1. Research Highlights:

A) BIOLOGICAL SCIENCES (Adish Dani, Aprotim Mazumder, Manish Jaiswal, Tamal Das)

- Auditory and visual sensory perception involves signal transmission via ribbon synapses. The cochlear ribbon synapse is a molecular machine specialized for rapid and continuous transmission of acoustic information to the brain. Adish Dani's lab measured organization of proteins at cochlear ribbon synapses using single molecule super-resolution microscopy. Their observations reveal localizations of proteins not seen with EM or confocal microscopy, as well as reorganization during developmental maturation of hearing function. These methods and data lay the foundation for ongoing structure-function studies to link ribbon synapse diversity and plasticity with mechanisms of congenital deafness and noise-induced hearing loss.

- DNA damage responses (DDR) is intimately linked to the emergence of cancers and to the cell cycle. Aprotim Mazumder's lab showed that it is the damage response that is cell cycle dependent and not DNA damage itself. Foci of phosphorylated H2AX in S phase cells correspond to sites of replication and not double strand breaks. They have also demonstrated the possibility of correlating the subnuclear position of a gene to its expression on a cell-by-cell basis.

It has previously been described how fluorescence anisotropy can be used to monitor chromatin compaction states. In this year, Mazumder's lab has combined this with laser-induced DNA damage to show an unexpected compaction of even undamaged DNA in response to localized double strand breaks, concomitant with the spread of damage markers monitored by immunofluorescence.

- A ubiquitin ligase Ben was found to negatively regulate mitochondrial fusion by inducing degradation of a mitochondrial fusion protein Marf in *Drosophila*. Loss of Ben protein resulted in increased Marf levels. To further understand the role of Ben in Marf degradation, a transgenic line was made to overexpress Ben protein fussed with small tag V5. Overexpression of ben was shown to rescue Ben loss of function mutants. It was found that the overexpression of Ben alone is not sufficient to degrade Marf suggesting the presence of unknown components that may trigger its activity. Traf6 and dSarm were identified as putative interactors of Ben in the regulation of Marf degradation and thereby novel regulators of mitochondrial size regulation.

In an effort to identify the regulators of mitochondrial dynamics during development, Achi and Vis, two *Drosophila* transcription factors were identified. Overexpression of Achi and Vis was found to induce mitochondrial fusion in Drosophila. Achi and Vis were known to regulate spermatogenesis and their loss resulted in male infertility in Drosophila. The mitochondrial fusion protein Marf gets down regulated during advanced stages of spermatogenesis and Marf expression correlated with the

activity of Achi/Vis suggesting that Achi and Vis could regulate spermatogenesis by the regulation of Marf expression.

- Tamal Das' group focused on understanding how cellular forces affect the collective dynamics of epithelial cells during cell competition and collective cell migration. On cell competition, they found that stiffening of extracellular matrix inhibited the competitive elimination of HRAS oncoprotein-expressing cells, and that this inhibition depended on a change in the intracellular localization of a competition-associated protein, filamin and nuclear force-sensing. On collective migration, Das' group studied how cellular organelles, including Golgi apparatus and lysosomes, reorganized as the sedentary cells started migrating. They found that from an apical location, Golgi first disintegrated, then scattered around, and finally reassembled at one side of the cell nucleus. They also found that as the cells migrated, lysosomes increasingly accumulated at the leading edge. Both Golgi and lysosome reorganization depended on the rearrangement of actin cytoskeleton. Finally, polarization of these organelles was discovered to be crucial for the efficient turnover of cell-matrix adhesion molecules.

B) CHEMICAL SCIENCES: (Anukul Jana, Jagannath Mondal, Kalyaneswar Mandal, Kanchan Garai, P. K. Madhu, Kaustubh R. Mote, Vipin Agarwal, Pushpita Ghosh, Pramodh Vallurupalli, V. Chandrasekhar, T. N. Narayanan, Raghunathan Ramakrishnan)

- Diphosphene, a phosphorus phosphorus double bonded compound was reversibly coordinated to an N-heterocyclic carbene, a Lewis base. This was used to bind to gold(I) hydride affording a compound which readily activates carbon dioxide at room temperature yielding the corresponding gold(I) formate. The latter could also be generated by a dehydrogenative coupling of the gold(I) hydride with formic acid. This established formic acid as a chemical hydrogen storage material.

Utilizing putative cyclic(alkyl)(amino)carbene, generated in situ, diradical analogues known in aromatic hydrocarbons have been synthesized and structurally characterized. This paves way for the creation of a new family of organic materials with potential applications in diverse areas ranging from molecular electronics to redox-reagents.

- Over the last one year, Jagannath Mondal's research group has made important strides in understanding the mechanism of drug resistance in kinase and predicting more potent kinase inhibitors via molecular simulations and enhanced sampling simulations. Additionally, in collaboration with Ruchi Anand's crystallography group at IIT Bombay, they have elucidated the role of allosteric regulation in proteins. On a fundamental level, the group has provided key insights in the role of solvent in a popular model system of hydrophobic cavity-ligand recognitions. They have extended their ongoing investigation on exploring optimised collective variables for enumerating the key conformations of macromolecules. Towards this end, Mondal and colleagues have explored the conformational landscape of monomeric amylose and its assembly of dimers across multiple force fields using the unbiased molecular dynamics simulation and Markov state model. In a joint effort with Surajit Sengupta's group, they have investigated a new collective variable called global non-affine parameter for its ability to explore protein's conformational landscape. They have also investigated the mechanisms of hydrogen evolution reactions from key materials, in collaboration with T. N. Narayanan's group.

- Techno-economically, hydrogen (H2(g)) based energy production is one of the most promising substitutes for fossil fuel. The electrochemical hydrogen evolution reaction (HER) is the cleanest method for hydrogen production. The usage of expensive metal-based electrochemical catalysts for HER is restricted by their paucity and short lifetime. Kalyaneswar Mandal and colleagues designed

highly effective metal-free HER catalysts by utilizing protein functionalized carbon nanotubes (CNTs) that were durable in acidic medium, scalable for industrial application, and obtained from inexpensive precursors thereby reducing the production cost. They observed multifold enhancement in the HER current density due to electrochemical protein denaturation induced by the acidic medium used for HER. Their findings open up new avenues in carbon-based metal-free HER catalysis which will have a very high impact on the field of electrochemical catalysis, and related energetics.

- Amyloid aggregation has attracted a lot of attention in the recent past due to involvement in multiple human diseases. The goal is to understand how endogenous proteins influence amyloid aggregation. Two functional proteins, viz, apolipoprotein E and the chaperone protein Hsp70 have been used to characterize its role on aggregation of amyloid β peptides. To characterize amyloid aggregation, Kanchan Garai's group developed two major single molecule techniques, viz, cuvette-FCS and Total Internal Reflection Fluorescence Microscopy (TIRFM). These techniques help detection of the rare and small amyloid fibrils allowing characterization of the earliest phase of the aggregation process. The researchers observed that both these proteins inhibit aggregation of Aβ. However, these proteins interact strongly with the oligomeric forms of Aβ but weakly with the monomeric forms.

Apolipoprotein E4 is the strongest risk factor for Alzheimer's disease, while apoE3 is normal and apoE2 is protective. The apoE isoforms differ by single amino acid substitutions but its effect on the functions of apoE is tremendous. A major hypothesis in the field has been that the apoE isoforms differ in terms of domain interactions. However, little is understood about this interaction. To characterize the isoform specific differences in the domain interaction, Garai's lab prepared several mutants of apoE. They characterized the domain interaction using stability of the isoforms and by interdomain FRET (Forster resonance energy transfer).

Additionally, the cuvette-FCS set up is being developed further by Garai's lab to perform Life-time Fluorescence correlation spectroscopy (Life time FCS).

- Measuring distances and understanding molecular motion is one of the most important applications of solid state NMR spectroscopy. The primary measurement unit of this in solid-state NMR is the dipolar coupling, which is inversely proportional to the cube of the distance between nuclei. P. K. Madhu, Kaustubh R. Mote and colleagues describe a new pulse sequence that allows the measurement of very high dipole dipole couplings by scaling these in a systematic manner. This method will find use in determining dynamics in proteins as well as small molecules.

The researchers have also developed a technique that will allow as many as 8 experiments to be simultaneously collected so that one can complete all required experiments within a time period that is ~2-3 times shorter than required with individual experiments

In addition, the researchers have used the newly developed SERP sequence to study different crystal forms of the drug albendazole and showed how fast magic-angle spinning frequencies and proton detection can be used to distinguish between different forms of the same compound.

- Spin-diffusion (SD) is used to spatially transfer polarization between dipolar-coupled nuclear spins and is routinely employed for structural characterization of molecules with solid-state NMR. It is well established that the diagonal and cross-peaks have the same sign during SD polarization transfer and is a result of the dipolar Hamiltonian. Proton SD spectra recorded on small molecules such as crystalline Histidine show negative cross-peaks in the spectrum. Cross-relaxation due to rapid tumbling of small molecule on the picosecond time scale typically result in negative cross-peaks in the SD equivalent NOESY experiment in solution. Vipin Agarwal and colleagues explored the coherent or the incoherent origin of the negative peaks in the proton SD spectra of histidine through theory, numerical simulations and experiments. The unusual features in the spectra were explained using

the four-spin, double flip-double flop, terms in the third-order average Hamiltonian combined with special arrangement of isotropic chemical shifts.

- Proteins are dynamic entities, populating a range of conformations with varying populations and lifetimes. Often a dominant `visible' major state is in exchange with `invisible' minor states that cannot be detected by standard biophysical techniques. However, these minor states can be crucial to understand protein folding, function, misfolding and diseases. Pramodh Vallurupalli's group is developing NMR experiments to detect and characterize these `invisible' states. Recently, they developed a double-resonance CEST experiment to study multistate exchange. This new double-resonance CEST approach was applied to study the exchange of T4L between the dominant native state (F) and two minor states, the unfolded state (U) and a second minor state (B), each populated to only ~4%. Double resonance CEST data unequivocally showed that T4L can fold directly from U to F. They have also developed a new methyl 1H CPMG experiment that can be used to study the dynamics of megadalton sized macromolecular machines.

- Pushpita Ghosh investigates thermodiffusion-induced spatiotemporal instabilities in reaction-diffusion system following activator-inhibitor kinetics. The interaction among reaction, diffusivity and the imposed constant thermal gradient gives rise to the formation of traveling waves and directional motion of stationary spatial inhomogeneity. The instability regions in the appropriate parameter space is derived and examined. This study shows how an imposed temperature gradient can generate spatiotemporal instability by destabilizing the otherwise homogeneous steady state. These results were also reproduced by numerical simulations using the general Brusselator and Chlorine-dioxide iodine malonic acid (CDIMA) reaction-diffusion models.

- Experimentally noted molecular conduction selectivity trends across isomeric spacer groups have been captured in electron dynamics simulations based on time-dependent configuration interaction (TDCI). Raghunathan Ramakrishnan and colleagues take this approach which gives a real-time perspective on electron density migrating from one end of a molecular junction to another. Results are reported for isomer benzene clarifying the meta-vs-para selectivity, and for azulene isomeric spacers, where experimental trends in conductivity have been captured.

- V. Chandrasekhar’s group has been working on molecular complexes involving transition metal ions and lanthanide metal ions for studying their magnetic properties. Both mono- and polynuclear complexes have been studied. Also, they have examined heterometallic complexes containing 3d/4f systems. One of the key aspects of this study has been the design of the ligand which allowed the specific synthesis of these systems. Examples of such systems included dinuclear homometallic complexes, mononuclear complexes prepared from a NNO ligand and heterobimetallic Co(II)/Y(III) complexes. The latter were assembled by a novel ligand that was assembled by using ferrocene as a scaffold. These heterometallic complexes were shown to be single-ion magnets because the magnetic properties observed in these systems is due to the Co(II) ion alone.

- The crystalline and amorphous of Cr2O3 were developed by T. N. Narayanan and colleagues using a novel method. The motivation behind the development of amorphous structures was their applicability in catalysis, where this will be beneficial in long term performance. It was also shown that these layers have synergistic augmented hydrogen evolution performance when made interfaces with metals like gold and platinum. In another work, edge engineered atomic layers of transition metal dischalcogenides was developed using a kinetically controlled growth process, where it was shown that both tri-angle shaped large area layers and their dendritic structures can be grown by modifying the method. These structures were shown for their application in hydrogen evolution in acid medium and shown that engineering edge has important role in catalysis. Different interfaces with atomic layers, such as graphene, and graphene and hBN, developed and such interfaces include both covalent and non-covalent ones. Se atom was used to couple two graphene sheets and it was shown that such a system undergo a 4 electron transfer assisted oxygen reduction reaction.

C) PHYSICAL SCIENCES: (Kabir Ramola, Karthik V. Raman, M. Krishnamurthy, Mustansir Barma, Prasad Perlekar, G. Rajalakshmi, Ram Gopal, Surajit Sengupta, Smarajit Karmakar, Pranav. R. Shirhatti, Saroj Nandi)

- The mechanics and rigidity of naturally abundant amorphous solids such as granular materials and structural glasses are not described by the conventional paradigm of broken symmetry that defines crystalline elasticity. Instead, local constraints of mechanical equilibrium describing them leads to a generalized electromagnetism that has a natural description in terms of tensor fields. Such emergent elasticity from constraints offers a new paradigm for systems with no broken symmetry, analogous to emergent gauge theories of quantum spin liquids. In addition to developing a field theory for such systems, Kabir Ramola and colleagues presented numerical and experimental evidence that force chains in granular media are sub-dimensional excitations of amorphous elasticity similar to fractons in quantum spin liquids. They also focussed on near-crystalline athermal systems and derived exact results for the fluctuations. They showed that forces in such systems display constrained fluctuations, characterized by non-Gaussian distributions, a feature absent in their thermal counterparts. They developed a 'field-charge' mapping which is quite general and will be applicable in a variety of situations, including in systems involving active forces. Since situations involving athermal disorder find relevance across disparate fields where the techniques of statistical mechanics are presently inapplicable, these results are of relevance to theorists as well as experimentalists studying athermal materials.

- Karthik V. Raman's group has developed proximity effect studies at the surface of ferromagnets and topological insulators. In the case of ferromagnetic surfaces, using molecular adsorption studies they have shown a new phenomenon of molecular crane-pulley effect - whereby the surface 2D supra-molecular magnetic layer (SML) decouple from the underneath Fe layer giving rise to a robust exchange-bias effect with a surprisingly large in-plane biaxial anisotropy and switching field in excess of 7T. On the other hand, their study on magnetic proximity of EuS with a high quality c-axis oriented strain-free layered film of topological insulator, Bi2Se3 has provided a direct evidence of gate-controlled enhanced interface magnetism in EuS arising from the carrier mediated RKKY interactions across the Bi2Se3/EuS interface.

- M. Krishnamurthy's group explored how the transient absorption of laser pulse changes when matter is coagulated in the form of solid density clusters compared to the gaseous systems. They showed that for pulse widths smaller that 100fs, absorption can be explained completely by single particle phenomenon.

A nanocluster ionized by an intense fs pulse sets up an electron cloud that oscillates with respect to the ion cloud. Most theoretical frameworks on understanding cluster ionization are built on this dipole oscillation model. M. Krishnamurthy's group has set up the experiment to probe this transient dipole by pump-probe absorption spectroscopy. The polarization dependence of the probe pulse absorption gives a direct measure of the asymmetry and ellipticity in the dielectric permitivity. Their results show that orthogonally polarized pump-probe pulses absorb about 18% less compared to the parallel case at the peak of the linear plasma resonance.

Electron spectrometry where a pair of magnets deflect negatively charged particles and detected by image plates have been in use in the laser-plasma studies for more than 2 decades. The conventional wisdom is that electrons are the only negatively charged particles detected in the scheme. This may not be true as the latest experiments have proved. In almost all the experiments, accelerated negative ions are invariably generated in intense laser plasmas. M. Krishnamurthy's research group found that the spectral assignment to electrons can be erroneous and they prove that negative ions of H- are detected in such a well-practised scheme. A course correction based on these results is

perhaps important to most of the measurements in intense plasma studies that routinely uses this method.

- Particles on fluctuating interfaces are widely used as simple models to study variety of systems. The interactions between the particles and the interface is two-fold, the particles can push or pull the surface and the fluctuations in the surface can dictate the particle motion. Mustansir Barma and colleagues studies the following two problems:

(i) Active particles on an interface which resemble energy-consuming proteins embedded in the cell membrane, responsible for membrane deformation and cell movement. A simple model was introduced in which the active particle overturns local valleys of the interface into hills, simulating growth, while itself sliding and seeking new valleys. In one dimension, the particle moves much faster than diffusively in the transverse direction while pulling the immobile interface upward. Numerical simulations show that with time a tent-like profile develops, which has simple scaling properties and shows large fluctuations. Pullers on two-dimensional surfaces also show same properties. By contrast, pushers move slower than diffusively, leading to a separation of time-scale of pusher motion and interface response.

(ii) Sliding particles on a fluctuating energy landscape were studied using both numerical and analytical tools to look for new universality classes predicted by recent analytic work. The study revealed that the system is rich enough to show several new universality classes as the strengths of the coupling were varied. The finite size of the system leads to strong corrections to the predicted power law decay, which holds exactly only for an infinite size system.

- Pranav R. Shirhatti's group has been working on developing an imaging technique based on scattering of low energy (< 1 eV) neutral atoms/molecules from surfaces namely, `neutral atom/molecule microscopy (NAM)'. This method presents several unique features such as being 'non-destructive' and 'universal'. Improving the spatial resolution and understanding contrast generating mechanisms are key questions being studied. In order to address these questions, they have designed and developed an atom/molecule beam scattering machine. Proof of concept has been demonstrated by imaging objects by measuring the scattered flux. Dynamics of molecule - surface collisions and energy transfer are also being studied. These require quantum state specific preparation and detection of molecules. Radiation sources for such experiments need to be high intensity (MW/cm^2), narrow linewidth and frequency stable (~ 1 ppm) and in the mid-IR range. Shirhatti's group is developing such a source based on the `Master Oscillator Power Amplifier' (MOPA) approach. A master oscillator cavity using KTP as the nonlinear medium has been built and narrow linewidth operation has been demonstrated. Further efforts are being directed towards single longitudinal mode operation and frequency stabilization. In parallel, development of a wavemeter, capable of measuring wavelengths to ppm level accuracy and precision has been undertaken.

- Multiphase fluid flows such as binary-mixtures, bubbly flows, and suspensions of droplets or aerosols appear in a variety of natural and industrial processes. In many cases, the presence of a different phase dramatically alters the transport properties of a flow. Using direct numerical simulations, Prasad Perlekar's group has investigated and characterized the statistical properties of turbulence in:

a) Buoyancy-driven bubbly flows.
b) Binary-fluid mixtures driven by external forcing.

c) Two-dimensional dusty-gas turbulence.

- Atomic magnetometers based on Nonlinear Magneto-Optical Rotation (NMOR) have sensitivities as low as fT.Hz^(-1/2) . Typical magnetometers use balanced polarimetry to detect the polarisation rotation signal. G. Rajalakshmi and colleagues use this as well as other more quantum coherence

enabled methods to get nT to PT sensitivity to magnetic fields. In addition, these methods enable polarisation rotation measurements at microradian levels, with high bandwidth especially in the 0.1-100KHz regime.

- Generally, molecular ions have the tendency to align themselves in an external field. However, Ram Gopal and colleagues observed, in a homonuclear molecule, O2, that at certain experimental conditions the molecular ions oppose the alignment and hence the molecular ion appears frozen. This feature can be attributed to the negative polarizability of a molecular ion. Velocity map spectroscopic measurements of the fragmentation following dissociative ionization of the molecule were performed by scientists and students from TIFR Hyderabad, IIT Hyderabad and IISER Pune. By analyzing its fragmentation pattern in intense laser fields, the polarizability of the excited states of the molecular ion, O2+ were extracted. These fragmentation patterns inherently contain information of the rotation of the molecular ion in the field, which is mediated by the polarizability of the molecule. This approach has the advantage of experimental access to the properties of the excited states in a molecular ion, leading to this singular observation of negative polarizability.

- Glassy dynamics are usually characterised by stretched-exponential relaxations (SER) of the two-point density-density auto-correlation functions. However, SER can stem from many different processes and which one is relevant for glasses remains elusive. Saroj Nandi and colleagues have studied the effect of rapid quench to zero temperature in a model with competing interactions, evolving through double spin flip dynamics that conserves the staggered magnetization. In a certain regime of model parameters, they find that the model belongs to the broader class of kinetically constrained models, however, the dynamics is different from that of a glass. The system shows SER with the unusual feature that the relaxation time diverges as a power of the system size; the relaxation dynamics is a consequence of domain wall diffusion and Nandi and colleagues have termed it as size-stretched exponential relaxation (SSER).

- Quite contrary to what we are usually taught in school, a solid is never truly rigid. If it is deformed at an extremely slow rate then all solids begin to flow. Surajit Sengupta's group has discovered that this happens due the presence of a new kind of phase transition - similar to freezing or boiling. This picture gives us a fundamentally new viewpoint on the phenomenon of yielding, i.e. the loss of rigidity of a crystal when deformed beyond a limit. The phenomenon of yielding is now simply the nucleation of bubbles of a stress free solid within the body of the rigid crystal. An outcome of this theory is that the yield point is always a weak function of the rate of deformation and vanishes in the limit of zero deformation rate. The analytic form derived by us for the yield point as a function of the rate of deformation is able to explain experimental data over 15 orders of magnitudes in time. The researchers believe that their insight will lead to better design of nano-structures that are subjected to deformation over extremely long periods of time.

- Glasses are ubiquitous in nature. Many food items (such as ketchup, cosmetic products, toothpaste) and metallic glasses are examples of glassy materials whose rheological properties matter in our daily life. Smarajit Karmakar's group has demonstrated that one can tune the yielding phenomena in these amorphous solids from being heterogeneous to homogeneous by embedding inclusions which have relaxation timescales much larger than that of the amorphous matrix. This will have important implications in understanding micro-alloying that is done to modify the material properties experimentally. They have also studied a direct relationship between short and long time dynamical relaxation processes in glass-forming liquids. Short time relaxations are assumed to be one of the main mechanisms for ageing and rejuvenation in glassy solids as well as an important component to understanding bio-preservation.

Another study by this group highlights that both the relaxation processes are important to understand the preservation of biomolecules and drugs. They have also studied how dynamic heterogeneity in disordered system evolves over time and our results suggest that heterogeneity in

these systems develops fully at short timescales and then remains active over timescales much larger than the characteristic timescales of the system under consideration.

D) SCIENCE EDUCATION:

Curiosity is a basic human drive which is crucial for learning. Unfortunately, in Indian schools, there is an observed lack of questioning among students. The school outreach program of TIFR Hyderabad provided a conducive setting for students to express their curiosity. Analysis of 678 questions collected by volunteers over two years showed that these questions were often drawn from everyday phenomena. Prominent fields of questioning were biology (37%) (especially human physiology) and physics (27%) (especially astronomy and light). There were questions on religion, society, humankind, and life and career matters (26%). Explanatory- type questions predominated followed by complex factual and open-ended ones. Interaction with scientists elicited more factual-type questions.

Students' questions give adults a window into their thinking and show us more effective ways to design learning experiences. 'Sawaliram 2.0' is being developed as a multilingual online repository of questions asked by school students, collected with the aim of providing credible answers, fostering curiosity, analysing the questions for insights into their interests and motivations, and eventually contributing to curriculum development. The project is collaborative with Eklavya, an NGO based in Bhopal, Madhya Pradesh. The open source website (sawaliram.org) provides a dashboard for students' questions to be submitted, answered, queried and translated into multiple languages. The current repository of over 2000 questions has been sourced from diverse groups of students across the country.

3. Science communication and outreach:

- Sawaal-Jawaab: Conversations on Science: TIFR Hyderabad has strengthened its efforts in public engagement and science outreach. The flagship event of our community science outreach is a Science Café called `Sawaal-Jawaab: Conversations on Science'. These sessions provide an informal platform for the general public to interact with a scientist. `Sawaal-Jawaab' has been steadily gaining popularity, thus, increasing our reach to the general public in Hyderabad. The Sawaal-Jawaab programme is coordinated by Anusheela Chatterjee.

Sessions conducted between April 2019 and March 2020:

1) Mar 07, 2020, “Growing food in the face of salinity and drought”, M. K. Mathew, NCBS Bangalore
2) Feb 15, 2020, “How do raindrops form and grow?”, Rama Govindarajan, ICTS Bangalore
3) Feb 8, 2020, “The Coronavirus Pandemic”, Gautam Menon, Ashoka University, Sonepat and IMSc, Chennai
4) Nov 9, 2019, “Astrophotography- the art of capturing the ancient light”, Vinita Navalkar, CBS Mumbai
5) Oct 12, 2019, “New views of the Moon from Chandrayaan-2”, P. Sreekumar, ISRO
6) Sep 14, 2019, “Why Engineers need Greek Philosophy”, Surajit Sengupta, TIFR Hyderabad
7) Jul 13, 2019, “Black Holes- Heard three years ago and seen three months ago”, Rajaram Nityananda, Azim Premji University
8) May 4, 2019, “Superbreakfast for Superheroes and other stories”, Arnab Bhattacharya, TIFR Mumbai

- During the course of this year, TIFR Hyderabad has taken initiatives in providing science writing and illustration skills to students belonging to institutes in Hyderabad.

1) SciComm101: TIFR Hyderabad hosted the workshop `SciComm101' on campus. This workshop was conducted by instructors from the Wellcome Trust- DBT India Alliance and included carefully crafted modules on the basics of science communication, writing manuscripts and grants, research ethics, presenting one's research through posters or slides, and various career opportunities in science. Initially, the workshop was meant to be a one-day event catering to a group of 60-80 participants. However, we received an overwhelming response to the call for registrations. Thus, there were two iterations of this workshop, one on August 26, 2019 and the other on August 28, 2019, for more than 185 participants. We received participation from institutions such as University of Hyderabad, Osmania University, CSIR-Centre for Cellular and Molecular Biology, Centre for DNA Fingerprinting and Diagnostics, National Institute of Animal Biotechnology, IIT Hyderabad and CSIR- Indian Institute of Chemical Technology. (Organiser: Anusheela Chatterjee)

2) Science Illustration workshop: On March 05 and 06, 2020, Dr. Ipsa Jain conducted a two-day science illustration workshop at TIFR Hyderabad. This workshop was attended by 18 students and post-doctoral fellows from institutions/universities in Hyderabad. Day 1 included discussions on what art and design entails, what is science illustration, and sketching exercises that highlighted the importance of observation. On Day 2, participants were divided into teams. Each team had to come up with a science illustration on an assigned topic. (Organiser: Anusheela Chatterjee)

- Outreach with neighbouring government schools:

A strong association with schools is essential for any science education research. In 2019-20, the 3rd year of the school outreach program, volunteers from TIFR Hyderabad and University of Hyderabad conducted a total of 75 weekend visits with 207 classroom sessions in 5 nearby schools: 3 Telangana Social Welfare Residential schools, 1 Zilla Parishad and 1 Mandal Parishad school. The sessions included concept discussions, library, lab and life skills sessions. Students' questions collected by volunteers were added to the 'Sawaliram' repository. A highlight of the practical sessions since 2017 has been the use of Foldscopes, or low-cost paper microscopes. The Foldscope engagement was extended to PG students at the University of Hyderabad and it continues to be reported online at https://microcosmos.foldscope.com/?author=1733.

2. Staff Strength:

Faculty- 26 + 3 (Visiting faculty- 1, No. of Emeritus faculty- 1, No. of INSPIRE faculty- 01)
Research Scholars- 115
Junior Research Fellows- 31
Senior Research Fellows- 15
Post-doctoral Fellows- 41
Visiting students- 03
Scientific Staff- 15
Technical Staff – 12 (3 out sourced out of 12)
Admin Staff – 22 (5 out sourced out of 22)
Auxillary staff- 01

3. Awards and distinctions:

1) Anukul Jana - INSA Medal for Young Scientist (December 2019)

2) P. K. Madhu - ISMAR Fellow, International Society of Magnetic Resonance, In recognition of the contributions to the field of magnetic resonance (January 2020)

3) M. Krishnamurthy - Elected Fellow of the Indian National Science Academy, Delhi

4) Mustansir Barma - R. D. Birla Memorial Award in Physics, Indian Physics Association, For pioneering contributions over the past four decades to some fundamental problems in Statistical Physics and Condensed Matter Physics, focusing on the way cooperative effects arise and manifest themselves in interacting systems both in and out of equilibrium (November 2019)

5) Smarajit Karmakar - Swarna Jayanti Fellowship, Department of Science and Technology (DST), India (January 2020)

6) T. N. Narayanan - Recognition from Journal of Materials Chemistry A - 2020 Emerging Investigators Themed Issue, Royal Society of Chemistry (January 2020)

7) Tamal Das - Merck Young Scientist Award (Finalist) Merck GmbH (December 2019)

8) V. Chandrasekhar - Elected Vice-president, Indian National Science Academy, New Delhi (2019-2022)

4. Number of students graduated: 7

5. Publications:

1. Khumukcham, S.S., Samanthapudi, V.S.K., Penugurti, V., Kumari, A., Kesavan, P.S., Velatooru, L.R., Kotla, S.R., Mazumder, A. and Manavathi, B., 2019. Hematopoietic PBX-interacting protein is a substrate and an inhibitor of the APC/C–Cdc20 complex and regulates mitosis by stabilizing cyclin B1. Journal of Biological Chemistry, 294(26), pp.10236-10252.

2. Jana, A., Mandal, D., Chandra, S., Neuman, N.I., Sarkar, A., Kundu, A., Anga, S., Rawat, H., Schulzke, C., Mote, K.R. and Sarkar, B., 2020. Activation of Aromatic C-F Bonds by a N-Heterocyclic Olefin (NHO). *Chemistry–A European Journal*.

3. Nayak, M.K., Stubbe, J., Neuman, N.I., Narayanan, R.S., Maji, S., Schulzke, C., Chandrasekhar, V., Sarkar, B. and Jana, A., 2020. N, N′-Ethylene-Bridged Bis-2-Aryl-Pyrrolinium Cations to E-Diaminoalkenes: Non-Identical Stepwise Reversible Double-Redox Coupled Bond Activation Reactions. *Chemistry–A European Journal*.

4. Maiti, A., Stubbe, J., Neuman, N.I., Kalita, P., Duari, P., Schulzke, C., Chandrasekhar, V., Sarkar, B. and Jana, A., 2020. CAAC-Based Thiele and Schlenk Hydrocarbons. *Angewandte Chemie*, 132(17), pp.6795-6800.

5. Santra, B., Kalita, P., Chandra, S., Mandal, D., Kumar, V., Narayanan, R.S., Dey, A., Chrysochos, N., Huch, V., Biswas, S. and Ghoshal, D., 2020. Molecular enneanuclear Cu II phosphates containing planar hexanuclear and trinuclear sub-units: syntheses, structures, and magnetism. *Dalton Transactions*, *49*(8), pp.2527-2536.

6. Dhara, D., Das, S., Kalita, P., Maiti, A., Pati, S.K., Scheschkewitz, D., Chandrasekhar, V. and Jana, A., 2020. Influence of N-heterocyclic carbenes (NHCs) on the hydrolysis of a diphosphene. *Dalton Transactions*, *49*(4), pp.993-997.

7. Mandal, D., Gupta, V., Santra, B., Chrysochos, N., Bhoyare, V.W., Maiti, A., Kar, A., Guha, A., Thakur, P., Narayanan, R.S. and Patil, N.T., 2019. Solvent-assisted monomeric molecular structure of the phosphate diester and the synthesis of menthol-based phosphate diesters. Journal of Chemical Sciences, 131(12), p.121.

8. Dhara, D., Das, S., Pati, S.K., Scheschkewitz, D., Chandrasekhar, V. and Jana, A., 2019. NHC-Coordinated Diphosphene-Stabilized Gold (I) Hydride and Its Reversible Conversion to Gold (I) Formate with CO2. *Angewandte Chemie International Edition*, *58*(43), pp.15367-15371.

9. Mandal, D., Dolai, R., Kumar, R., Suhr, S., Chrysochos, N., Kalita, P., Narayanan, R.S., Rajaraman, G., Schulzke, C., Sarkar, B. and Chandrasekhar, V., 2019. Influence of N-Substitution on the Formation and Oxidation of NHC–CAAC-Derived Triazaalkenes. *The Journal of organic chemistry*, *84*(14), pp.8899-8909.

10. Santra, B., Narayanan, R.S., Kalita, P., Kumar, V., Mandal, D., Gupta, V., Zimmer, M., Huch, V., Chandrasekhar, V., Scheschkewitz, D. and Schulzke, C., 2019. Modulation of the nuclearity of molecular Mg (ii)-phosphates: solid-state structural change involving coordinating solvents. *Dalton Transactions*, *48*(24), pp.8853-8860.

11. Klemmer, L., Huch, V., Jana, A. and Scheschkewitz, D., 2019. An anionic heterosiliconoid with two germanium vertices. *Chemical Communications*, *55*(68), pp.10100-10103.

12. Santra, B., Kumar, V., Kalita, P., Gupta, V., Mandal, D., Chandra, A., Joshi, M., Choudhury, A.R., Jana, A. and Chandrasekhar, V., 2019. Molecular di-and tetra-nuclear zinc (II) phosphates with sterically hindered aryl phosphate mono esters ligands. *Polyhedron*, *172*, pp.216-225.

13. Mukherjee, M. and Mondal, J., 2019. Osmolyte-Induced collapse of a charged macromolecule. *The Journal of Physical Chemistry B*, *123*(22), pp.4636-4644.

14. Bawari, S., Pal, S., Pal, S., Mondal, J. and Narayanan, T.N., 2019. Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. *The Journal of Physical Chemistry C*, *123*(28), pp.17249-17254.

15. Koneru, J.K. and Mondal, J., 2019. Quantitative assessment of amylose dimerization process across force fields. *JOURNAL OF THE INDIAN CHEMICAL SOCIETY*, *96*(7), pp.949-956.

16. Mukherjee, M. and Mondal, J., 2019. Osmolyte-induced macromolecular aggregation is length-scale dependent. *The Journal of Physical Chemistry B*, *123*(41), pp.8697-8703.

17. Koneru, J.K., Zhu, X. and Mondal, J., 2019. Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. *Journal of Chemical Theory and Computation*, *15*(11), pp.6203-6212.

18. Ahalawat, N., Bandyopadhyay, S. and Mondal, J., 2020. On the role of solvent in hydrophobic cavity–ligand recognition kinetics. *The Journal of Chemical Physics*, *152*(7), p.074104.

19. Sharma, N., Ahalawat, N., Sandhu, P., Strauss, E., Mondal, J. and Anand, R., 2020. Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation. *Science Advances*, *6*(14), p.eaay7919.

20. Vinutha, H.A., Ramola, K., Chakraborty, B. and Sastry, S., 2020. Timescale divergence at the shear jamming transition. *Granular Matter*, *22*(1), pp.1-8.

21. Merrigan, C., Ramola, K., Chatterjee, R., Segall, N., Shokef, Y. and Chakraborty, B., 2020. Arrested states in persistent active matter: Gelation without attraction. *Physical Review Research*, *2*(1), p.013260.

22. Acharya, P., Sengupta, S., Chakraborty, B. and Ramola, K., 2020. Athermal fluctuations in disordered crystals. *Physical Review Letters*, *124*(16), p.168004.

23. Nampoothiri, J.N., Wang, Y., Ramola, K., Zhang, J., Bhattacharjee, S. and Chakraborty, B., 2020. Emergent Elasticity in Amorphous Solids. *arXiv preprint arXiv:2004.02230*.

24. Mannuthodikayil, J., Singh, S., Biswas, A., Kar, A., Tabassum, W., Vydyam, P., Bhattacharyya, M.K. and Mandal, K., 2019. Benzimidazolinone-Free Peptide o-Aminoanilides for Chemical Protein Synthesis. *Organic letters*, *21*(22), pp.9040-9044.

25. Ghosh, S., Sil, T.B., Dolai, S. and Garai, K., 2019. High-affinity multivalent interactions between apolipoprotein E and the oligomers of amyloid-β. *The FEBS journal*, *286*(23), pp.4737-4753.

26. Jain, M.G., Rajalakshmi, G., Agarwal, V., Madhu, P.K. and Mote, K.R., 2019. On the direct relation between REDOR and DIPSHIFT experiments in solid-state NMR. *Journal of Magnetic Resonance*, *308*, p.106563.

27. Kupče, Ē., Mote, K.R. and Madhu, P.K., 2019. Experiments with direct detection of multiple FIDs. *Journal of Magnetic Resonance*, *304*, pp.16-34.

28. Sharma, K., Madhu, P.K., Agarwal, V. and Mote, K.R., 2020. Simultaneous recording of intra-and inter-residue linking experiments for backbone assignments in proteins at MAS frequencies higher than 60 kHz. *Journal of Biomolecular NMR*, pp.1-9.

29. Jain, M.G., Mote, K.R. and Madhu, P.K., 2019. NMR Crystallography at Fast Magic-Angle Spinning Frequencies: Application of Novel Recoupling Methods. *Crystals*, *9*(5), p.231.

30. Jain, M.G., Rajalakshmi, G., Madhu, P.K., Agarwal, V. and Mote, K.R., 2020. Overcoming Prohibitively Large Radiofrequency Demands for the Measurement of Internuclear Distances with Solid-State NMR under Fast Magic-Angle Spinning. *The Journal of Physical Chemistry B*, *124*(8), pp.1444-1451.

31. Agarwal, V., 2020. The origin of negative cross-peaks in proton-spin diffusion spectrum of fully protonated solids at fast MAS: Coherent or incoherent effect?. *Journal of Magnetic Resonance*, *311*, p.106661.

32. Mandya, A.S., Cheramangalam, R.N. and Jaiswal, M., 2019. Understanding Neurodegeneration and Neuroprotection Through Genetic Screens in Drosophila. In *Insights into Human Neurodegeneration: Lessons Learnt from Drosophila* (pp. 55-88). Springer, Singapore.

33. Sarkar, S., Gopal, R., Anand, M., Kumar, M.P. and Krishnamurthy, M., 2019. On the importance of field driven single particle processes in short pulse absorption of clusters. *Scientific reports*, *9*(1), pp.1-7.

34. Sarkar, S., Gopal, R., Kundu, M., Gope, K., Anand, M. and Krishnamurthy, M., 2019. Measurement of asymmetric electron cloud in cluster nano-plasma. *Physics of Plasmas*, *26*(7), p.070703.

35. Bisht, P. and Barma, M., 2019. Interface growth driven by a single active particle. *Physical Review E*, *100*(5), p.052120.

36. Chakraborty, S., Chatterjee, S. and Barma, M., 2019. Dynamics of coupled modes for sliding particles on a fluctuating landscape. *Physical Review E*, *100*(4), p.042117.

37. Barma, M., Majumdar, S.N. and Mukamel, D., 2019. Fluctuation-dominated phase ordering at a mixed order transition. *Journal of Physics A: Mathematical and Theoretical*, *52*(25), p.254001.

38. Vallurupalli, P., Tiwari, V.P. and Ghosh, S., 2019. A double-resonance CEST experiment to study multistate protein conformational exchange: an application to protein folding. *The journal of physical chemistry letters*, *10*(11), pp.3051-3056.

39. Yuwen, T., Huang, R., Vallurupalli, P. and Kay, L.E., 2019. A Methyl-TROSY-Based 1H Relaxation Dispersion Experiment for Studies of Conformational Exchange in High Molecular Weight Proteins. *Angewandte Chemie International Edition*, *58*(19), pp.6250-6254.

40. Perlekar, P., 2019. Kinetic energy spectra and flux in turbulent phase-separating symmetric binary-fluid mixtures. *Journal of Fluid Mechanics*, *873*, pp.459-474.

41. Pandey, V., Perlekar, P. and Mitra, D., 2019. Clustering and energy spectra in two-dimensional dusty gas turbulence. *Physical Review E*, *100*(1), p.013114.

42. Pandey, V., Ramadugu, R. and Perlekar, P., 2020. Liquid velocity fluctuations and energy spectra in three-dimensional buoyancy-driven bubbly flows. *Journal of Fluid Mechanics*, *884*.

43. Ghosh, P., 2019. Emergent spatiotemporal instabilities in reactive spatially extended systems by thermodiffusion. *Physical Review E*, *100*(4), p.042217.

44. Tchoufag, J., Ghosh, P., Pogue, C.B., Nan, B. and Mandadapu, K.K., 2019. Mechanisms for bacterial gliding motility on soft substrates. *Proceedings of the National Academy of Sciences*, *116*(50), pp.25087-25096.

45. Ramakrishnan, R., 2020. Charge-transfer selectivity and quantum interference in real-time electron dynamics: Gaining insights from time-dependent configuration interaction simulations. *The Journal of Chemical Physics*, *152*(19), p.194111.

46. Kilaj, A., Gao, H., Tahchieva, D.N., Ramakrishnan, R., Bachmann, D.G., Gillingham, D., von Lilienfeld, A., Küpper, J. and Willitsch, S., 2020. Quantum-chemistry-aided identification, synthesis and experimental validation of model systems for conformationally controlled reaction studies: Separation of the conformers of 2, 3-dibromobuta-1, 3-diene in the gas phase. *Physical Chemistry Chemical Physics*.

47. Francis, T.V., Suna, R.R., Madhu, P.K., Viswanathan, N.K. and Rajalakshmi, G., 2019. Ultra-sensitive single-beam atom-optical magnetometer using weak measurement method. *AIP Advances*, *9*(6), p.065113.

48. Sen, A., Sairam, T., Sahu, S.R., Bapat, B., Gopal, R. and Sharma, V., 2020. Hindered alignment in ultrashort, intense laser-induced fragmentation of O2. *The Journal of Chemical Physics*, *152*(1), p.014302.

49. Mandal, Suddhasattwa, Ram Gopal, S. R. Krishnan, Robert Richter, Marcello Coreno, Marcel Mudrich, Hemkumar Srinivas, Alessandro D'Elia, Bhas Bapat, and Vandana Sharma. "Photoionization of Acetylene Doped in Helium Nanodroplets by EUV Synchrotron Radiation." In *Quantum Collisions and Confinement of Atomic and Molecular Species, and Photons*, pp. 230-238. Springer, Singapore, 2019.

50. Nandi, S., Deviri, D., Bajpai, G. and Safran, S., 2019, July. Multivalency of proteins in cellular phase separation. In *EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS* (Vol. 48, pp. S73-S73). 233 SPRING ST, NEW YORK, NY 10013 USA: SPRINGER.

51. Bhowmik, B.P., Chaudhuri, P. and Karmakar, S., 2019. Effect of pinning on the yielding transition of amorphous solids. *Physical review letters*, *123*(18), p.185501

52. Mukherjee, M., Mondal, J. and Karmakar, S., 2019. Role of α and β relaxations in collapsing dynamics of a polymer chain in supercooled glass-forming liquid. *The Journal of chemical physics*, *150*(11), p.114503.

53. Bhowmik, B.P., Karmakar, S., Procaccia, I. and Rainone, C., 2019. Particle pinning suppresses spinodal criticality in the shear-banding instability. *Physical Review E*, *100*(5), p.052110

54. Srivastava, A., Karmakar, S. and Debnath, A., 2019. Quantification of spatio-temporal scales of dynamical heterogeneity of water near lipid membranes above supercooling. *Soft Matter*, *15*(47), pp.9805-9815.

55. Tah, I. and Karmakar, S., 2020. Signature of Dynamical heterogeneity in Spatial Correlations of Particle displacement and its Temporal evolution in Supercooled liquids. *Physical Review Research*, *2*(2), p.022067.

56. Popli, P., Kayal, S., Sollich, P. and Sengupta, S., 2019. Exploring the link between crystal defects and nonaffine displacement fluctuations. *Physical Review E*, *100*(3), p.033002.

57. Shankaraiah, N., Sengupta, S. and Menon, G.I., 2019. Orientational correlations in fluids with quenched disorder. *The Journal of Chemical Physics*, *151*(12), p.124501.

58. Reddy, V.S., Nath, P., Horbach, J., Sollich, P. and Sengupta, S., 2020. Nucleation Theory for Yielding of Nearly Defect-Free Crystals: Understanding Rate Dependent Yield Points. *Physical Review Letters*, *124*(2), p.025503

59. Shankaraiah, N., Sengupta, S. and Menon, G.I., 2020. Disorder-induced enhancement of local hexatic correlations in two-dimensional fluids. *Journal of Physics: Condensed Matter*, *32*(18), p.184003.

60. Prakashchand, D.D., Ahalawat, N., Bandyopadhyay, S., Sengupta, S. and Mondal, J., 2020. Nonaffine displacements encode collective conformational fluctuations in proteins. *Journal of Chemical Theory and Computation*, *16*(4), pp.2508-2516.

61. Sharma, R., Sahoo, K.R., Rastogi, P.K., Biroju, R.K., Theis, W. and Narayanan, T.N., 2019. On the Synthesis of Morphology-Controlled Transition Metal Dichalcogenides via Chemical Vapor Deposition for Electrochemical Hydrogen Generation. *physica status solidi (RRL)–Rapid Research Letters*, *13*(12), p.1900257

62. Narayanan, S.P., Thakur, P., Balan, A.P., Abraham, A.A., Mathew, F., Yeddala, M., Subair, T., Tiwary, C., Thomas, S., Narayanan, T.N. and Ajayan, P.M., 2019. Two-Dimensional Amorphous Cr2O3 Modified Metallic Electrodes for Hydrogen Evolution Reaction. *physica status solidi (RRL)–Rapid Research Letters*, *13*(12), p.1900025.

63. Guha, A., Narayanaru, S. and Narayanan, T.N., 2018. Tuning the hydrogen evolution reaction on metals by lithium salt. *ACS Applied Energy Materials*, *1*(12), pp.7116-7122.

64. Rastogi, P.K., Sahoo, K.R., Thakur, P., Sharma, R., Bawari, S., Podila, R. and Narayanan, T.N., 2019. Graphene–hBN non-van der Waals vertical heterostructures for four-electron oxygen reduction reaction. *Physical Chemistry Chemical Physics*, *21*(7), pp.3942-3953.

65. Pal, S., Bawari, S., Veettil Vineesh, T., Shyaga, N. and Narayanan, T.N., 2019. Selenium-Coupled Reduced Graphene Oxide as Single-Atom Site Catalyst for Direct Four-Electron Oxygen Reduction Reaction. *ACS Applied Energy Materials*, *2*(5), pp.3624-3632.

66. Ozden, S., Bawari, S., Vinod, S., Martinez, U., Susarla, S., Narvaez, C., Joyner, J., Tiwary, C.S., Narayanan, T.N. and Ajayan, P.M., 2019. Interface and defect engineering of hybrid nanostructures toward an efficient HER catalyst. *Nanoscale*, *11*(26), pp.12489-12496.

67. Bawari, S., Pal, S., Pal, S., Mondal, J. and Narayanan, T.N., 2019. Enhanced Photo-Electrocatalytic Hydrogen Generation in Graphene/hBN van der Waals Structures. *The Journal of Physical Chemistry C*, *123*(28), pp.17249-17254.

68. Guha, A., Narayanaru, S., Kaley, N.M., Rao, D.K., Mondal, J. and Narayanan, T.N., 2019. Mechanistic insight into high yield electrochemical nitrogen reduction to ammonia using lithium ions. *Materials Today Communications*, *21*, p.100700.

69. Kumar, V., Acharya, J., Kumar, P., Gupta, V., Kalita, P., Biswas, S., Narayanan, R.S., Santra, B., Anga, S., Jana, A. and Chandrasekhar, V., 2020. Organotin Phosphates Assembled from a Sterically Hindered Organophosphate, ArOP (O)(OH) 2,(Ar= 2, 6-(CHPh2) 2-4-i-Pr-C6H2): Syntheses and Structures. *Crystal Growth & Design*.

70. Kalita, P., Acharya, J. and Chandrasekhar, V., 2020. Mononuclear pentagonal bipyramidal Ln (III) complexes: Syntheses and magnetic properties. *Journal of Magnetism and Magnetic Materials*, *498*, p.166098.

71. Senapati, T., Dey, A., Kumar, V. and Chandrasekhar, V., 2020. Metalation Studies of Carbophosphazene-Based Coordination Ligands: Metallacages to Polymeric Networks. *Crystal Growth & Design*, *20*(4), pp.2660-2669.

72. Chelike, D.K., Alagumalai, A., Acharya, J., Kumar, P., Sarkar, K., Thangavelu, S.A.G. and Chandrasekhar, V., 2020. Functionalized iron oxide nanoparticles conjugate of multi-anchored Schiff's base inorganic heterocyclic pendant groups: Cytotoxicity studies. *Applied Surface Science*, *501*, p.143963.

73. Acharya, J., Sarkar, A., Kumar, P., Kumar, V., Gonzalez, J.F., Cador, O., Pointillart, F., Rajaraman, G. and Chandrasekhar, V., 2020. Influence of ligand field on magnetic anisotropy in a family of pentacoordinate Co II complexes. *Dalton Transactions*, *49*(15), pp.4785-4796.

74. Dey, A., Acharya, J. and Chandrasekhar, V., 2019. Heterometallic 3d–4f Complexes as Single-Molecule Magnets. *Chemistry–An Asian Journal*, *14*(24), pp.4433-4453.

75. Acharya, J., Swain, A., Chakraborty, A., Kumar, V., Kumar, P., Gonzalez, J.F., Cador, O., Pointillart, F., Rajaraman, G. and Chandrasekhar, V., 2019. Slow Magnetic Relaxation in Dinuclear CoIIYIII Complexes. *Inorganic chemistry*, *58*(16), pp.10725-10735.

76. Sengupta, D., Chandrika, D., Dey, B.K. and Ramadas, J., 2020. THE CONDITIONS, CONTEXT AND CHARACTER OF CHILDREN'S QUESTIONS IN AN OUTREACH PROGRAM. *epiSTEME 8*.

6. Conferences organised:

- Science Illustration Workshop, Host institution: TIFR-Hyderabad, Venue: Hyderabad, Dates: 05-03-2020 and 06-03-2020

- Symposium on Intense Laser Application and Innovation, Host institution: TIFR-Hyderabad, TIFR-Mumbai, STFC RAL, and IIT Madras, Venue: Hyderabad, Dates: 27-01-2020 to 29-01-2020

- National Workshop on Fluorescence and Raman Spectroscopy, Host institution: TIFR-Hyderabad, TIFR-Mumbai, Venue: Hyderabad, Dates: 16-12-2019 to 21-12-2019

- 2nd Indo-Japanese Bilateral Meeting on Magnetic Resonance, Host institution: TIFR-Hyderabad, Venue: Hyderabad, Dates: 09-12-2019 and 10-12-2019

- Pressing for progress 2019: An IPA national conference towards gender equity in Physics Host institution: TIFR-Hyderabad, Indian Physics Association, University of Hyderabad, Venue: Hyderabad, Dates: 19-09-2019 to 21-09-2019

- Science Communication workshop, Host institution: TIFR Hyderabad (workshop conducted by The Wellcome Trust / DBT India Alliance), Venue: Hyderabad , Dates: 26-08-2019 and 28-08-2019

- Structural Biology Meeting 2019, Host institution: TIFR-Hyderabad, Venue: Hyderabad, Dates: 21-08-2019

7. Invited talks:

1. Aprotim Mazumder, *Microscopic investigation of DNA damage responses and associated chromatin and transcriptional changes*, MAHE - Erasmuc MC, Rotterdam International Symposium on Genome Instability: from bench to bedside, MSLS, Manipal Academy of Higher Education, Manipal, India, January 2020.
2. Aprotim Mazumder, *Investigating DNA damage responses and associated chromatin remodeling and gene expression with tools of microscopy*, FCS2019 meeting, TIFR Hyderabad, Hyderabad, India, December 2019.
3. Aprotim Mazumder, *DNA damage responses, cancer and aging (and degeneration?),* Junior Science Club, University of Hyderabad, Hyderabad, India, August 2019.
4. Aprotim Mazumder, *Approaches to Image Segmentation*, Building Bharat-Boston Biosciences (B4) Bioimaging Workshop, IISER Pune, Pune, India, August 2019.
5. Anukul Jana, *Reversibly NHC-Coordinated Diphosphene: Synthon for Low-Valent Phosphorus Compounds and Ligand for Au(I)-Complexes,* Seminar, University of Stuttgart, Stuttgart, Germany, November 2019.
6. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals*, Seminar, Jadavpur University, Jadavpur, India, October 2019.
7. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals*, Seminar, Contai P. K. College, Contai, India, October 2019.
8. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals,* Seminar, Mahishadal Raj College, Mahishadal, India, October 2019.
9. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals,* Seminar, Indian Institute of Engineering Science and Technology Shibpur , Shibpur, India, October 2019.
10. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals*, Seminar, IISER Thiruvananthapuram, Thiruvananthapuram, India, September 2019.
11. Anukul Jana, *Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals*, Seminar, Saarland University, Sarrbrücken, Germany, May 2019.
12. Jagannath Mondal, *Computer simulation of bimolecular recognitions in real time*, 30th Mid-year meeting of Indian Academy of Sciences, IISc Bangalore, Bangalore, India, June 2019.
13. Jagannath Mondal, *Mapping substrate recognition pathway in Cytochrome P450*, Annual meeting of Chemical Research Society of India (CRSI), IIT Kanpur, Kanpur, India, July 2019.

14. Jagannath Mondal, *Quantifying Biomolecular recognitions*, DST-JSPS meeting, Kobe University, Kobe, Japan, October 2019.
15. Jagannath Mondal, *Protein-ligand binding*, Annual Chemistry symposium, IIT Gandhinagar, Ahmedabad, India, January 2020.
16. Jagannath Mondal, *Capturing protein-ligand binding in coarse-grained simulation*, Michael Klein 80th birthday celebration, JNCASR Bangalore, India, February 2020.
17. Kabir Ramola, *Stress and Geometric Response of Sheared Frictional Networks,* International Workshop on Granular and Particulate Networks, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, July 2019.
18. Kalyaneswar Mandal, *Asexual blood stage infection: invasion and adhesion*, Seminar as a resource person (MHRD-GIAN workshop on 'Malaria control strategies: drug design and vaccine development'), School of Life Sciences, University of Hyderabad, Hyderabad, India, August 2019.
19. Kalyaneswar Mandal, *Mirror-image proteins: novel protein inhibitors of natural protein-protein interactions*, Seminar (Structural Biology Meeting 2019), TIFR Hyderabad, Hyderabad, India, August 2019.
20. Kalyaneswar Mandal, *Mirror-image protein inhibitors to interfere with red blood cell invasion by Plasmodium falciparum merozoites,* Seminar (30th National Congress on Parasitology & Global Summit on Malaria Elimination), Jawaharlal Nehru University, New Delhi, India, September 2019.
21. Kanchan Garai, *Single molecule fluorescence techniques for real-time monitoring of early stages of protein aggregation*, Dr. Reddy's Laboratories, Hyderabad, India, May 2019.
22. Kanchan Garai, *Developing single-molecule techniques to study aggregation of Alzheimer's amyloid-β peptides*, Ashoka University, Delhi, India, October 2019.
23. Kanchan Garai, *Real time monitoring of amyloid aggregation to determine the microscopic rate constants*, Pan TIFR meeting, TIFR Hyderabad, Hyderabad, India, August 2019.
24. Karthik V. Raman, *Magnetic proximity effect study at the surface of a topological insulator Bi2Se3/EuS,* QMH Conference 2020, India, February 2020.
25. Karthik V. Raman, *Magnetic proximity effect study at the surface of a topological insulator Bi2Se3/EuS,* Rugters University, NJ, USA, March 2020.
26. P. K. Madhu, *Recoupling schemes in solid-state NMR in a new light,* Plenary Lecture, NTU, Singapore, Singapore, July 2019.
27. P. K. Madhu, *Nuclear magnetic resonance methods for biomolecular structure-function-dynamics,* Plenary Lecture, Jayamukhi College of Pharmacy, Warangal, India, September 2019.
28. P. K. Madhu, *Nuclear magnetic resonance: An ubiquitous spectroscopy,* Plenary Lecture, NIT Trichy, Trichy, India, September 2019.
29. P. K. Madhu, *Recoupling schemes in solid-state NMR in a new light and new avenues,* Seminar, Univ. of Leipzig, Germany, October 2019.
30. P. K. Madhu, *Nuclear magnetic resonance: Principles to hardware,* Seminar, NIT Kozhikode, Kozhikode, India, October 2019.
31. Vipin Agarwal, (Plenary Talk) *Novel1H-1H Recoupling Approaches in Fully Protonated solids at very Fast Magic Angle Spinning*, Alpine Conference on Magnetic Resonance in Solids, Chamonix Mount-Blanc, France, September 2019.
32. Vipin Agarwal, *Lab-Frame 1H-1H-Spin Diffusion in Fully Protonated Solids at Fast Magic Angle Spinning NMR,* 15thEUROMAR/19thISMAR, Berlin, Germany, August 2019.

33. Vipin Agarwal, *Novel solid-state NMR methods for protein structure determination of crystalline and non-crystalline solids at nanomolar concentration,* IIT Bombay, Mumbai, India, August 2019.
34. Vipin Agarwal, *Novel Proton-Proton Recoupling Approaches in Fully Protonated solids at very Fast Magic Angle Spinning,* 8thAsia-Pacific NMR meeting, Nanyang Technological University, Singapore, July 2019.
35. M. Krishnamurthy, *Dynamic structures enable relativistic electron generation in Microdroplets*, High energy density science (HEDS), Optics & Photonics International Congress 2019; Laser Society of Japan, Yokohoma, Japan.
36. M. Krishnamurthy, *Nano particles in intense laser matter interaction*, SERB summer school, RRCAT, SERB summer school, RRCAT Indore, India.
37. M. Krishnamurthy, *How to convert a dazzling drop to a micro-accelerator,* Dept of Physics, Annual day colloquium, IIT Hyderabad, Hyderabad, India .
38. Mustansir Barma, *Fluctuation-dominated order in an Ising model with log-range interactions,* (Plenary speaker) Workshop on Quantum and Classical Systems with Long Range Interactions, International Institute of Physics, Natal, Brazil, July 2019.
39. Mustansir Barma, *Interface growth driven by a single active particle,* (Plenary speaker) Conference on Recent topics in Statistical Mechanics, NISER Bhubaneswar, India, December 2019.
40. Mustansir Barma, *Clustering and correlations in fluctuating environments,* University of Edinburgh, Edinburgh, United Kingdom, April 2019.
41. Mustansir Barma, *Clustering and correlations in fluctuating environments,* NISER Bhubaneswar, India, November 2019.
42. Mustansir Barma, *Fluctuations and order in and out of equilibrium,* Science Day Lecture, University of Hyderabad, Hyderabad, March 2020.
43. Prasad Perlekar, *Coarsening in two-dimensional dry active matter,* Presidency University, Kolkata, India, September 2019
44. Prasad Perlekar, *Pseudo-turbulence in three-dimensional buoyancy driven bubbly flows*, IIT Kanpur, Kanpur, India, December 2019.
45. Pushpita Ghosh, *Self-organized pattern formation in Chemistry and Biology,* Indian Institute of Technology-Hyderabad, Hyderabad, India, February 2020.
46. Pushpita Ghosh, *Self-organized pattern formation in complex system*, The Institute of Mathematical Sciences, Chennai, India, February 2020.
47. Pushpita Ghosh, *Nonlinear dynamics of chemical systems under far-from-equilibrium,* TIFR – Homi Bhabha Centre for Science Education(HBCSE), Mumbai, India, December 2019.
48. Raghunathan Ramakrishnan, *Charge-transfer selectivity and quantum interference in real-time electron dynamics*, Spectroscopy and Dynamics of Molecules and Clusters, Udaipur, India, February 2020.
49. Raghunathan Ramakrishnan, *Charge-transfer selectivity and quantum interference in real-time electron dynamics,* National Symposium on Recent Advances in Chemistry, Pondicherry University, Pondicherry, India, February 2020.
50. Raghunathan Ramakrishnan, *Data-driven discoveries in chemical compound space: Trends and Challenges*, International Conference on Synergy of Sciences, Saastra University, Tanjore, India, February 2020.
51. Raghunathan Ramakrishnan, *Data-driven discoveries in chemical compound space: Trends and Challenges*, Machine learning in natural sciences, IIIT Hyderabad, Hyderabad, India, November 2019.

52. Surajit Sengupta, *The Thermodynamic Cause of Solid Rigidity or Why Engineers Need Greek Philosophy*, School of Physics, Jawaharlal Nehru University, Delhi, India, September 2019.
53. Surajit Sengupta, *The Thermodynamic Cause of Solid Rigidity or Why Engineers Need Greek Philosophy,* Department of Physics, IISER, Mohali, Chandigarh, India, September 2019.
54. T. N. Narayanan, *Functional Mesoscopic Junctions: Applications from Catalysis to Electronics*, National Conference on Soft matter and Functional Materials (SMFM2020), NIT Calicut, Kozhikode, India, March 2020.
55. T. N. Narayanan, *Molecular Interfaces for Energy Applications*, First Prof. Chellamma Mathew Memorial Lecture, Thoma College Thiruvalla, Kerala (as a part of the Diamond Jubilee Celebration), Thiruvalla, India, February 2020.
56. T. N. Narayanan, *Role of Microstructure Studies in Energy Devices*, 12th Asia-Pacific Microscopy Conference (APMC-2020), Hyderabad, India, February 2020.
57. T. N. Narayanan , *Importance of Mesoscopic Structures: From Catalysis to Electronics,* 11th Vidyasagar Satyendra Nath Bose National Workshop on Physics of Novel Functional Materials, Vidyasagar University , Midnapur, India, January 2020.
58. T. N. Narayanan , *Mesoscale Junctions: From Catalysis to Electronics,* SCICON '19 - 2nd International Conference on Advanced Materials held, Amrita Vishwa Vidyapeetham University, Coimbatore, India, January 2020.
59. T. N. Narayanan, *Importance of in situ Probes in Electrochemical Experiments,* 2nd Indo-Japanese Bilateral Meeting in Magnetic Resonance, TIFR-Hyderabad, Hyderabad, India, December 2019.
60. T. N. Narayanan, *Importance of Interfaces in Catalysis*, Indo-UK Researcher Links (Newton-Bhabha Workshop supported by British Council, RSC, and Newton Bhabha fund hosted by IISER Pune and University of Glasgow, UK), IISER Pune, Pune, India, December 2019.
61. T. N. Narayanan , *Engineered Atomic Layers: Importance of van der Waals Heterostructures in Catalysis & Devices*, 3rd FRIMS International Symposium on Frontier Materials, Nagoya Institute of Technology, Nagoya, Japan, November 2019.
62. T. N. Narayanan, *Tuning the Kinetics & Thermodynamics of Reactions by Nanostructuring*, International Conference on Physics of Materials & Nanotechnology (ICPN-2019), Mangalore University, Mangalore, India, September 2019.
63. T. N. Narayanan, *Two Dimensional Heterostructures in Catalysis & Devices*, A Meet on 2D Materials, S. N. Bose National Center for Basic Sciences, Kolkata, India, September 2019.
64. T. N. Narayanan, *Molecular Junctions for Catalysis and Beyond*, Kaleidoscope – 2019, Goa, India, July 2019.
65. T. N. Narayanan , *Mesoscopic Interfaces: Catalysis to Electronics*, International Conference on Advanced Materials (ICAM2019), Nirmalagiri College, Kannur, India, June 2019
66. Tamal Das, *Mechanobiology of Collective Cell Dynamics: Force-dependent Reorganization and Dynamics of Cellular and Multicellular Elements*, Molecular Motors, Transport and Trafficking (M2T2) Meeting, National Brain Research Center (NBRC), Manesar, India, October 2019.
67. Tamal Das, *Mechanobiology of Collective cell dynamics: Cell Migration and Competition in Epithelium,* Unraveling Cellular Processes - models and experiments, Indian Academy of Science (IAS), Coorg, India, December 2019
68. Tamal Das, *Mechanobiology of Collective cell dynamics: Cell Migration and Competition in Epithelium*, CompFlu 2019, IISER Bhopal, Bhopal, India, December 2019
69. Tamal Das, *Mechanobiology of Collective cell dynamics: Cell Migration and Competition in Epithelium*, FCS 2019, TIFR Hyderabad, Hyderabad, India, December 2019

70. Tamal Das, *Mechanobiology of Cell Competition: A Force-Perspective to Tumor Suppression,* Conference cum Workshop on Phenotypic Heterogeneity as a Driver of Cancer Progression, Indian Institute of Science (IISc), Bengaluru, India, January 2020
71. Tamal Das, *Mechanobiology of Collective Cell Migration,* Cell Migration: Biophysical and Mathematical perspective, Savitribai Phule Pune University, Pune, India, February 2020.
72. Nitin Paul, D. Chandrika & Jayashree Ramadas, *The 'What, Why and How?' of building 'Sawaliram*', The International Institute of Information Technology, Hyderabad, India, September 2019
73. Jayashree Ramadas, *The many tongues of 'Sawaliram'*, A celebration of 25 years of Jantar Mantar, Tamil Nadu Science Forum, Institute of Mathematical Sciences, Chennai, India, November 2019.
74. Jayashree Ramadas and D. Chandrika, *A lifespan view of curiosity and questioning*, Azim Premji University Undergraduate Campus, Bangalore, India, February 2020.
75. Jayashree Ramadas and D. Chandrika, *Exploring gaps in curiosity and education: clues from recent Indian studies*, Azim Premji University Postgraduate Campus, Bangalore, India, February 2020.
76. Pranav R. Shirhatti, *Quantum state selective preparation and detection of molecules*, SCOP-2019, Physical Research Laboratories, Ahmedabad, India, September 2020.
77. Pranav R. Shirhatti, *Neutral atom/molecule scattering: A soft and universal probe for surfaces*, Workshop on modern topics in Chemical Physics, Max Planck Institute for Biophysical Chemistry, Meeting, Gottingen, Germany, May 2019.

8. New initiatives:

- An MoU was signed with Konstantin Ivanov, International Tomography Centre, Novosibirsk, Russia, and TIFR Hyderabad (with P. K. Madhu) for research activities in magnetometry and zero-field NMR, exchange of students, and organisation of workshops.

- A new project exploring how lysosomes might influence the emergence of leader cells during collective cell migration was initiated by Tamal Das and colleagues. Collective cell migration during embryonic morphogenesis, cancer metastasis, and wound healing critically depend on the selective emergence of few leader cells at the front. However, the intracellular changes that enable only a fraction of cells to become the leaders remain elusive. Guided by their preliminary results, Das' lab started a project addressing whether a specific organelle, lysosomes, might play a role in the emergence of leader cells. They discovered that the leader cells at the epithelial wound- margin indeed appeared through a force-responsive alteration of lysosome position and biochemistry. In these cells, lysosomes relocated to the cell periphery and promoted actin- branching by recruiting active Rac1 molecules. These results together indicated a broader role of lysosomes beyond their well-known catabolic activity and opened up new directions in lysosome biology and cell migration research.

- Smarajit Karmakar and Kalyan Kumar N have set up another small HPC facility (~40TF) partly from Smarajit Karmakar's SERB grant and partly from Institute to work on the mechanical properties of active amorphous solids. Karmakar and colleagues will be looking at the brittle to ductile transition under non-equilibrium active forces. This research will have importance in understanding the mechanical properties of biological systems like cell monolayer.

- Identification of roles of polyphosphate biology in multicellular organisms: Polyphosphates are important biomolecules and exist throughout evolution. While their function in bacteria is well studied, their function in multicellular organisms remains obscured. To study the function of Polyphosphate in multicellular organisms, Manish Jaiswal's lab initiated developing a model system using fruit flies. Initial goals are to develop methods to detect Polyphosphate in flies followed by methods to develop genetic manipulation of Polyphosphate levels. Towards this goal, they have standardized methods to measure Polyphosphate in flies using a biochemical approach. Jaiswal and colleagues have also created transgenic fly lines to deplete polyphosphates in tissue specific manner, which will allow them to study the impact of Polyphosphates depletion during development and physiology.

- The following initiatives were taken up by Adish Dani: 1) Operationalizing and development of the SPF mouse facility at TFR Hyderabad with the idea of starting mouse sperm cryo preservation and in-vitro fertilization (IVF) to preserve and reserve specific mouse lines (with help from Gopalkrishna, SO). 2) Conceptualization and implementation of a Basic Molecular Biology training course for Covid-19 diagnosis (along with other faculty and SOs).

9. Significant achievements:

1. The NMR group (P. K. Madhu, Kaustubh R. Mote, Vipin Agarwal) made contributions in the direction of geometry elucidation and resolution enhancement in solid-state NMR with high magic-angle spinning (MAS) experiments. The MAS frequency was around 100-110 kHz, the fastest such in the country. Efforts are on now to find structures of molecules with minimal amount of sample.

2. Graphene oxide (GO) based catalysts promise cheap, renewable, and light alternatives to commercial metal-based catalysts. In this effort, researchers uncovered the differences that boron and nitrogen doping in GO, synthesized in different permutations, can have on its structure. In a collaboration between T. N. Narayanan, Jagannath Mondal and P. K. Madhu, doped GO was synthesised, and subsequently characterised by solid state-NMR spectroscopy. A reactive molecular dynamics approach, shows the change in the micro-structure of a catalyst as it is formed at high temperatures. Utilising insight from these simulations, coupled with experimental characterisation, the authors were able to explain differences in hydrogen evolution which occur when the catalyst is formed in different ways.

3. Atomically thin sheets, like MoS2, are on the forefront as electronic devices with enhanced functionality not possible with traditional silicon electronics. In this work, a collaborative effort uncovers the possibility of inducing magnetism in non-magnetic MoS2 by layering with Iron. After growth of MoS2/Fe and preliminary magnetic measurements in T. N. Narayanan and K. V. Raman's labs, subsequent measurements of the spin hall effect of light (SHEL) were performed in Nirmal Vishwanathan's lab at University of Hyderabad. Magnetisation of MoS2, by simple Iron layering, increase the repertoire of applications that MoS2 can be used in.

4. Proteins, apart from their functional properties, comprise of various types of functional groups which can have implications in other fields of research. Researchers from K. Mandal's lab synthesised proteins mounted on carbon nanotubes, which are stable and conducting templates. These supported proteins, when studied as hydrogen evolution catalysts in T. N. Narayanan's lab, showed promising activity which enhances as the protein unfolds. A clear correlation with conducting and/or nitrogen containing amino acids, with hydrogen evolution was also seen for protein functionalized CNTs.

5. Metal-ligand complexes afford different functionalities to a central metal atom just on the basis of the ligands surrounding it. In this work, Co complexes with minor differences in the Co environment,

developed in V. Chandrashekhar's lab, showed enormous differences in the water oxidation process, studied in T. N. Narayanan's lab.

6. Jagannath Mondal and Surajit Sengupta’s groups identified the kinetics behind the slowly evolving conformational changes in biomacromolecules. The quantifier for non-affinity, Global non-affinity parameter, holds the promise of acting as an optimal CV for accurately projecting the free energy landscape.