1. Research Highlights:

- Structural Characterization of RNA Triple Helix: (Anand Teertha Vaidya)
  The central aspect of life involves conversion of DNA to RNA and RNA to protein. Though some RNA molecules are not converted to protein, they still play an important role in controlling the process of DNA to RNA to protein. This places RNA as a central component of life. Along with a double helical structure, RNA also adopts complex 3D shapes, which are important for its function. Many RNA molecules have a chemical attachment called the poly(A) tail that is important for its stability. A new type of RNA called ENE forms triple helix structures with the poly(A) tail and protects the RNA from degrading. The crystal structure of this new class of ENE called 'double ENE' was determined. This provided key insights into new RNA-RNA interactions. Along with the triple helix, a new RNA pocket was discovered that binds the end of the poly(A) and protects it.

- Investigating Gene Expression and DNA damage responses at a single cell resolution: (Aprotim Mazumder)
  Mazumder's lab is broadly interested in processes of DNA damage responses (DDR) and gene expression. Understanding DDR is critical for elucidating cancer emergence. The group's experiments indicated that DNA damage response peaks in the S phase, and not primary damage. Mazumder's lab also optimized a method for combining DNA and RNA smFISH to interrogate gene position and expression at the same time. In another study, using single molecule mRNA detection in the context of EGFR signaling in the fruit-fly, this group provided critical insight into cell-type emergence during organismal development. Also, the researchers had previously described how fluorescence anisotropy can be used to monitor chromatin compaction states. They showed compaction of even undamaged DNA in response to localized double strand breaks.

- Anionic Boron- and Carbon-Based Hetero-Diradicaloids Spanned by a p-Phenylene Bridge: (Anukul Jana)
  The design and synthesis of open-shell singlet diradicals have attracted much interest due to their synthetic challenges and unique physical properties, making them interesting for potential applications in materials science. Jana's group disclosed the synthesis and characterization of first anionic heteronuclear boron- and carbon-based Kekulé diradicaloids spanned by a p-phenylene bridge. In contrast to homonuclear carbon-based Thiele's

hydrocarbon, a closed-shell singlet system, heteronuclear boron- and carbon-based Kekulé diradicaloids showed an appreciable population of the triplet state at room temperature, as evidenced by both NMR and EPR spectroscopy. The work provides a novel structural motif of π-conjugated molecules with small singlet-triplet gaps involving an electron-deficient heteroatom. Moreover, en route to these anionic boron- and carbon-based hetero-diradicaloids, the formation of an isolable diamino(4-diarylboryl-phenyl)methyl radical was achieved. Given the modular synthetic methodology established in this study, different kinds of diradicaloids can be envisioned which merit further investigation into their potential applications in functional materials.

- Computer simulation at the interface of chemistry and biology: (Jagannath Mondal)
  Mondal's group focusses on computer simulations of certain chemical and biologically relevant phenomena. The investigation has shed light into the protein/drug recognition processes. The simulation highlighted the role of conformational diversities in protein/substrate recognition. A certain direction elucidated the role of osmolytes in stability of protein. In another study, the group developed a model of bacterial cytoplasm. The project integrated experimental data in a model and discovered macrodomain segregation inside bacterial chromosome. The researchers also initiated a collaboration on exploring host-guest interaction in caged molecules for developing sensors. An existing collaboration led to discovery of allosteric switches in an ammonia-sensing protein. Finally, a continued collaborative effort led to the observation of structural evolution in doped graphene oxide systems.

- Stability and Response of Athermal Amorphous Solids: (Kabir Ramola)
  Kabir Ramola's group has been studying the mechanics and rigidity of naturally abundant amorphous solids such as granular materials and structural glasses: materials that are not described by conventional paradigms of broken symmetry. In collaboration with other researchers, they developed a field theory for amorphous systems that shows a remarkable agreement with numerical simulations as well as experiments. In other recent work, they have also analytically demonstrated the presence of long-range correlations in such athermal systems that arise from disorder at the microscopic scale. Recently, analytic results were also derived for the Hessian matrices that govern the stability of such solids. Additionally, recent numerical work with collaborators has also highlighted the importance of choosing the right ensemble from which configurations are sampled when studying the vibrational properties of amorphous solids.

- A radically simplified total chemical protein synthesis utilizing Fmoc-group as an N-masking group of reactive cysteine (Kalyaneswar Mandal)
  Easy access to multi-segment, fully convergent or one-pot, native chemical ligations greatly facilitates total chemical synthesis of proteins. A robust and operationally simple method for total chemical protein synthesis has been developed exploiting the Fmoc moiety as a temporary masking group of the N-terminal reactive Cys residue of Cys-peptide thioester segment(s). The Fmoc group was found to be fully compatible with harsh oxidative conditions frequently used to generate peptide thioesters from hydrazide or o-aminoanilide. The ready availability of the Fmoc-Cys(Trt)-OH, routinely used in Fmoc chemistry solid phase peptide synthesis, where the Fmoc group is pre-installed on cysteine residue, minimized additional steps required for the temporary protection of the N-terminal cysteinyl peptides.

Notably, the exceedingly efficient method demonstrated in this study would be very useful for high yielding chemical protein synthesis and will be widely accepted by the chemistry and chemical biology community worldwide.

- Study of protein aggregation using single molecule techniques: (Kanchan Garai)
  Aberrant aggregation of proteins is involved in the pathology of multiple debilitating human diseases. Early intermediates or the soluble oligomers are considered the proximal cytotoxic species. However, study of these oligomers is challenging due to rare population and heterogeneity. Garai's lab has developed two single molecule techniques, viz, superresolution fluorescence microscopy and two-color coincidence detection to detect and characterize the early aggregates and the soluble oligomers respectively. Recently, they have shown that molecular chaperone Hsp70 interacts with the oligomers but not the monomers of IAPP, which is involved in the pathology of type2 diabetes. Using superresolution microscopy, the researchers have also detected the complexes of apoE and amyloid-beta peptide, which is involved in Alzheimer's disease. These studies open up the possibility of screening of potential drug candidates that may alter the interaction of endogenous proteins with the amyloidogenic peptides.

- Proximity effect studies in quantum materials: (Karthik V. Raman)
  The group demonstrated proximity effect studies between organic molecules and ferromagnets by introducing a new mechanism of crane-pulley effect. The work showed that molecules when placed on magnetic surfaces can magnetically detach the surface magnetism from the bulk magnetism giving rise to an exchange-bias effect. In another study, the researchers explored proximity effect studies between topological insulator and ferromagnetic insulators showing that surface states of topological insulators can enhance the Curie temperature of the ferromagnet via the conduction electron mediated RKKY interactions. Raman's group successfully demonstrated the establishment of a world's first cryogen free scanning tunneling microscopy integrated to a cryogen-free vector-superconducting magnet. Also, they explored Berry-curvature effect studies in sputter deposited polycrystalline films of kagome material Manganese Platinum.

- Structural Biology of Active Transporters and Actins: (Kaustubh R. Mote)
  The main focus of the lab is to study how membrane proteins and actins function. To do this, Mote's group uses a combination of solid-state NMR spectroscopy and other biophysical techniques. In the past year, they have achieved the following: (1) Refolding of a membrane protein MPC for downstream structural biology work using solid and solution NMR studies. They have developed an assay to monitor its activity in vitro. (2) Expressed and purified a bacterial actin ParM. The researchers have developed assays for downstream structural biology work. (3) They applied their recently developed NMR techniques based on the rotational-echo double resonance sequence to determine protein dynamics at very fast MAS frequencies. (4) They have developed a technique to simultaneously acquire assignments and structural restraints under slow magic-angle spinning, which will help speed up much of the work on the above topics.

- Direct two electron attachment to fast hydrogen: (M. Krishnamurthy)
  Direct two electron attachment is an extremely weak process that has eluded most terrestrial observations in atomic physics. Three body recombination of H to H- is a fundamental process that is relevant in astrophysical measurements but the conflicting

requirements of high electron density with low temperature with low quasi-static fields have made this observation impossible thus far. In continuation with the researchers' interests in electron ion recombination in high contrast and high intense lasers, they found this inconceivable reaction take place. Its observation has only been possible now in this research group's experiments due to their enhanced gated- Thomson parabola spectrometry developed in house recently. Krishnamurthy and colleagues established that recombination of ions that co-propagate with electrons in a universal scheme prevalent in all the intense laser experiments and in fundamental to all the studies, just that these processes have been missed in the 3 decades of this research.

- Polyphosphates: (Manish Jaiswal)
  Inorganic polyphosphate (polyP), orthophosphate residues of varying chain lengths, is found in all living organisms. Its functions in metazoans are largely underexplored. However, the major limitation in testing the functions of polyP in metazoans has been the lack of knowledge of the genes involved in polyP synthesis and turnover, which restricts modulation of polyP levels in vivo. Manish Jaiswal's lab has developed a Drosophila model to study the functions of polyP. They showed that polyP exists in flies and that its levels are developmentally regulated during embryogenesis. Further, through phylogenetic analysis, a putative exopolyphosphatase Prune was identified. A significantly higher level of polyP was found in prune mutants as compared to wild-type flies. Since mutations in prune were shown to be linked to neurodegeneration, this work suggested that the Prune mediated regulation of polyP is crucial for the protection of neurons among many other processes in a multicellular organism.

- Strategies for Survival: (Mustansir Barma)
  How should dispersal strategies be chosen to increase the likelihood of survival of a species? Barma and colleagues obtain the answer for the spatially extended versions of three well-known models of two competing species with unequal diffusivities. Though identical at the mean-field level, the three models exhibit drastically different behavior leading to different optimal strategies for survival, with or without a selective advantage for one species. When the total particle number is fixed, dispersal has no effect on survival probability. With a fluctuating number, faster dispersal is advantageous if species competition is present between members of the same species, while moving slower is the optimal strategy for the disadvantaged species if there is no intra -species competition: it is imperative to include fluctuations to properly formulate survival strategies.

- Enhancing resolution and information content in and from solid-state NMR spectra: (P. K. Madhu)
  This group has developed methods in solid-state nuclear magnetic resonance to improve spectral resolution and easy extraction of geometry parameters over a wide range of experimental conditions currently in vogue. The methods help in obtaining internuclear distances and order parameters in a given molecule. These lead to structural and dynamics information, the latter being a unique aspect of NMR spectroscopy. Salient features of these methods include robustness to various experimental parameters, less to no parameters to optimise, ease of extraction of information, and targeting couplings in both strong and weak regimes. The methods have been shown to be useful in a variety of molecular systems, from small molecules to proteins.

- Confronting the Invisible: Assignment of Protein $^{1}H^{N}$ Chemical Shifts in Cases of Extreme Broadening: (Pramodh Vallurupalli)
  Vallurupalli's group is mainly interested in studying the conformational dynamics of proteins as it is critical to their function, folding, misfolding etc. Two accomplishments in 2020-2021 are:
  1) Development of a new NMR method to detect amide 1H nuclei that cannot be detected in IDPs etc due to solvent exchange.
  2) Development of a new CEST experiment to study slow conformational exchange at Gly 1Halpha sites.

- Imaging single atomic layer thin films using atom scattering as a probe: (Pranav R. Shirhatti)
  A neutral atom scattering based surface probe technique for imaging surfaces was developed. The work involved testing and characterization of the experimental setup in order to optimize the signal to noise ratio and measurement speed. Using the soft and universal nature of slow (65 meV) Helium atom scattering, Shirhatti's group was able to demonstrate that ultra thin MoS_2 films as thin as a single monolayer, can be successfully imaged. Based on a comparison with Kr atom scattering, the researchers hypothesized that the contrast generation occurs due to the different local roughness of the SiO_2/Si and the ultra thin films of MoS_2. This work paves the way for future developments and studies in 'neutral atom scattering based microscopy'.

- Instabilities and turbulence in complex fluids: (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. Perlekar and colleagues consider groups of motile organisms in a bulk fluid medium. Using linear stability analysis, and numerical simulations, they are investigating the physics of complex spatiotemporal flow patterns that are generated in these systems.

  The flow of suspension of deformable objects (bubbles or droplets) is omnipresent in a variety of natural and industrial processes. The presence of bubbles dramatically alters the rheological and thereby mixing properties of flows. In the absence of bubbles, a nonlinear transfer of energy (maintaining constant energy flux) from forcing to dissipation range characterizes turbulence. How does the presence of bubbles modify this flow? Using Direct Numerical Simulation (DNS) and tools from statistical physics, Perlekar and colleagues are investigating the underlying energy transfer mechanisms.
- Waves and patterns in spatially-extended systems: (Pushpita Ghosh)
  During this year, research efforts were carried out across two different areas under a common theme to explore the spatiotemporal dynamics of complex systems of chemical and biological interest. Pushpita Ghosh investigated thermodiffusion induced emergent traveling and shock waves in a self-propelled colloidal system. The study has provided a route towards development of shock waves by adjusting the initial and boundary conditions. Along the same lines, another study was conducted to explore the role of time-delay of diffusive flux in a one-variable reaction-Cattaneo system. This work is particularly important in the context of biological population dynamics where a better description of dispersion is needed rather than standard diffusion. Another study was conducted to explore the collective

spatiotemporal dynamics of bacteria, which differ, only by their cell-aspect ratio. The study reveals that both shorter and longer bacteria exhibit slow dynamics whereas the fastest motion is obtained for intermediate aspect ratios as observed in some of the recent experimental studies.

- Nonlinear magnetoelectric effect in atomic vapor: (G. Rajalakshmi)
  Magnetoelectric (ME) effect refers to the coupling between electric and magnetic fields in a medium that causes the magnetic fields to induce electric polarization and vice versa. So far, the exclusive studies on the nonlinear ME effect are mostly concerned with the investigation of second-harmonic generation in chiral materials. G. Rajalakshmi and colleagues demonstrated nonlinear wave mixing of optical electric fields and radio-frequency (rf) magnetic fields in thermal atomic vapor, which is the consequence of the higher-order nonlinear ME effect in the medium. The experimental results are explained by comparing with density matrix calculations of the system. They also experimentally verified the expected dependence of the generated field amplitudes on the rf field magnitude as an evidence of the magnetoelectric effect. This study can open up the possibility for precision rf-magnetometry due to its advantage in terms of larger dynamic range and arbitrary frequency resolution.

- Glassy dynamics and aggregation in cellular and intra-cellular systems: (Saroj K. Nandi)
  Saroj Nandi's group theoretically studies the physical principles behind the slow dynamics and aggregation in different biological systems. In two recently published articles, they have studied two distinct problems with long-standing applications in biology. a) The first problem investigates the principles of how protein-protein interactions and their valency affect the intracellular phase separation. A multidisciplinary approach was undertaken with experimentalists from Weizmann Institute of Science, Israel. Through a combination of theory, simulation and expressing synthetically designed proteins in yeast cells, this study yielded intriguing results on how interaction strength determines the extent of phase separation whereas valency determines its symmetry. b) The second problem looks at glassy dynamics in a confluent monolayer. This dynamics is indispensable in morphogenesis, wound healing, bronchial asthma, and many others; and therefore, a detailed theoretical framework for such a system is important. Nandi's group combines numerical simulations of such a model system and an analytical study based on one of the most successful theories of equilibrium glass (the random first order transition theory) to develop a comprehensive theoretical framework for a confluent glassy system.

- Signature of dynamical heterogeneity in spatial correlations of particle displacement and its temporal evolution in supercooled liquids: (Smarajit Karmakar)
  Dynamic heterogeneity (DH) is believed to be one of the hallmarks of glass transition. Numerous studies have been performed to understand this at alpha-relaxation timescale of the liquid. Karmakar and colleagues have shown that DH develops completely at very short timescale and survives much beyond the alpha-relaxation time. Temperature dependence of DH length scale is found to remain same for all timescales but the magnitude of the length scale reaches maximum at alpha-relaxation time for molecular liquids. In contrast for models that undergo jamming transition like colloidal model, length scale continues to grow much beyond alpha-relaxation time, where other measures of DH dies out completely.

- Understanding mechanism of Cu-based bidirectional catalyst for O2/H2O conversion: (Soumya Ghosh)
  This work highlights the underpinnings of one of the rare examples of a bidirectional catalyst. This Cu-based complex can catalyze both reduction of dioxygen to water and oxidation of water to dioxygen depending on the applied voltage. Experimental observations indicated the in situ formation of a dimeric complex during both the oxidation and reduction cycles. Extensive computational studies supported the feasibility of a binuclear mechanism both for oxidation and reduction pathways. Computational studies further explored the structural flexibility of the associated ligand framework that supports various oxidation states of the two Cu-centers in the intermediate complex that facilitates the catalysis. In addition, the computations predicted the existence of Cu(III) species during reduction, even though the cycle started with Cu(II) oxidation cycle. This prediction was also confirmed experimentally.

- Rechargeable Respiratory Mask using Graphene Oxide: (T. N. Narayanan)
  Electrostatically rechargeable respiratory masks having the standards of 'N95' have been developed using graphene oxide based ink. It has been shown that such a low cost mask can effectively stop the sub-micron sized particles with good quality factor, a measure ensuring the breathability with the mask. The melt-spun polypropylene, available in a conventional N95 mask, modified with graphene oxide and polyvinylidene fluoride mixture containing paste using a simple solution casting method acts as active filtration layer. The efficacy of this tri-layer system toward triboelectric rechargeability using small mechanical agitations is demonstrated here. These triboelectric nanogenerator assisted membranes have high electrostatic charge retention capacity (~1 nC/cm2 after 5 days in ambient condition) and high rechargeability even in very humid conditions (>80% RH).

- Collective dynamics of cells: A mechanobiological perspective (Tamal Das)
  Collective cell dynamics refers to the process of many cells acting as a cohesive unit. Das' group addressed how cell-generated forces govern the collective dynamics of cells during cell competition and collective cell migration, using numerous biophysical methods and super-resolution microscopy techniques. In cell competition, it was found that the competition between HRAS oncogene-transformed cells and their normal neighbors was determined by cell generated forces and the elasticity of extracellular matrix, with pathologically stiffened matrix abrogating the competitive removal of transformed cells. In collective cell migration, cell-cell forces were found to govern the structure, localization, and dynamics of intracellular organelles, including the Golgi complex, lysosomes, and the endoplasmic reticulum. Taken together, importance of mechanical forces on cell competition and collective cell migration was established by their research efforts.

- Single-molecule and single-ion magnets: (V. Chandrasekhar)
  Single-molecule magnets are a family of molecular magnets that encompass other subsets including single-ion magnets and single-chain magnets. Two factors seem to govern the properties: the magnetic anisotropy and the overall spin. V. Chandrasekhar's group has been focusing on these by appropriate design of the ligand that allow assembly of such complexes.

- Proton Triple Quantum Spectroscopy at fast MAS: (Vipin Agarwal)
  Proton triple quantum (TQ) has been challenging in the solid-state mainly due to poor excitation efficiencies (4-8%) and prominent t1- noise. TQ improve structural understanding of systems with complicated spin topology. Agarwal and colleagues have designed five TQ

recoupling sequences ((RNnvRNn-v)31) that employ second-order Hamiltonian that minimize t1-noise and have 3-4 fold higher TQ excitation efficiency. The TQ terms was generated as a cross-term between the T2±2j,k and T2±1j,k operators in the second-order Hamiltonian. The three-dimension TQ-DQ-SQ proton spectrum on unlabeled samples can be recorded in less than 1.5 days that would otherwise take a week of measurement time. The improved experiment allows the characterization of spin-topology in unlabeled samples.

- Molecular Biology of Vomeronasal system and Molecular architecture of auditory ribbon synapses: (Adish Dani)
  A. The vomeronasal organ is an important model sensory system to understand how sensory stimuli elicit innate behaviors. Dani and colleagues have developed a combination of RNA sequencing approaches to understand the transcriptomes of sensory neurons. These approaches revealed novel molecular components that are being investigated further.
  B. Using a single molecule microscopy, Dani and colleagues imaged specialized ribbon synapses in the mouse cochlea with a goal to understand their molecular architecture and how noise induced hearing loss can affect these synapses.

- Electronic properties of halide perovskite and organic semiconductors: (Pabitra K. Nayak)
  Nayak and colleagues contributed to the understanding of the role of vibronic modes in charge carrier dynamics in halide perovskites. They showed how photoinduced vibrations contribute towards an ultrafast structural distortion in lead halide perovskite. In a similar study, they showed how intermolecular vibrations facilitate the singlet fission in pentacene. Using solid state NMR technique, Nayak's group provided information on the role of piperidinium salt towards the stabilization of metal-halide perovskite solar cells. Using Kelvin probe based measurements, the researchers unraveled the types of defects present in double halide perovskite Cs2AgBiBr6 and their impact on the solar cell performance.

- Mechanical properties of Materials: (Surajit Sengupta)
  Sengupta's group was actively involved in the development of a theoretical model that takes a new approach to classify atomic fluctuations viz. affine and non-affine. This alternative classification has not only provided new insights into materials physics but finds its application in programmable active matter and frontiers of biology. A few of these applications include protein conformation and drug binding. In the former, the yielding of crystalline solids upon deformation due to an externally applied mechanical load was investigated. Combined with extensively large in-house computations, the theoretical model predicts experimentally observed yield points over the fourteen orders of magnitude of deformation rates. Intriguingly, the study reveals that yielding of a defect free crystal is, in fact, a hidden first order phase transition. These surprising results demand a review of widely accepted viewpoints on the phenomena of yielding or, in general, physics of materials. The group further advanced the knowledge and show a swarm of programmable active matter, such as drones can be stabilised in any desired pattern, whatsoever, against the destabilising turbulent weather. The crucial ingredient here involves suppressing a certain class of fluctuations, non-affine displacements that are responsible for the disruption of pattern while simultaneously allowing trivial translations and rotational capabilities to the swarm.

- Gateway Vectors for Efficient Protein Production based on Kanamycin and Streptomycin Selection in *Escherichia coli:* (Deepa Balasubramanian, Protein expression and purification study with Sreejith Rarankurrussi)

Balasubramanian helped Rarankurrussi modify the existing gateway cloning technique by creating a kanamycin based entry clone so that insoluble protein and soluble protein can easily be expressed.

- RT-LAMP: A Simple Calorimetric Diagnostic Tool for COVID-19 Viral RNA Detection: (Manish Jaiswal, Sreejith Rarankurrussi, Sunayana Sarkar and Deepa Balasubramanian)
  Loop-mediated isothermal amplification (LAMP) is a single-tube technique for the amplification of DNA and a low-cost alternative to detect certain diseases. In LAMP, the target sequence is amplified at a constant temperature of 60–65 °C using either two or three sets of primers and a polymerase with high strand displacement activity in addition to a replication activity. Typically, 4 different primers are used to amplify 6 distinct regions on the target gene, which increases specificity. An additional pair of "loop primers" can further accelerate the reaction. Currently, the researchers are testing the sensitivity of LAMP-based assay against PCR based amplification which is widely used for testing SARS-COV-2 samples.

  Additionally, Balasubramanian participated in the COVID training program conducted by the institute carried out following activities under the guidance of Manish Jaiswal -
  a) arranged and provided the materials that were required for the training program.
  b) instructed volunteers to perform the required experiments
  c) carried out the experiments such as RNA extraction followed by Realtime PCR and data analysis with the registered volunteers.
  d) coordinated the planning activities required for the training.
  e) arranged for the indents and purchase requirements along with Sreejith Rarankurrusi for the training.

- Sreejith Rarankurrusi actively participated in the research design and execution of the NMR group's entire protein production efforts. He prepared close to 100 new plasmids and re-engineered many existing protein constructs in the laboratory to suit the large-scale protein production efforts. He standardized the expression and purification protocols for many proteins that are produced in the laboratory. Fusion proteins and other molecular biology tools like proteases for tag removal are also regularly prepared for the entire laboratory. Rarankurrussi is also involved in various method developments to promote better expression and purification of labeled proteins in *E. coli*.

- Deepa S. has been involved in the SEC/FFF MALS studies on Hsp 70 protein & amylin peptide (for Kanchan Garai's research group) and AC monomer/dimer protein (for Vipin Agarwal's research group) along with the regular LC MS spectra recordings and other biophysical instruments assistance for different research groups.

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

Faculty	: 27 + 4 (Emeritus -1, Visiting Faculty-2, Inspire Faculty-1)
Research Scholars	: 114
Junior Research Fellows	: 30
Senior Research Fellows	: 22
Post-doctoral fellow	: 45
Project Associates	: 08
Visiting Students	: 13

Visiting Fellows	: 01
Short Term Visitors	: 04
Scientific Staff	: 23 (01 out sourced out of 23)
Technical Staff	: 09 (04 out sourced out of 09)
Admin Staff	: 25 (02 out sourced out of 25)
Auxillary Staff	: 66 (65 outsourced out of 66, Security-12, HK-15, Canteen-15, HVAC-07, Gardener-02, Electrical & Fire safety-09, Plumbing Staff-03, STP operator-01, Carpenter-01)

3. Awards/Distinctions:

No.	Name of the Awardee	Scope (National/ International)	Name of the Award	Awarding / Electing Body	Date
1.	Anand T. Vaidya	National	Ramalingaswami Fellowship	DBT, Govt. of India	March 2021
2.	Anusheela Chatterjee and Aprotim Mazumder	National	The 1st IndiaBioscience Outreach Grant Award	IndiaBioscience	September 2020
3.	Karthik V. Raman	National	INSA young Scientist award	INSA	October 2020
4.	P. K. Madhu	International	Member, Advisory Editorial Board Team	Magnetic Resonance in Chemistry	December 2020
5.	T. N. Narayanan	International	Journal of of Materials Chemistry A - 2020 Emerging Investigators	Royal Society of Chemistry	2020
6.	T. N. Narayanan	National	Prof. Prakash P. Karat Endowment Lecture - 2021	St. Aloysius College, Mangalore, Karnataka	2021

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

Ph.D. : 9

M.Sc. : 1

5. Publications:

1) Torabi, Seyed-Fakhreddin, Anand T. Vaidya, Kazimierz T. Tycowski, Suzanne J. DeGregorio, Jimin Wang, Mei-Di Shu, Thomas A. Steitz, and Joan A. Steitz. "RNA stabilization by a poly (A) tail 3′-end binding pocket and other modes of poly (A)-RNA interaction." *Science* 371, no. 6529 (2021).

2) Dhuppar, Shivnarayan, Sitara Roy, and Aprotim Mazumder. "γH2AX in the S phase after UV irradiation corresponds to DNA replication and does not report on the extent of DNA damage." Molecular and cellular biology 40, no. 20 (2020). *(selected for cover image)*

3) Dhuppar, Shivnarayan, and Aprotim Mazumder. "Investigating cell cycle-dependent gene expression in the context of nuclear architecture at single-allele resolution." Journal of Cell Science 133, no. 12 (2020).

4) Kesavan, P. S., Darshika Bohra, Sitara Roy, and Aprotim Mazumder. "Monitoring global changes in chromatin compaction states upon localized DNA damage with tools of fluorescence anisotropy." Molecular biology of the cell 31, no. 13 (2020): 1403-1410.

5) Chandradoss, Keerthivasan Raanin, Bindia Chawla, Shivnarayan Dhuppar, Rakhee Nayak, Rajesh Ramachandran, Sreenivasulu Kurukuti, Aprotim Mazumder, and Kuljeet Singh Sandhu. "CTCF-Mediated Genome Architecture Regulates the Dosage of Mitotically Stable Mono-allelic Expression of Autosomal Genes." Cell Reports 33, no. 4 (2020): 108302.

6) Male, Gurranna, Pallavi Deolal, Naresh Kumar Manda, Shantam Yagnik, Aprotim Mazumder, and Krishnaveni Mishra. "Nucleolar size regulates nuclear envelope shape in Saccharomyces cerevisiae." Journal of Cell Science 133, no. 20 (2020).

7) Maiti, Avijit, Fangyuan Zhang, Ivo Krummenacher, Moulika Bhattacharyya, Sakshi Mehta, Michael Moos, Christoph Lambert et al. "Anionic Boron-and Carbon-Based Hetero-Diradicaloids Spanned by ap-Phenylene Bridge." Journal of the American Chemical Society 143, no. 10 (2021): 3687-3692.

8) Jana, Anukul, Debdeep Mandal, Shubhadeep Chandra, Nicolás I. Neuman, Arighna Sarkar, Abhinanda Kundu, Srinivas Anga et al. "Activation of Aromatic C-F Bonds by a N-Heterocyclic Olefin (NHO)." *Chemistry–A European Journal* (2020).

9) Mandal, Debdeep, Felix Stein, Shubhadeep Chandra, Nicolás I. Neuman, Pallavi Sarkar, Shubhajit Das, Abhinanda Kundu et al. "Trisubstituted geminal diazaalkene derived transient 1, 2-carbodications." *Chemical Communications* 56, no. 59 (2020): 8233-8236.

10) Anga, Srinivas, Shubhadeep Chandra, Pallavi Sarkar, Shubhajit Das, Debdeep Mandal, Abhinanda Kundu, Hemant Rawat et al. "Facile One-Pot Assembly of Push–Pull Imines by a Selective C–F Substitution Process in Aryl Fluorides." *European Journal of Organic Chemistry* 2020, no. 48 (2020): 7445-7449.

11) Maiti, Avijit, Shubhadeep Chandra, Biprajit Sarkar, and Anukul Jana. "Acyclic diaminocarbene-based Thiele, Chichibabin, and Müller hydrocarbons." *Chemical Science* 11, no. 43 (2020): 11827-11833.

12) Sharma, Nandini, Navjeet Ahalawat, Padmani Sandhu, Erick Strauss, Jagannath Mondal, and Ruchi Anand. "Role of allosteric switches and adaptor domains in long-distance cross-talk and transient tunnel formation." *Science advances* 6, no. 14 (2020): eaay7919.

13) Dandekar, Bhupendra R., and Jagannath Mondal. "Capturing Protein–Ligand Recognition Pathways in Coarse-Grained Simulation." *The Journal of Physical Chemistry Letters* 11, no. 13 (2020): 5302-5311.

14) Mukherjee, Mrinmoy, and Jagannath Mondal. "Unifying the Contrasting Mechanisms of Protein-Stabilizing Osmolytes." The Journal of Physical Chemistry B 124, no. 30 (2020): 6565-6574.

15) Mukherjee, Mrinmoy, and Jagannath Mondal. "Bottom-Up View of the Mechanism of Action of Protein-Stabilizing Osmolytes." The Journal of Physical Chemistry B 124, no. 50 (2020): 11316-11323.

16) Ahalawat, Navjeet, and Jagannath Mondal. "An Appraisal of Computer Simulation Approaches in Elucidating Biomolecular Recognition Pathways." *The Journal of Physical Chemistry Letters* 12 (2020): 633-641.

17) Som, Arka, Meenakshi Pahwa, Sumit Bawari, Nilanjana Das Saha, Ranjan Sasmal, Monica Swetha Bosco, Jagannath Mondal, and Sarit S. Agasti. "Multiplexed optical barcoding of cells via photochemical programming of bioorthogonal host–guest recognition." *Chemical Science* 12, no. 15 (2021): 5484-5494.

18) Dandekar, Bhupendra R., Navjeet Ahalawat, and Jagannath Mondal. "Atomic Resolution Mechanism of GTP Recognition by GTPase." *Biophysical Journal* 120, no. 3 (2021): 121a.

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6. Conferences organized:

- March 03 – 05, 2021, TIFR Annual Chemistry Conference (Organising committee from TIFRH: Anukul Jana, Anand T. Vaidya, Soumya Ghosh, Pramodh Vallurupalli, Jagannath Mondal)
- February 10 – 12, 2021, ICONS-2021, Intercontinental NMR Conference (Organiser from TIFRH: P. K. Madhu)
- December 16 – 18, 2020, Conference on Advances in Catalysis, Energy, and Environmental Research (Organising committee from TIFRH: T. N. Narayanan, Jagannath Mondal, Pranav R. Shirhatti, Pabitra K. Nayak)
- August 26 – 28, 2020, ICONS2020, Intercontinental NMR Conference on Methods and Applications, Organisers: TIFR-H, ITC, Novosibirsk, TU-Darmstadt, ENS, Paris (Organiser from TIFRH: P. K. Madhu)
- May 05, 2020 onwards, Virtual Conference on Aspects of Condensed Matter Physics in Quantum Computing & Sensing (Organiser from TIFRH: Karthik. V. Raman, Dhavala Suri, Kabir Ramola)
- April 08, 2020 onwards, Intercontinental NMR seminar series on various topics in NMR initiated by TIFR-H, ITC, Novosibirsk, TU-Darmstadt, and ENS, Paris (Fridays, 1530 IST) (Organiser from TIFRH: P. K. Madhu)

7. Invited lectures given:

- Aprotim Mazumder, Panel member for a discussion on Theoretical Biology, 'Thirsting for Theoretical Biology 2021' online meeting, ICTS, January 2021.
- Anukul Jana, e-Workshop on Advancements in the Molecular World: Materials and Catalysis
- (AMWMC-2021), National Institute of Technology Karnataka (NITK), Surathkal, February, 2021. Title: Low-Valent Low-Coordinated Carbon Compounds: Emerging New Class of Synthons
- Anukul Jana, TIFR Annual Chemistry Conference (TACC-2020), TIFR, March, 2021. Title: Low-Valent Low-Coordinate Main-Group Compounds: Emerging Novel Class of Synthons
- Pramodh Vallurupalli, NMR online seminar series, October 2020. Title: A methyl 1H SQ-CPMG experiment to study conformational exchange in large systems: Lessons from a methyl 1H DQ-CPMG experiment

- Pramodh Vallurupalli, Emerging topics in biomolecular NMR, September 2020. Title: New CEST Experiments to study protein conformational exchange
- Raghunathan Ramakrishnan, IACS-Kolkata, April 2021. Title: Data-driven discoveries in chemical compound space: Trends and Challenges
- Tamal Das, Soft Matters: Young Investigators e-Meet 2020
- Tamal Das, Institute of Smart Structures and Systems
- Kalyaneswar Mandal, 8th Indian Peptide Symposium (virtual symposium), Indian Institute of science, Bangalore, March 2021.
- Kalyaneswar Mandal, TIFR Annual Chemistry Conference (virtual), TIFR Hyderabad, March 2021
- Kalyaneswar Mandal, Online Refresher Course on Chemistry (virtual), one of the Resource persons in the Refresher course, University of Hyderabad, February 2021.
- P. K. Madhu, Emerging Topics in Biomolecular Magnetic Resonance (Virtual) Meeting Series, August 2020. Title: Heteronuclear spin decoupling for all (commercial) MAS frequencies: Methods and recipes
- P. K. Madhu, MIT Weekly SSNMR and DNP Webinars, August 2020. Title: Recoupling schemes in solid-state NMR in a new light
- P. K. Madhu, SRIBS, KSCSTE, Kottayam, Kerala, August 2020. Title: Principles of nuclear magnetic resonance spectroscopy
- P. K. Madhu, SRIBS, KSCSTE, Kottayam, Kerala, 2020. Title: Two-dimensional NMR spectroscopy
- P. K. Madhu, VI International School for Young Scientists, Novosibirsk, Russia, September 2020. Title: Principles of nuclear magnetic resonance spectroscopy
- P. K. Madhu, VI International School for Young Scientists, Novosibirsk, Russia, September 2020. Title: Relaxation in nuclear magnetic resonance: Phenomenology
- P. K. Madhu, Experimental NMR Conference (ENC), Asilomar (Virtual), March 2021. Title: Recent advances in heteronuclear spin decoupling
- T. N. Narayanan, Prof Prakash P. Karat Endowment Lecture -2021, St. Aloysius College (Autonomous), Mangaluru, March 2021. Title: Role of New Materials in Energy Crisis: Present and Future
- T. N. Narayanan, World Nano Congress on Advanced Science and Technology (WNCST), March 2021. Title: Role of Electrode-Electrolyte Interface Engineering in Electrodics
- T. N. Narayanan, Pan-TIFR Chemistry Meet, March 2020. Title: Role of Electrode-Electrolyte Interface Engineering in Electrodics
- T. N. Narayanan, Science People Delhi Online Platform, January 2021. Title: ഊർജ്ജ പ്രതിസന്ധി: ചില പ്രായോഗിക ചിന്തകൾ (Future Energy Challenges)
- T. N. Narayanan, the talk given during the program for high school science teachers of Telangana Social Welfare Residential Educational Institutions Society (TSWREIS), January 2021. Title: Learning Science from Nature: Bio-Inspired Technologies
- T. N. Narayanan, Atal Tinkering Lab, A. K. N. M. M. A. Memorial High School Kattukulam, Kerala, India, December 2020. Title: Biomimicry in Emerging Technologies
- T. N. Narayanan, 10th Year of TIFR-Hyderabad, October 2020. Title: Rechargeable Respirator Mask & A Device to Test Mask Efficiency
- Manish Jaiswal, Webinar series, IISER Berhampur, August 2020. Title: Tales of the fly and the human: Understanding Biology and Diseases, LA Vida

8. New initiatives:

- Unravelling the Molecular Basis of Mitochondrial Cristae Dynamics (Anand T. Vaidya)
  Mitochondria are small sacs or organelles in almost all of our cells. They are the engines of a cell, where the food we eat and the oxygen we breathe combine to generate energy for our body. Not surprisingly, dysfunctional mitochondria are involved in a wide range of diseases, including cancer. 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. Vaidya's research plan is to understand the atomic and molecular details of the MICOS complex that will help understand how cristae are formed and how their shapes change. This would not only answer fundamental questions in biology, but could also lead to new medical therapies.

- New projects are underway in Aprotim Mazumder's lab, which will further their understanding of DDR in terms of cell to cell heterogeneity and live cell dynamics. Mazumder's lab is exploring the roles of cellular response to damage to rDNA and more broadly roles of the nucleolus in stress responses. They are also investigating the differential roles of heterochromatin proteins and LLPS in DDR, and using live cell FRET-based tools for investigating double strand break responses. These studies are likely to be more advanced in the coming report period.

- Kanchan Garai's lab is trying to understand how the E4 isoform of apolipoprotein E interacts with the amyloid beta peptide and alter its aggregation behavior. This is important since apoE4 is the strongest risk factor for Alzheimer's disease (AD). Currently, there is no cure for AD. Garai's lab is developing biophysical techniques, primarily fluorescence based single molecule techniques to study the interaction of apoE with the intermediates of amyloid beta. Single molecules techniques offer the advantage of detecting and characterizing the individual species, viz, the free monomers, the oligomers and the complexes of the proteins involved in the amyloid aggregation pathway. These studies are aimed at understanding the biophysical properties of the intermediates and also at examining the effects of potential drug candidates on these particles.

- Karthik V. Raman
  a) Exploring anomalous Hall effect in non-collinear kagome antiferromagnets, b) Exploring Skyrmion physics at the interface between topological insulator and magnetic insulator

- Structural Biology of MPC (ongoing) (Kaustubh R. Mote)
  A major focus of the lab is to understand how the mitochondrial pyruvate carrier (MPC) transports pyruvate across the mitochondrial membrane. The work in the near future will focus on trying to address the activation, inhibition and coupling mechanism of this transporter using a combination of biophysical assays and NMR spectroscopy. Interaction of MPC with the intrinsically-disordered protein PUMA is currently also being planned.

- Structural Biology of Actins (Kaustubh R. Mote)
  The lab is working towards studying atomistic details of actin dynamics by targeting a bacterial actin homologue ParM for structural studies using NMR spectroscopy. In particular, the researchers aim to use very fast magi-angle spinning NMR to address questions about

nucleotide-dependent conformational changes in actin, actin stabilization by capping and dynamic instability.

- NMR Methods (Kaustubh R. Mote)
  The lab has developed a number of techniques in the past 2 years to measure dipole-dipole couplings in solid samples using the REDOR experimental block. The group will explore ways to extract information about the amplitude of motions using this experiment by tailoring these techniques study the abovementioned proteins.

- Extreme photonics innovation center (M. Krishnamurthy)
  Extreme photonics innovation center (EPIC) setup in collaboration with Rutherford Appleton Laboratory with funding from UKRI, UK has expanded with four major streams of work: a) Control systems development b) New detectors for laser based plasma studies c) Novel high repetition rate targetry. D) Development of opto-mechanical components for high powered high repetition rate laser studies. The project now employs over a dozen engineers and scientists. The work is also multi-institutional with some activities spread to IIT Mumbai and IIT Chennai in addition to TIFR, Mumbai.

- In vivo detection of polyphosphates (polyp) - Development of new tools to manipulate and detect polyphosphate in a live organism. (Manish Jaiswal)
  Jaiswal's lab plans to develop FRET-based tools to identify polyp location and levels in flies. This will help investigate developmental regulation of polyp as well as screening the regulators of the polyP. These tools can also be employed in other organisms as well. Once the group develops this tool successfully, they will use it for setting up a genetic screening platform to identify genes regulating polyP levels. This screen will help in the identification of crucial genes involved in PolyP synthesis and degradation in multicellular organisms.

- Spin Locking of Half-Integer Spin Quadrupole Nuclei and Feasibility of Cross-Polarisation (P. K. Madhu)
  Cross-polarisation with magic-angle spinning (CP-MAS) is an important method in solid-state NMR with the former transferring polarisation from abundant spins to rare spins. This increases the sensitivity of the rare spin spectra. This also leads to structural information in the form of correlation and distances. However, for CP to be effective, the two relevant nuclear spins should be locked in an appropriate frame. Whilst this is routine in case of spins-1/2, transferring polarisation to quadrupolar spins (spin quantum number greater than ½) has been always difficult as it is tough to lock the latter. Madhu and colleagues have introduced phase-modulated pulses to achieve effective spin locking of the quadrupolar spins under a wide range of MAS frequencies and radiofrequency (RF) irradiation. They have further shown that with such a scheme, CP also is effective for quadrupolar spins. The new scheme has been tested successfully on samples of glycine, Al(acac)3, and borax. The researchers observe a large number of resonance conditions between the applied RF, MAS, and the quadrupole frequency. Currently, they plan to check the scheme for a wider range of MAS frequencies on a few more samples and quadrupolar nuclei. Further, they are making use of numerical simulations and average Hamiltonian theory to understand the mechanism of spin locking and CP transfer with the phase-modulated pulses.

- Developing methods to explore the free Energy Surface of Proteins (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. Vallurupalli's group is developing CEST based NMR methods to explore the free energy surface of the protein by detecting process with rates varying 10 s-1 to 10,000 s-1 and populations as low as 0.1%.

- Structures of minor folding intermediates (Pramodh Vallurupalli)
  The FF domain from HYPA/FBP11 folds on a rugged free energy surface with multiple folding intermediates. Vallurupalli and colleagues are attempting to obtain the structures of some of these sparsely populated intermediates to obtain an unprecedented view of protein folding.

- 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.

- Quantum state resolved molecule surface scattering experiments for understanding elementary chemical processes in surface chemistry (Pranav R. Shirhatti)
  In order to understand state selective chemical reaction dynamics, one needs the capability to prepare molecules in a quantum state specific manner. Shirhatti and colleagues have built a broadly tunable and narrow linewidth (sub-ppm) and high power radiation source (optical parametric oscillator and amplifier) working in the near IR range. A detailed characterization of the oscillation threshold, narrow line width and conversion efficiency showed excellent performance as required for molecular beam experiments (linewidth better than 0.5 ppm). Alongside, they have also built a very simple, low cost wavemeter which can do precise wavelength measurements (sub-ppm). The performance of the combined OPO/A and the wavemeter system showed promising results for high resolution spectroscopy and optical pumping experiments. Direct tests of the performance for optical pumping experiments and extension of this system to work in mid IR wavelength region is being looked into currently.

- Zero-Ultra Low field NMR of powdered solid samples (G. Rajalakshmi, P. K. Madhu)
  Zero- to ultralow-field nuclear magnetic resonance (ZULF NMR) provides an alternative to standard high-field NMR to study spin systems in a regime dominated by inter-/intra-nuclear spin-spin interactions. Some of the early experiments in this regime by Pines and coworkers tried to employ zero field experiments for studying dipole coupling in powdered solid samples by overcoming the line broadening caused by the random orientation of the dipoles with respect to the applied magnetic field. In these experiments, the researchers use filed cycling techniques to measure the low-field evolution in high field by inductive detection. Atomic magnetometers are the preferred choice to study the magnetisation evolution directly at zero field. The fT sensitivity and few 100 Hz bandwidth of atomic magnetometers make them ideally suited for j-spectroscopy in liquid samples. In solid samples, however, the dominant dipole interactions are in the 1-30 KHz regime. The researchers have built an atomic magnetometer that has pT sensitivity with a bandwidth of about 30 KHz. They are currently involved in attempts to use this atomic magnetometer to directly detect ZULF NMR in solid samples.

- Active Glasses (Smarajit Karmakar)

Karmakar's group is trying to understand the dynamical and mechanical properties of active glass forming liquids via simulations and analytical theory. Their recent results suggest that dynamic heterogeneity in active glass-forming systems is inherently different from their equilibrium behavior. Understanding the effect of non-equilibrium active external driving on the dynamics of glass-forming liquids is one of the sought-after questions that a significant fraction of the physics community is actively researching in the last decade. One of the main reasons for this problem to be so widespread in the science community is its ubiquitous presence in a wide variety of systems - ranging from frictional driven granular matter to collection of bacteria to cell migrations. Thus, these studies are of importance both from fundamental science and industrial application perspectives. In this study, Karmakar and colleagues show that the effect of active force on the dynamical behaviour of the complex glass-like system is qualitatively different from the equilibrium glasses. They then extended the Mode Coupling Theory formalism to this non-equilibrium scenario to successfully rationalize all the observed results in their simulations. For the first time, this work highlights that dynamic heterogeneity in complex glassy systems is qualitatively different from its equilibrium behaviour.

- Yielding in Amorphous solids (Smarajit Karmakar)
  This is a joint project with collaborators from IMSc, IIT-Roorkee and IIT-Palakkad and TIFR-Hyderabad. The project is funded by National Supercomputing Mission (NSM) to develop a meso-scale computer model to understand mechanical failure mechanisms in amorphous solids, which can be used to design materials in future.

- Multi-scale model for electrochemical reactions (Soumya Ghosh)
  Understanding the molecular details of electrochemical reactions is an important and challenging problem. The detailed understanding of the structure of the solid-electrolyte interface will help us engineer improved electrocatalysts, and batteries. In general, simulating a set-up that constitutes the electrode material, reactants and the electrolyte using first principles molecular dynamics (also called ab initio molecular dynamics) is extremely expensive. The main aim of this work is to replace a part or whole solvent with a statistical description (3D-reference interaction site model). The 3D-RISM description is also capable of incorporating the effect of the electrolyte ions. The set-up will be implemented in the open source software CP2K.

- Modelling Au grain boundaries (Soumya Ghosh, Nandana Pal Chowdhury)
  Recent studies have shown that Au grain boundaries are orders of magnitude more reactive towards CO_2 reduction that the more commonly studied Au(111) surface. This begs the question what kind of structural motifs are responsible for this enhanced reactivity. In this project, several models of grain boundaries between Au(111), Au(100), and Au(110) will be generated at first with well-established strategies. Next, a correlation will be sought between the 5D parameters that describe the grain boundaries and their energies using machine learning tools. Furthermore, CO_2 reactivity will be tested for representative structures of these grain boundaries. Finally, a structure function map will be created by correlating the extent of CO_2 activation with the local structural motif.

- Computing wannier centers at metal-water interface (Soumya Ghosh)
  Wannier centers encode crucial information about instantaneous effective electronic positions. This localized, Lewis dot like picture provides a fairly accurate description of electronic polarization and hence, is a very important tool to obtain information about instantaneous molecular dipole moments. The dipole-dipole autocorrelation function, computed over a trajectory length, can be employed to estimate the frequency dependent infra-red absorption coefficient, and hence, the spectra. The standard methodologies, however, do not work for a metallic system. In this project, a new method to compute the wannier centers close to the metallic surface will be implemented in CP2K. This method has been shown to work for molecules adsorbed on metal surface but has never been employed for charged metal-water interface.

9. Science Communication and Public Outreach:

A) The second issue of the TIFR Hyderabad newsletter was released in July 2020. With this issue, the institute newsletter goes multilingual. The issue features articles, starting with Jishan Bari's article about his research on the crystallin protein in the eye, where mutations can lead to congenital cataracts. Meanwhile, Anku Guha's article talks about his work on synthesizing ammonia to store hydrogen, which is a great fuel source. Parswa Nath discusses the science of supernovas, and how these dying stars have fascinated humans since the dawn of civilization. Following this, Ipsa Jain talks to us about her career choice as a science illustrator, and how illustration can do wonders by bringing more clarity into scientific concepts. Lastly, we have a section called 'Blue-Sky' that showcases art and photography.

A team of volunteers came forward to translate the articles in multiple languages- Hindi, Telugu, Bengali and Malayalam- a concerted effort to reach out to as many people as possible.

Link to newsletter: https://www.tifrh.res.in/~newsletter/

Chief Editor: Anusheela Chatterjee

Student Editors: Sumit Bawari, Aishwarya Mandya

B) On October 19, 2020, Prof. V. Chandrasekhar launched the Science Media Centre website of TIFR Hyderabad. Over the past few months, the media centre website has hosted articles, interviews, research highlights, media mentions and short videos, in an effort to communicate science to all. Link to website: https://ftp.tifrh.res.in/~sciencemedia/

C) IndiaBioscience Outreach Grant: Anusheela Chatterjee and Aprotim Mazumder are one of the recipients of the First IndiaBioscience Outreach Grant. Project title: 'Stories from the Life Sciences: A multifaceted approach in interactive science communication'

The aim of this project is to bring researchers, illustrators, and writers together to create short videos covering basic scientific concepts and the latest research from TIFR Hyderabad in the area of life sciences.

D) Sawaal-Jawaab: Conversations on Science (Popular science café organized by TIFR Hyderabad)

In view of the COVID-19 pandemic, our Science Café 'Sawaal-Jawaab' went online. The following sessions were held:

August 21, 2020: 'Your brain on stress', Vidita Vaidya (TIFR Mumbai)

October 21, 2020: 'The 2020 Nobel Prizes' (Three scientists, Krishnan Harshan, P. Ajith and Sonal Nagarkar Jaiswal, steered a discussion on this year's Nobel Prizes.)
'Taming a deadly viral pathogen-Hepatitis C virus' (Speaker: Krishnan Harshan, CCMB-Hyderabad)
'Black holes on the horizon' (Speaker: P. Ajith, ICTS Bangalore)
'Crispr/cas9: A quantum leap in genome editing' (Speaker: Sonal Nagarkar Jaiswal, CCMB-Hyderabad)

November 21, 2020: 'When, What and How much to eat: Understanding how diet impacts our health and ageing', Ullas S. Kolthur (TIFR Mumbai)

May 15, 2021: 'Math and numbers: Why are they important?', Sujatha Ramdorai (University of British Columbia, Canada)

E) TIFR Hyderabad set up a Molecular Diagnostic Training facility to boost the capacity of healthcare professionals in performing PCR based diagnostic tests, which is primarily used for COVID-19 diagnosis. The training effort is supported by the Prime Minister's Scientific Advisor's office and funded by Bill & Melinda Gates Foundation. The participants trained at TIFR Hyderabad were lab technicians, in-service doctors, government undergraduate lecturers, researchers, medical students from seven states across India. The three-week 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 a 12-hour rtPCR diagnostic online module by FIND India for all participants. ESIC Medical College and Hospital was the local collaborator in Hyderabad where participants could visit the BSL 2-3 lab facility for COVID-19 diagnosis and research. This workshop was organized by Manish Jaiswal, Anand Vaidya and Adish Dani. Over 180 trainees have attended and completed the training programme. Many of these trainees are now working in COVID-19 diagnostic labs in various parts of the country.

F) COVIDGyan: TIFR Hyderabad was actively involved in a multi-institutional science communication effort called COVIDGyan– a digital platform for communicating scientifically accurate information about COVID-19. In order to realise the goals of COVIDGyan, multiple members of the institute were involved in ideation, editing, content creation,

communication strategy and translation of the articles. The members of the institute involved in this effort are mentioned below:

- Coordinating Committee: V. Chandrasekhar, Anand Vaidya
- Editorial Team: Anand Vaidya (Convenor), Aprotim Mazumder
- Content Team: Anusheela Chatterjee
- Communication Strategy Team: Anusheela Chatterjee
- Translation Coordinator (Odia Team): Pabitra K. Nayak

G) Popular Science Lectures by faculty: (Speaker: Anand Vaidya)

- '*Covid-19 - What? Where? How? Why?*' organized by the Science Gallery Bengaluru and Azim Premji Foundation - January 2021
- '*DNA, RNA and Protein*' as a part of TIFR Hyderabad's training program on RT-PCR based testing for healthcare workers – October 2020 to April 2021

H) Vipin Agarwal has given introductory online classes in the field of Solid-state NMR spectroscopy

- Tutorial: Solid-state NMR course at the Federal University of Rio de Janeiro, Brazil 15th March, *(2021)*
- Teaching and Learning of NMR spectroscopy for Structure determination. 19th – 24th February, National Institute of Technology, Warangal. (2021) Online Tutorial

10) Any other significant achievement:

- Smarajit Karmakar has received the National Supercomputing Mission (NSM) grant for developing mesoscale model of amorphous plasticity.

- P. K. Madhu is an Advisory Editorial Board Member of the journal, *Magnetic Resonance in Chemistry* (December 2020).