrogen and Go Electric", IIT-Mandi, (March 17, 2022) [Invited Talk]

- T. N. Narayanan, 'Science for Sustainable Future: Importance of Integrated Approaches in Science & Technology', Dr. PAARIVENDHAR RESEARCH COLLOQUIUM (DPRC) SRM Institute of Science & Technology, Chennai, March 25, 2022. [Keynote Lecture]

- T. N. Narayanan, 'Science for Sustainable Future', National Day Celebration 2022, MA College Kothamangalam, Kerala, (March 01, 2022) [Invited Lecture]

- T. N. Narayanan, 'Engineering Interfaces Towards Catalysis', Indo-Norwegian International Online Conference on "Functional materials for energy, environment and biomedical applications" "FARAON - 2022", February 2, 2022. [Invited Talk]

- T. N. Narayanan, 'Electrochemistry as a tool for evaluating materials for energy', Online Symposium on "Advanced Techniques on Nanomaterials Characterisation", CSIR-AMPRI, Bhopal, (January 27, 2022) [Invited Lecture]

- T. N. Narayanan, 'Interface & Morphological Engineering of Two-Dimensional Materials for Energy Devices', E-Workshop on 'Advanced Spectroscopy for Emerging Materials", CSIR-NPL, New Delhi (December 22, 2021) [Invited Talk]

- T. N. Narayanan, 'Synergistic Effects of Atomic Interfaces in Enhanced Device Performance', Materials Research Society of India-AGM 2021, (December 20, 2021) [Invited Talk]

- T. N. Narayanan, 'Role of Interface Engineering in Emerging Energy Technology', International Conference: Advanced Materials for Better Tomorrow (AMBT 2021), IIT Banaras Hindu University, India (July 13, 2021) [Invited (online) Talk]

- T. N. Narayanan, 'Physics of Nanomaterials: Applications in Energy and Electronics', FDP on "Functional Materials for Energy, Environment and Healthcare", School of Materials Science and Engineering, National Institute of Technology Calicut, (June 21, 2021) [Invited Lecture]

- Vipin Agarwal, 'Mapping interatomic 1H-1H distances at fast MAS', 27th National Magnetic Resonance Society Meeting, IIT Gandhinagar, (March 6-9, 2022) [Online Talk]

- Vipin Agarwal, 'Mapping interatomic 1H-1H distances/correlations at fast MAS', Griffin Zoominar Series organized by Prof. Griffin at MIT, (November 30, 2021) [Online Talk]

- Vipin Agarwal, 'Different approaches to generate 1H-1H structural restraints for pharmaceuticals and biomolecules at fast MAS', ISMAR-APNMR-NMRSJ-SEST, (August 22-27, 2021) [Online Talk]

8. New initiatives:

- Transcriptional diversity of the Vomeronasal neuroepithelium (Devakinandan GVS and Adish Dani): The vomeronasal organ (VNO), part of the vertebrate accessory olfactory system, is an important sensory system model to understand how pheromones and kairomones elicit innate behaviors such as mating, aggression, predator avoidance. In similarity with the main olfactory system, VNO neurons regenerate throughout life, but they express completely different and diverse families of GPCRs, MHC and other signaling components. Here, Dani's group used a single cell transcriptional profiling approach to identify the diversity of cell types in the VNO sensory epithelium. Their results identify genes that help define neuronal sub-populations as well as cell types such as glia and supporting cells, that throw light on the function of various cell types within the organ. (Manuscript in preparation.)

- Aprotim Mazumder's group is 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 FRET-based 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 may also be dependent of cytoskeletal elements. FRET-based sensing of tension across the nuclear envelope is now standardized. Newer approaches are being developed for investigating ultraviolet damage dynamics in cells and for high throughput microscopic image acquisition.

- Chemical biology strategies for targeted modulation of microglial cells (Pikaso Latua, Aneesh T Veetil): In this project, the researchers will develop new chemical reagents using organic synthesis to target microglial cells in the brain.

- Synthesis of photoactivatable lipids for cell biology investigations (Sushreeta Chakraborty, Aneesh T Veetil): In this work, the researchers will photocage lipids that are involved in immune signaling to spatiotemporally release them within the cells to investigate their role in cell signaling.

- Microbial protease for targeted protein degradation of signaling proteins (Payal Chuabey, Aneesh T Veetil): In this project, the researchers will develop stable proteases as therapeutics to degrade proteins that are causing inflammation.

- The major ongoing project in Kanchan Garai's lab is the study of liquid-liquid phase separation (LLPS) of amyloid proteins. LLPS of proteins and protein-RNA complexes have been found to be involved in various functions *in vivo*. Additionally, it is also found to be involved in aberrant aggregation of proteins such as microtubule associated protein tau. Currently, Kanchan Garai's lab is using their home built superresolution microscope to study formation of LLPS of tau in presence of RNA. They expect that real-time high resolution monitoring of LLPS will provide important insights into the mechanism of the amyloid formation of tau *in vivo*.

- Membrane protein biophysics (Pravin Taware, Sudarshan Bandopadhyay, and Kaustubh R Mote): This is studying active transport across membranes using mitochondrial and bacterial carrier proteins. This work uses a combination of biophysical tools such as development of new protein expression tools, new assays to detect transport, and solid- and solution state NMR spectrosocpy tools to study dynamics in proteins.

- Actin Dynamics (Pragyan Parida and Kaustubh R Mote): This group is studying how actin polymerization and depolymerization is orchestrated at the molecular level using a combination of solid-state NMR spectroscopy and biophysical experiments.

- REDOR in dynamics and distances (Mrudula Nikam and Kaustubh R Mote): This group is developing solid-state NMR methods to study dynamics in proteins as well as measure multiple nm-scale distances in proteins.

- Development of fly models to study the biological function of Polyphosphates in multicellular organisms (Manish Jaiswal): Manish Jaiswal's group has initiated a new line of work to identify the biological processes that are regulated by polyphosphates in multicellular organisms. The group has, so far, developed tools to detect and manipulate polyphosphate in *Drosophila*. They have also found that the depletion of polyphosphate does not affect development of *Drosophila* but causes an accelerated aging. This suggests that polyphosphate may have some homeostatic function in multicellular organism. Currently, the lab is trying to identify the cellular and physiological defects induced by polyphosphate depletion that causes accelerated aging. This work will help in identifying cellular and physiological function of polyphosphates that are required for healthy ageing.

- M. Krishnamurthy's group shall be setting up new experiments to measure energy resolved electron angular dirstributions to further unravel the physics of relativitistic electron acceleration with non-relativistic laser intensities. This group would also be developing new methods to collimate the electron beams from the laser acceleration in micro-droplets and improvise the ability of generated pencil like beams with narrow divergence.

- Spin-locking of half-integer quadrupole spins in solid-state NMR (P. K. Madhu): Spin-locking quadrupole spins is difficult in solid-state NMR under magic-angle spinning. The phenomenon is important to transfer magnetisation to and from such spins which in turn sheds information on coupling and connectivity. P. K. Madhu's group will be looking at amplitude- and/or phase-modulated pulses to achieve this. Such an approach will be beneficial to materials science applications as many

such materials have NMR active quadrupole nuclei. The researchers will also try to understand the phenomenon from a Floquet theoretical point of view and in terms of energy-level crossings.

- Materials science applications (P. K. Madhu): P. K. Madhu and colleagues will be expanding their current work to a range of materials, both batteries-related and perovskites for solar cell applications, making use of modern solid-state NMR methods and zero-field NMR techniques. A combination of both of these is expected to give structural and dynamic information of the materials and a quick diagnostic aspect as well. Zero-field NMR methods will be expanded to solid materials to probe interactions such as scalar, dipole-dipole, and quadrupole couplings. Here, the researchers will make use of their home-built magnetometry apparatus with NMR sample shuttling methods incorporated.

- Buoyancy driven bubbly flows (Prasad Perlekar): The canonical text “An album of Fluid mechanics” by Van Dyke shows several remarkable realizations of turbulent flows. An otherwise laminar flow turns turbulent as it moves past a body. The flow behind an array of cylinders or a grid, either moving or stationary, provides an ideal testbed to verify and scrutinize the statistical theories of turbulence. What is the flow generated when a fluid is stirred by a dilute suspension of bubbles as they rise due to buoyancy? This question has intrigued researchers for the past three decades due to their occurrence in both industrial and natural processes. Prasad Perlekar’s group continues to investigate this problem using tools borrowed from nonequilibrium physics, statistical mechanics, and high resolution numerical simulations.

- What activates a protein molecule to cross a barrier? (Pramodh Vallurupalli): This group is experimentally studying the role of internal friction and solvent in the interconversion of proteins between compact conformations.

- De novo design of multivariate, epitaxial nanochannels for chemical separation (Ritesh Haldar): Chemical separation is an industrially important process, and currently most widely used technology is distillation. This process is highly energy intensive and have substantially high carbon footprint. A sustainable solution with much lower energy input can be membrane based separation technology. To make the membrane technology as efficient as distillation, following points need to be addressed: i) mechanical and chemical selectivity of the membrane, ii) selectivity vs permeability trade-off. Ritesh Haldar’s group aims to develop new membrane design principles, which can overcome the selectivity vs permeability trade-off.

- Dynamics in confluent biological systems (Saroj K. Nandi): Recent experiments have revealed that glassiness in a cellular monolayer is indispensable in morphogenesis, cancer metastasis, wound healing, bronchial asthma, etc. Three of the most popular models to study dynamics in such a confluent system, where there is no vacant space, are cellular Potts model, vertex model and voronoi model. The group’s long-term goal in this project is to develop a comprehensive theoretical framework to study dynamics in such a system. (a) *Random first order transition (RFOT) theory for confluent systems*: Currently, the group is studying the equilibrium glassy dynamics in confluent model systems; activity, cell division and apoptosis will be included later. They have extended one of the most popular theories of equilibrium glassy systems, the RFOT theory, for a confluent system and find excellent agreement when compared to their simulation results. One of the important control parameters in such systems is the target perimeter, P_0, that controls the inter-cellular interaction potential. The study reveals two regimes of the dynamics, characterised by super- and sub-Arrhenius relaxations. The researchers find that the perimeter constraint is crucial for the unusual sub-Arrhenius relaxation and constraint of confluency alone is not sufficient for such behaviour. (b) *Shape distribution of cells in confluent monolayer:* An interesting recent experimental finding is that

distribution of shapes, characterised via the aspect ratio of individual cells, in a confluent cellular monolayer follow a universal distribution in diverse systems. In this project, the researchers provide a theoretical understanding how such a distribution appears. They analytically obtain the distribution of aspect ratio in a confluent monolayer and then compare the analytical results with simulations and existing experiments. The study suggests that the universal distribution comes from the local geometric constraint on the cells (in the form of perimeter constraint) and not from the global constraint (in the form of confluency). These works are carried out by Souvik Sadhukhan (graduate student) and Saroj K. Nandi's group has collaborated with Profs. Mustansir Barma and Sumedha on the second part of the work.

- Effects of inclusions on the dynamical and rheological properties of disordered systems and understanding plasticity at Nano scale (Smarajit Karmakar): This project has components that deal with fundamental research as well as possible applications of these researches. One aspect is to study the plasticity in amorphous solids at nano-scale samples via uni-axial tensile simulations. The other aspect is to probe dynamical and rheological properties of disorder systems via inclusions in the form of impurity pinning sites and rod-shaped molecules. Plasticity at nano-scale especially in metallic glasses is very important to understand due to the industrial importance of metallic glasses as design materials. The project focuses on how these systems at small-scale yields under uniaxial elongation or compression. The second aspect will be to dope the glassy solids with random pinning in the forms of "soft" as well as "hard" pinning sites to tune the mechanical properties of these materials including tuning the yield strain value. Smarajit Karmakar's group found that yielding process in these disorder solids can be tuned from heterogeneous (fracture like shear banding process) to homogeneous (localised plastic processes) process using random pinning sites. This process in industry is known as "micro-alloying" and we expect to understand this micro-alloying process from microscopic point of view to possibly improve it for future material designing.

- Dynamical and Mechanical Properties of Active Glassy Systems – Heterogeneity, Plasticity and Yielding at Bulk and Nano Scale (Smarajit Karmakar)
This project focuses on dynamical and mechanical properties of active matters at bulk as well as small-scales, where surface relaxation becomes very important. The questions like - how active forces modify plasticity and yielding transition in these active amorphous solids under simple shear and uniaxial shear deformation, will be explored in complete details in order to develop a theoretical understand. The other aspect is to probe dynamical and micro- rheological properties of disorder systems by introducing small amount of active particles of varying shapes and sizes (spherical to rod like) as a perturbation to the system and looking at the response of the system due to this perturbation. One of the specific questions that will be addressed here is the effect of activity on the brittle-ductile transition in active glassy systems. Finally, study of the response of the system in the presence of small concentration of active particles of varying shapes from spherical to rod like to probe the local rheological properties of the medium will also be looked at.

- T. N. Narayanan's group has been involved in the following research projects:
1. DST-SERB Scientific and Useful Profound Research Advancement (SUPRA) Grant (2021-2024) Topic: "Development of Spin-correlation Engineered Transition Metal Dichalcogenides and Novel Light-assisted Methods for Probing them". (80 Lakhs) Role: Principal Investigator with Co-PIs: Prof. Nirmal K. Viswanathan (University of Hyderabad), Dr Rajalakshmi G., and Dr. Karthik V. Raman.
2. Infosys-TIFR "Leading Edge" Research Grant (18 Lakhs for 2.5 Years (2021)), Solar Metal-Ion Batteries and in situ Diagnostics Using Atomic Magnetometer, T. N. Narayanan [PI], G. Rajalakshmi [Co-PI], Pabitra K. Nayak [Co-PI], Soumya Ghosh [Co-PI], and P. K. Madhu [Co-PI].

3. IoE Directorate, Institution of Eminence University of Hyderabad Research Fund for "Complex Shifts of Optical Wave-Beam-Field in Complementary Domain to Probe Spin-orbit Interactions in 2D Materials", Prof. Nirmal K. Viswanathan (PI) and T. N. Narayanan (Co-PI). (50 Lakhs) (2021 December - 2024 March).

- Mechanics of Epidermal Development (Sanak Banerjee, Praver Gupta, Tamal Das, Dapeng Bi (Northeastern University, USA), Friedhelm Serwane (LMU, Germany)): Our knowledge of Cell and tissue mechanics mainly stems from experiments and theories of 2D epithelial monolayer and is limited to static elastic properties. Such knowledge is, however, unable to predict the events occurring inside a dynamic and viscoelastic 3D multilayer epithelial structure, such as the skin, where cells constantly move from one layer to another. To this end, pieces of evidence suggest that there may be a graded mechanical profile across different epidermal layers responsible for homeostasis and inter-layer cell movement. However, a direct evidence of such gradient and its role in directed cell movement remain elusive, due to the difficulties in recording dynamic viscoelastic properties and crafting proper theoretical models in 3D. Tamal Das and colleagues are trying to quantify the time-dependent viscoelastic cell and tissue mechanics in 3D epidermis during the development of this tissue. Their integrative approach, consisting of novel genetic, optogenetic, biophysical tools and 3D multiscale modeling, will bring a quantitative understanding to epidermal differentiation, oncogenesis and wound healing.

- 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 us answer the question how the same protein can enable different diseases.

- 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's group has been developing new solid-state NMR experiments to decipher structural information. Most notably amongst them being the ability to directly measure 1H-1H distances.

9. Science Communication and Public Outreach:

1) The science communication efforts at the TIFR Hyderabad Science Media Centre have taken the form of talks, articles, videos, illustrations, press releases and social media engagement. The media centre activities have been listed below: (reported by Anusheela Chatterjee (Programme Head, Science Media Centre))

- **'Stories from the Life Sciences: A multifaceted approach in interactive science communication', 1st IndiaBioscience Outreach Grant**

  In an effort to showcase how a researcher thinks about their science, four research stories from the institute were highlighted. Each story has been conveyed from a researcher's perspective, gradually introducing the project, after a brief overview of the basic concept. These stories have been communicated in the form of short videos. Key experiments were filmed, and illustrations and motion graphics were incorporated in the videos to tell the story in a lucid manner. The following stories were covered:

  A. How do lysosomes and golgi help in healing a wound? Part 1
  B. How do lysosomes and golgi help in healing a wound? Part 2
  [Projects A and B showcase how two researchers have taken separate directions to investigate collective cellular migration. These videos have a common introduction. These two stories would be uploaded on the TIFR Hyderabad YouTube channel once the studies are published.]

  C. What does glass and a dense layer of cells have in common?
  This story is a series of three videos [Video 1, Video 2 and Video 3] and is available on the TIFR Hyderabad YouTube channel.

  D. How do we extract polyphosphates from fruit flies?
  This story is available on the TIFR Hyderabad YouTube channel.

  The TIFR Hyderabad members who were involved in this project are: Anusheela Chatterjee, Basil Thurakkal, Souvik Sadhukhan, Purnati Khuntia, Rituraj Marwaha, Sunayana Sarkar, Anugraha A., Tarana Anand, M. R. Jishnu Seshadri, Antik Bhattacharya, Janmey Jay Panda

- **Articles:**
  - Opening doors and inducing changes: Binding of a substrate to the Cytochrome P450cam enzyme, Anusheela Chatterjee, *Research Highlight (short article)*
  - Plastic electronics: Ushering in the next generation of technology, Anusheela Chatterjee, *Research Highlight and Press release*
  - Searching for a super-thin stable photosensor, Anusheela Chatterjee, *Research Highlight (article)*
  - A 'tonic' that helps zinc-air batteries live longer, Anusheela Chatterjee, *Research Highlight (article)*
  - Recent advances on engineering compact solar batteries, Anusheela Chatterjee, *Press release (article)*
  - Investigating epithelial defence against cancer (EDAC), Praver Gupta, *Press release (article)*
  - Tamal Das receives the prestigious Human Frontier Science Program (HFSP) research grant, Anusheela Chatterjee, *Press release (article)*

- **Media Mentions** (in Eenadu, The Hindu, Telangana Today, AzoMaterials, Optics and Photonics News etc.):
  Some of the media mentions have been listed below:
  - Researchers Tweak Low-Cost Semiconductors for Increased Electroconductivity, AzoMaterials, April 2021
  - New light on how insulin signalling affects tissue health, The Hindu, October 2021
  - Toward Next-Gen Photo-Rechargeable Batteries, Optics and Photonics News, December 2021
  - TIFR Hyd faculty bags 9 cr research grant, Telangana today, March 2022

- **Sawaal-Jawaab:** Conversations on Science (Popular science café organized by TIFR Hyderabad)
  The sessions held during this period have been listed below (online mode only):
  - Insects in the Anthropocene, Shannon Olsson (NCBS Bengaluru), September 04, 2021
  - Math and Numbers: Why are they important?, Sujatha Ramdorai (University of British Columbia, Canada), May 15, 2021

- A series of popular science talks on the 2021 Nobel Prizes was organised. The details of the event are as follows:

  Date: November 25, 2021 (Thursday)
  Time: 4:00 PM - 5:30 PM
  Venue: TIFR Hyderabad auditorium and online via zoom

  Talks:
  "New Tool Kits for Molecular Carpentry"
  Speaker: V. Chandrasekhar

  "Physics of Disordered Systems – Works of Giorgio Parisi"
  Speaker: Smarajit Karmakar

  "Hot, Cold and the nuances of touch"
  Speaker: Adish Dani

- National Science Day celebrations: On National Science Day, 2022, a social media thread of science themed images, accompanied by descriptions, was started. A team of students participated in a science writing exercise and came up with descriptions of the science behind each of these images.
  Link to twitter thread: https://twitter.com/TIFRH_buzz/status/1498304357468708871

2) In an effort to reach out to high school students, TIFR Hyderabad set in motion a series of interactive sessions with researchers from the institute. The following sessions were held:
   - ‘A Journey to the Quantum World’, Dhavala Suri, August 14, 2021
   - ‘Birds, Babies and COVID: Role of Haemoglobin in Life and Medicine’, Anand T. Vaidya, August 28, 2021

- ‘Metabolism : Complex, but not chaotic’, Saptarnab Ganguly and Snigdha Nadagouda, September 11, 2021

3) Molecular Diagnostic Training at TIFR Hyderabad (Oct 2020-July2021)
TIFR Hyderabad set up a Molecular Diagnostic Training facility to boost the capacity of performing PCR based diagnostic tests, which is primarily used for COVID-19 diagnosis. The training effort is supported by the Principal Scientific Advisor’s office and funded by the Bill & Melinda Gates Foundation. The COVID-19 diagnostic training program at TIFR Hyderabad was organized by Manish Jaiswal, Anand T. Vaidya and Adish Dani along with Deepa Balasubramanian, Sreejith Rarankurussi and Gopalakrishna R. The participants trained at TIFR Hyderabad were lab technicians, in-service doctors, government undergraduate lecturers, researchers, medical students from seven states across India. The training session included one week of online theory sessions in collaboration with TIFR Mumbai, National Institute of Immunology, New Delhi and PanIIT Alumni Reach for India Foundation; and up to two weeks of wet-lab training session at the respective institutions. The program included an online module by FIND India and a visit to a BSL 2-3 lab facility for COVID-19 diagnosis and research at ESIC Medical College & Hospital. 200 trainees have completed the training programme. Many of these trainees are have worked in COVID-19 diagnostic labs in various parts of the country.

4) Popular science talks regarding Nobel Laureate Giorgio Parisi’s work were given by Smarajit Karmakar (who was a post-doctoral fellow at Giorgio Parisi’s group at the University of Rome). He gave these talks at TIFR Mumbai, TIFR Hyderabad, University of Hyderabad, and Society for Promotion of Science & Technology in India. Two popular science articles on Giorgio Parisi’s work have been published:
- Physics of Disordered Systems - Smarajit Karmakar, Resonance 27 (1), 19-38 (2022)
- Interplay of Disorder and Fluctuations in Physical Systems - Celebrating the Science of Giorgio Parisi, Physics Nobel laureate 2021, - S.K. Nandi and Smarajit Karmakar, Physics News 4 (2022).

5) Popular science talks given by TIFRH faculty in other institutions:

- Pabitra Kumar Nayak, ‘Let’s move to the sunny side, Chai & Why’, September 19, 2021.
- Pabitra Kumar Nayak, ‘Let’s move to the sunny side’, National Science day Lecture, KIIT University, Bhubaneswar, February 2022.
- T. N. Narayanan, ‘Higher Study in Science: How to Prepare’, Vaathayanam Talk for students, August 01, 2021. [Webinar]
- T. N. Narayanan, ‘Inspired to do Research’, Talk at St. Dominics School, Sreekrishnapuram, Kerala, July 31, 2021. [Webinar]
- Vipin Agarwal, ‘Solid-state NMR for Structural Characterization of Proteins’, Advancements in Biochemistry and Allied Sciences (four-day teacher-training workshop aimed updating teachers with the new area in biological sciences), Bhavan’s Vivekananda College of Science, Humanities and Commerce, Secunderabad, India, November 23-27, 2021.

10. Any other significant achievement:

- P. K. Madhu, Organiser of the Intercontinental Magnetic Resonance Seminar Series since April 8, 2020 (with Daniel Abergel, ENS, Paris, and Gerd Buntkowsky, TU Darmstadt, Germany).

- P. K. Madhu, Organiser of the on-line conference ICONS3, September 1-3, 2021, and ICONS4, February 9-11, 2022 (with Daniel Abergel, ENS, Paris, and Gerd Buntkowsky, TU Darmstadt, Germany).

- Raghunathan Ramakrishnan, External Research Grant secured: Department of Science and Technology, Government of India has sanctioned Rs. 43,34,260 for a period of three years for an INDO - SOUTH AFRICA joint project entitled: “Extremely Large Scale Modeling of Elementary Processes in Hydrocarbon Combustion using High-Throughout Atomistic Simulations and Data Science”. Project File No. DST/IBCD/SA/2021/6. The partner from a South African institute is Prof. Lydumila Moskaleva, University of the Free State.

- Saroj K. Nandi, SERB Grant SRG for Glassy dynamics in biological systems.

- Tamal Das received the HFSP Research Grant to work on “Dynamics of multilayer epithelial structures: Integrative mechanical characterization of epidermis” in collaboration with Friedhelm Serwane (LMU Munich, Germany) and Dapeng (Max) Bi (Northeastern University, USA).