1. Research Highlights:

A) COMPUTATIONAL MOLECULAR BIOPHYSICS (Jagannath Mondal)

- Mondal's group has been trying to capture the complete process of ligand binding to the designated cavity of a protein in a single Molecular Dynamics simulation trajectory. Utilizing the in-house GPU-based high performance computing facility, the group has been successful in deciphering the atomistic pathways of biomolecular recognitions in two popular protein/ligand system, namely Camphor binding to cytochrome P450 and recognition of benzene to solvent inaccessible cavity of L99A T4 Lysozyme.

- Glycine and Trimethyl N-oxide (TMAO) are known to stabilize a protein's folded conformation. By simulating the hydrophobic collapse of a macromolecule in aqueous solutions of these two osmoprotectants, Mondal's group has demonstrated that these two osmolytes can impart mutually contrasting effects towards hydrophobic interaction. While TMAO preserves its protectant nature across diverse range of polymer-osmolyte interactions, glycine is found to display an interesting cross-over from being a protectant at weaker polymer-osmolyte interaction to a denaturant at stronger polymer-osmolyte interactions.

B) CHEMICAL SCIENCES and Biophysics: (Kalyaneswar Mandal, Kanchan Garai)

- Mandal's group has been involved in the development of novel protein inhibitors that would interfere with the invasion of human red blood cells by malaria parasites. Malaria parasite uses two key proteins, AMA-1 and RON2, for the invasion process. They aimed to design the mirror-image protein inhibitor that would interfere with the interaction between AMA-1 and RON2. They successfully prepared the full-length polypeptide chain of the receptor binding domain of AMA-1 protein, consisting of 180-residue polypeptide chain with three disulfide bonds.

- Garai's group built a cuvette-FCS setup to detect and characterize the early intermediates of amyloid aggregation. This technique can extend the applications of FCS on various experiments, which are regularly performed in Spectrofluorometers. In addition, this group has built a superresolution optical microscope based on STORM for characterization of role of chaperone

proteins and apolipoprotein E on the growth of the amyloid fibrils of amyloid beta, alpha-synuclein and amylin.

C) CONDENSED MATTER PHYSICS and MATERIAL SCIENCES (Karthik V. Raman, T. N. Narayanan)

- Recent theoretical studies have showed that spin current can be generated by temperature gradient along superconducting hybrid structures in presence of Zeeman split density of states in the superconductor. Raman's group has successfully produced ultra-thin films (5nm) of Aluminium where a Tc of 2.6K has been observed (Tc~1.2K for bulk Al). Thin Niobium films, prepared by RF sputtering, have also showed superconducting behavior below 5.8K.

- In a recent study, Narayanan's group found that the surface modification of platinum (Pt) with an atomically thin layer corrosion resistive layer, such as hexagonal boron nitride (hBN), protects Pt from electrochemical erosion. At the same time, the activity of Pt towards hydrogen generation can be enhanced.

D) BIOLOGICAL SCIENCES: (Manish Jaiswal, Aprotim Mazumder, Tamal Das)

- Jaiswal's research efforts are focused on identifying the mechanism of mitochondrial quality control and its implications in neuronal health and diseases, using *Drosophila* as a model. In order to understand how cells regulate mitochondrial homestasis under stress conditions, they conducted a genetic screen and identified eight mutants that display increased mitochondrial abundance. These mutations mapped to genes that are primarily required for the regulation of mitochondrial function. These results indicated that the increased mitochondrial biogenesis is a possible a compensatory mechanism to counteract the effect of mitochondrial dysfunction.

- Mazumder's group has developed a microscopy-based assay for determining cell cycle stages over large cell numbers. An intriguing suppression of P53 transcription was found across different stages of the cell cycle with DNA damage. This method can be used to study cell-cycle-dependent DDR in cultured cells without the need for synchronization.

- Single molecule Fluorescence in situ Hybridization (smFISH) for mRNA provides a powerful quantitative handle on gene expression. While the method has been widely applied in cells in culture, applications to primary tissue samples remain fewer, and often use involved cryosectioning. Mazumder's group has developed a modified method of smFISH applicable on various primary whole-mount tissues from *Drosophila*.

- Tamal Das's group elucidated the effect of extracellular matrix stiffness (ECM) on the process of cell competition. ECM stiffness was shown to have an important role in modulating the kinetics of extrusion of mutant cells during cell competition. Experiments revealed that cell competition was suppressed at higher matrix stiffness. Further, this group found that the intracellular distribution of an actin-binding protein, Filamin, played a crucial role in regulating the kinetics of cell competition on different substrate stiffness.

- Das's group elucidated intrinsic cell-cell variability within a population of cells with single clonal origin. They discovered that the epithelial cells exhibited heterogeneity in the several geometric, biophysical, and biochemical parameters, including number density, cell shape, velocity,

monolayer stress landscape, and mitochondrial potential. All of these heterogeneities were correlated with the tissue-level force landscape. Together, it was established that the collective dynamic heterogeneity in various cellular parameters was an interesting biological property at tissue level.

D) THEORETICAL PHYSICS: (Prasad Perlekar, Smarajit Karmakar, Surajit Sengupta, Mustansir Barma, Pushpita Ghosh)

- Bubble laden flow appears in a variety of natural and industrial processes. Presence of bubbles dramatically alters the transport properties of a flow. A single bubble of diameter d, because of buoyancy, rises under gravity. Its trajectory and the wake flow depend on the density and viscosity contrast with the ambient fluid, and the surface tension. In this project, Perlekar and his group has investigated the complex spatiotemporal flow patterns generated by a suspension of such bubbles at moderate volume fractions.
- In nature, turbulent flows often include small particles (dust) embedded within the flow, typical examples are (a) proto-planetary disks (gas and dust), (b) clouds (air and water droplets), and (c) aeolian processes (wind and sand). Perlekar's group has investigated the clustering of dust in 2D turbulence.
- Intermittency, characterized by sudden bursts of activity, occurs in many non-equilibrium systems. Are there simple laws which govern the approach to an intermittent steady state? Barma and his colleague show that, for particles driven by fluctuating height fields, there is a length scale which grows with time and governs the amount of particle clustering, and thereby intermittency.
- Pushpita Ghosh has investigated thermodiffusion-induced spatiotemporal instabilities in reaction-diffusion system following activator-inhibitor kinetics. Studies show 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.
- Karmakar's group showed that the static and dynamics of glasses with medium range crystalline order are different from other glass forming liquids with no predominant local order. The group has studied the stability of a model polymer chain in a supercooled glass-forming liquid at different amount of supercooling in order to understand how dynamics of supercooled liquids influence the collapse behaviour of the polymer. This study showed that apart from long time relaxation processes (α relaxation), short time dynamics of the supercooled liquid, known as β relaxation plays an important role in controlling the stability of the model polymer. These observations are in stark contrast with the common belief that only long time relaxation processes are the sole player. This study presents convincing evidence that suggest that one may need to review the vitrification hypothesis which postulates that α relaxations control the dynamics of biomolecules and thus α-relaxation time should be considered for choosing appropriate bio-preservatives.
- While common sense says that solids are rigid, careful arguments show that all solids under infinitesimal strain must eventually flow. Resolution of this paradoxical result lies at the core of our understanding of the behaviour of solids under deformation. Sengupta's group provides a completely novel framework within which the paradox is reconciled and extract conditions wherein stable, rigid, crystalline solids are possible. Failure of ideal crystals is determined by a

kinetic process similar to the decay of supercooled phases following quenches across a first-order phase boundary. This fresh conceptual viewpoint curiously allows one to study failure of perfect crystalline solids in quantitative detail without invoking specifics of many-body, defect–defect interactions, raising hope of a more unified description of materials in the future.

E) THEORETICAL CHEMISTRY: (Raghunathan Ramakrishnan)

- Ramakrishnan's group has developed an analytic formalism, for two-electron atoms, to partition the many-body correlation energy into contributions along radial and angular terms. The resulting equations are useful to design new density functionals. In addition, novel machine learning approaches have been developed and utilised to statistically model electron correlation energy functionals that depend on Hartree—Fock pair densities. In the emerging discipline of Big-Data-driven inference of molecular/materials properties, this group's new contribution has been the characterisation of all possible boron, nitrogen substituted polycyclic aromatic hydrocarbon molecules that contain upto six aromatic rings. The resulting dataset contains 7,453,041,547,842 unique molecules of interest to solar-cell applications (this dataset is publicly accessible via the Big Data facility, MolDis- http://moldis.tifrh.res.in/index.html).

F) NMR SPECTROSCOPY and BIOPHYSICS: (P. K. Madhu, Pramodh Vallurupalli, Kaustubh R. Mote, G. Rajalakshmi, Vipin Agarwal)

- Heteronuclear spin decoupling is essential in solid-state NMR to improve resolution and sensitivity of the spectra of both rare and abundant spins. Madhu's group has thoroughly investigated the performance of various such decoupling methods in the regime of fast magic-angle spinning (MAS) and low radiofrequency (RF) amplitude irradiation. Whilst fast MAS helps in resolution enhancement, it should be accompanied by low-amplitude RF decoupling schemes as otherwise heating effects could be harmful to samples, particularly to most of the biological samples. The analysis has led to unifying most the existing schemes in vogue and rationalise them in a quantitative manner. This process has also enabled the group to identify solutions for new decoupling schemes which may offer better performance than the existing ones.

- Madhu's group has introduced certain unique versions of the commonly-used heteronuclear dipole-dipole recoupling schemes in MAS solid-state NRM, namely, REDOR (rotational-echo double resonance). The new methods aim at the measurement of strong dipole-dipole couplings, and thereby distances, by scaling down the interactions in a controlled fashion. Such scaling is necessary to avoid faster dephasing due the otherwise stronger couplings and to collect more data points. They have also modified the commonly-use DIPSHIFT (dipolar-chemical shift correlation spectroscopy) that is used for elucidation of order parameters in solid samples. They have unified both the REDOR and DIPSHIFT schemes which also have resulted in the expansion of the range of applications of the DIPSHIFT experiment.

- An Rb atomic magnetometer was developed by G. Rajalakshmi and colleagues using balanced polarimetry based method for optical rotation measurement. A new method for the optical rotation sensing was developed based on classical weak measurement concept and at its sensitivity and noise was compared with the standard balanced polarimetry. This group

demonstrated a dc field sensitivity of 1nT using this technique, an enhancement by a factor of 4 from standard polarimetry.

- Mote and colleagues were able to express and and purify components of the Mitochondrial Pyruvate Carrier in bacterial cells. Work is ongoing to reconstitute them in artificial lipid vesicles in a functional form.

- In a recent study, Agarwal's group experimentally demonstrated the feasibility of selective recoupling of two spins in a network of strongly coupled spins. They have also demonstrated how this method could benefit the structural characterization of both pharmaceutically relevant small molecules and structure of protein in the solid-state NMR.

- Building upon their previous work on using methyl triple quantum (TQ) CPMG experiments to study dynamics, Vallurupalli's group has introduced a DQ-CPMG experiment and experiments to measure exchange induced shifts. A combination of TQ, DQ and single quantum (SQ) CPMG data allows one to extract exchange rates and populations in a site-specific manner. A combination of the CPMG and exchange induced shift data allows one to detect minor conformers with populations as low as ~50 μs and reconstruct their spectra. This group has devised a new experiment that combines TQ-CPMG with PFG-diffusion techniques to measure the diffusion constants of these sparsely populated states.

G) SYNTHETIC CHEMISTRY: (Anukul Jana, V. Chandrasekhar)

- Jana's group studied the influence of N-heterocyclic carbenes (NHCs) on the hydrolysis of a diphosphene, a phosphorus-phosphorus double bonded compound.

- The addition reactions of N-heterocyclic carbenes (NHCs) with substrates are mostly known to occur through the carbenic centre (C2-centre) leading to a normal adduct. This study by Jana's group shows an abnormal addition of NHCDip (NHCDip = 1,3-(2,6-iPr2C6H3)-imidazole-2-ylidene) to a conjugate acid of CAAC, (CAACiPr = 1-iPr-3,3,5,5-Me¬4-pyrrolinium triflate).

- Synthesis of organic radicals is challenging due to their inherent instability. In recent years, cyclic(alkyl)(amino)carbene (CAAC)-derived 2-substituted pyrrolinium salts have been used as synthons for the synthesis of isolable carbon based radicals. Jana's group demonstrated a direct, easy and convenient method for the synthesis of 2-aryl substituted pyrrolinium salts without using CAAC as a precursor. This study may be effective for generating carbon-based radicals whose stability as well as reactivity can be varied.

- Chandrasekhar's group has been able to come out with new ligand designs to prepare single-ion and single molecule magnets. These are based on coordination complexes that contain 3d transition metal ions or 4f lanthanide metal ions or heterometallic complexes containing both 3d and 4f metal ions. Among the various systems that were studied include a pentagonal bipyramidal lanthanide complex containing axial chloride ligands. This complex was a single-ion magnet and the complex can be fine-tuned by variation of the axial ligands readily.

H) LASER PHYSICS: (M. Krishnamurthy, Pranav R. Shirhatti)

- In bulk targets, the presence of a prepulse a few nanoseconds prior to the mainpulse soft ionizes the target and leads to preplasmas with varying density gradients. With the use of 15 um liquid droplets, Krishnamurthy's group has been able to engineer not just density but also spatial modifcations in the pre-plasma. With this as the target for a moderate intensity (1016 W/cm2) main laser pulse, generation of energetic electrons, as high as 6 MeV has been observed. Protons with energies of 600keV have also been detected. In comparison, bulk targets at similar intensities lead to electrons of highest energy of only 300 keV. Evidence indicates that with such mass limited targets, these spatial modifications lead to not only increased laser coupling but also could provide sharp density gradients for relativistic electron acceleration.

- Laser-plasma particle accelerators have attracted widespread attention. Krishnamurthy's group is addressing the need to develop accelerators which can function with driving laser intensities at the levels available from 'university-class' milli-Joule femtosecond lasers. In this context, mass-limited targets when impinged with moderate intensity (1016 W/cm2) femtosecond lasers offer a novel system for study for laser plasmas in the absence of the usual energy dissipation channels of bulk condensed media. When the targets are mesoscopic in nature, with dimensions of the size similar to wavelength of the laser, coupling of laser energy is expected to be enhanced through linear and nonlinear Mie scattering type mechanisms. These targets are either 15 um liquid droplets in a jet or solid micro-particles injected into vacuum through an in-house custom built particle jet generator.

- Shirhatti's group has initiated two major research directions: (a) Exploring the possibility of using atomic/molecular collisions as a soft and universal probe for imaging surfaces, which promises to be a new microscopy technique complementary to the existing well established methods. (b) Understanding the dynamics of plasmon induced surface chemistry, where the efforts are directed towards understanding how light energy can be harnessed to drive chemical reactions on metallic nanoparticle surfaces. This group has designed the custom - built apparatus needed for both experiments. Currently, the atom/molecular scattering apparatus is under fabrication. The apparatus for the plasmon induced chemistry is currently being tested in the laboratory.

G) SCIENCE EDUCATION: (Jayashree Ramadas)

- Volunteers from TIFR Hyderabad and University of Hyderabad conducted a total of 72 weekend visits to three nearby TSWREIS schools i.e. Gowlidoddi (22 visits), Narsingi (22 visits) and Shaikpet (28 visits) in 2018-19. These visits majorly aimed to inculcate concept-based learning of Science and Mathematics among 6th to 9th grade students. Apart from textbook-based teaching, activity-based learning of concepts was encouraged and students were stimulated to interact freely and ask questions.

2. Staff Strength:

Faculty- 24 + 5 (Visiting faculty- 2, No. of Emeritus faculty- 1, No. of INSPIRE faculty- 2)
Research Scholars- 95
Junior Research Fellow- 21
Senior Research Fellow- 5
Post-doctoral Fellow- 31

Visiting students - 10
Scientific Staff- 20
Technical Staff - 06
Admin Staff - 15

3. Awards/Distinctions:

- Kalyaneswar Mandal: Wellcome Trust/DBT India Alliance Intermediate Fellowship award 2015. The Fellowship was activated on 1st June 2016, TCIS being the host Institute; and, based on the progress made in the first two years, successfully renewed to its 3rd year term in the year 2018.
- Mustansir Barma: Department of Atomic Energy Homi Bhabha Chair Professorship.
- P. K. Madhu: ISMAR (International Society for Magnetic Resonance) Council Member.
- V. Chandrasekhar: Elected Vice-president, Indian National Science Academy, New Delhi (2019-22).

4. Number of students graduated: M.Sc- 3, Ph.D -4

5. Publications:

1) A. Maiti, D. Mandal, I. Omlor, D. Dhara, L. Klemmer, V. Huch, M. Zimmer, D. Scheschkewitz, and A. Jana, *"Equilibrium Coordination of NHCs to Si(IV) Species and Exchange of Donor Exchange in Donor-Acceptor Stabilized Si(II) and Ge(II) Compounds"*, Inorg. Chem. 2019, 58, 4071–4075.

2) D. Mandal, S. Sobottka, R. Dolai, A. Maity, D. Dhara, P. Kalita, R. Suriya Narayanan, V. Chandrasekhar, B. Sarkar, and A. Jana*, "Direct Access to 2-Aryl Substituted Pyrrolinium Salts for Carbon Centre Based Radicals without Pyrrolidine-2-Ylidene alias cyclic(Alkyl)(Amino)Carbene (CAAC) as a Precursor"*, Chem. Sci. 2019, 10, 4077-4081.

3) B. Santra, D. Mandal, V. Gupta, P. Kalita, V. Kumar, R. S. Narayanan, A. Dey, N. Chrysochos, A. Mohammad, A. Singh, M. Zimmer, R. Dalapati, S. Biswas, C. Schulzke, V. Chandrasekhar, D. Scheschkewitz, and A. Jana, *"Structural Diversity in Supramolecular Organization of Anionic Phosphate Mono Esters: Role of Cations"*, ACS Omega 2019, 4, 2118–2133.

4) D. Dhara, T. Vijayakanth, M. K. Nayak, P. Kalita, R. Boomishankar, C. B. Yildiz, V. Chandrasekhar, and A. Jana, *"Contrasting reactivity of (boryl)(aryl)lithium-amide with electrophiles: N- vs. p-aryl-C-nucleophilic substitution",* Dalton Trans. 2018, 47, 14411−14415.

5) V. Gupta, B. Santra, D. Mandal, S. Das, R. S. Narayanan, P. Kalita, D. K. Rao, C. Schulzke, S. K. Pati, V. Chandrasekhar, and A. Jana, *"Neutral and Anionic Phosphate-Diesters as Molecular Templates for the Encapsulation of a Water Dimer",* Chem. Comm. 2018, 54, 11913−11916.

6) D. Mandal, R. Dolai, P. Kalita, R. S. Narayanan, R. Kumar, S. Sobottka, B. Sarkar, G. Rajaraman, V. Chandrasekhar, and A. Jana, *"Abnormal" Addition of NHC to a Conjugate Acid of CAAC: Formation of N-Alkyl Substituted CAAC",* Chem. Eur. J. 2018, 24, 12722−12727.

7) R. S. Narayanan, P. Thilagar, J. Acharya, P. Kumar, D. K. Rao, V. Chandrasekhar, and A. Jana, *"Reactions of 4-diphenylphosphino benzoic acid with organotin oxides and -oxy-hydroxide",* J. Chem. Sci. 2018, 130, 92.

8) D. Dube, N. Ahalawat, H. Khandelia, J.Mondal and S. Sengupta, *"On identifying collective displacements in apo-proteins that reveal eventual binding pathways",* PLOS Comput. Biol. 2019, 15, e1006665

9) N. Ahalawat and J. Mondal, *"Mapping the Substrate Recognition in Cytochrome P450",* J. Am. Chem. Soc. 2018, 140, 17743.

10) N. Ahalawat and J. Mondal, *"Assessment and optimization of collective variables for protein conformational landscape: GB1 β-hairpin as a case study",* J. Chem. Phys. 2018, 149, 094101 **(Featured Article) (Highlighted in AIP)**

11) M. Mukherjee and J. Mondal, *"Heterogeneous Impacts of Protein-Stabilizing Osmolytes on Hydrophobic Interaction"*, J. Phys. Chem. B, 2018, 122, 6922.

12) J. Mondal, N. Ahalawat, S. Pandit, L. Kay and P. Vallurupalli, *"Atomic resolution mechanism of ligand binding to a solvent inaccessible cavity in T4 lysozyme"*, PLOS Comput. Biol. 2018, 14, 5, e1006180

13) S. Bawari, T. N. Narayanan and J. Mondal, *"Atomistic Elucidation of Sorption Processes in Hydrogen Evolution Reaction on a van der Waals Heterostructure",* J. Phys. Chem. C, 2018, 122, 10034.

14) S. Bawari, N. M. Kaley, S. Pal, T. V. Vineesh, S. Ghosh, J. Mondal and T. N. Narayanan, *"On the hydrogen evolution reaction activity of graphene–hBN van der Waals heterostructures",* Phys. Chem. Chem. Phys. 2018, 20, 15007.

15) S. Mohapatra, S. Mathimalar, S. Chaudhary, K.V. Raman, *"Observation of zero-bias conductance peak in topologically trivial hybrid superconducting interfaces"*, Journal of Physics Communications, 2019 (accepted manscript) https://doi.org/10.1088/2399-6528/ab14a7.

16) P. Bielytskyi, D. Gräsing, K. R. Mote, K. B. S. S. Gupta, S. Vega, P. K. Madhu, A. Alia. & J. Matysik, *"13C→ 1H transfer of light-induced hyperpolarization allows for selective detection of protons in frozen photosynthetic reaction center",* J. Magn. Reson. 2018, 293, 82-91.

17) D. Dhara, P. Kalita, S. Mondal, R.S. Narayanan, K. R. Mote, V. Huch, M. Zimmer, C. B. Yildiz, D. Scheschkewitz, V. Chandrasekhar, and A. Jana, *"Reactivity enhancement of a diphosphene by reversible N-heterocyclic carbene coordination",* Chem. Sci. 2018, 9(18), 4235-4243.

18) K. R. Mote, and P. K. Madhu, *"Simultaneous Homonuclear and Heteronuclear Spin Decoupling in Magic-Angle Spinning Solid-State NMR"*, Solid State Nucl. Magn. Reson. 2018, 90, 7–12.

19) K. R. Mote, J. Thomas, and A. Ramanan, *"Crystal engineering of molecular to nonmolecular metal malonates in presence of piperazine: Role of metal ions in tuning architectures",* Indian Journal of Chemistry, 2018, 57A, 1081–1090.

20) P. Bielytskyi, D. Gräsing, S. Zahn, K. R. Mote, A. Alia, P. K. Madhu, and J. Matysik, *"Assignment of NMR resonances of protons covalently bound to photochemically active cofactors in photosynthetic reaction centers by 13C–1H photo-CIDNP MAS-J-HMQC experiment",* J. Magn. Reson. 2019, 298, 64-76.

21) S. Li, C. Xu, Y. Fu, P. Lei, Y. Yao, Y. Zhang, M. P. Washburn, L. Florens, M. Jaiswal, M. Wu and M. Mohan, *"DYRK1A interacts with Histone Acetyl Transferase p300 and CBP and localizes to enhancers",* Nucleic Acids Res. 2018, 30; 46(21):11202-11213.

22) S. S. Balakrishnan, U. Basu, D. Shinde, R. Thakur, M. Jaiswal and P. Raghu, *"Regulation of PI4P levels by PI4KIIIa during G-protein coupled PLC signaling in Drosophila photoreceptors",* J. Cell Sci. 2018, 3;131(15).

23) D. Li-Kroeger, O. Kanca, P. T. Lee, S. Cowan, M. Lee, M. Jaiswal, J. L. Salazar, Y. C He and H. J. Bellen, *"An expanded toolkit for gene tagging based on MiMIC and scarless CRISPR tagging in Drosophila",* elife, 2018, e38709.

24) T. Singha, & M. Barma, *"Clustering, intermittency, and scaling for passive particles on fluctuating surfaces",* Phys. Rev. E, 2018, 98(5), 052148.

25) T. Singha, and M. Barma, "*Comment on- Replica Symmetry Breaking in Trajectories of a Driven Brownian Particle",* 2018, arXiv preprint arXiv:1806.06824.

26) A. Pandey, M. K. Verma, & M. Barma, *"Reversals in infinite-Prandtl-number Rayleigh-Bénard convection",* 2018, Phys. Rev. E, 98(2), 023109.

27) R. Singh, N. Bayal, A. Maity, D. J. Pradeep, J. Trebosc, P. K. Madhu, O. Lafon, V. Polshettiwar, *"Probing the interfaces in nanosilica supported TiO2 photocatalysts by solid-state NMR and in-situ FTIR",* ChemNanoMet, 2018, 4, 1231-1239.

28) P. Bielytskyi, D. Graesing, A. Das, R. Kundu, J. Matysik, S. Maiti, P. K. Madhu, "*Precise in situ photo-induced pH modulation during NMR spectrometry",* Chem. Phys. Lett. 2018, 16, 665-668.

29) A. B. Gopalan, T. Yuwen, L. E. Kay, & P. Vallurupalli, *"A methyl 1 H double quantum CPMG experiment to study protein conformational exchange",* J. Biomol. NMR, 2018, 72(1-2), 79-91.

30) A. B. Gopalan, and P. Vallurupalli, *"Measuring the signs of the methyl 1 H chemical shift differences between major and 'invisible'minor protein conformational states using methyl 1 H multi-quantum spectroscopy",* J. Biomol. NMR, 2018, 70 (3), 187-202.

31) T. Yuwen, A. Sekhar, A. J. Baldwin, P. Vallurupalli, & L. E. Kay, *"Measuring Diffusion Constants of Invisible Protein Conformers by Triple-Quantum 1H CPMG Relaxation Dispersion"*, Angew. Chem. Int. Ed. Engl. 2018, 130(51), 17019-17022.

32) V. P. Tiwari, S. Pandit, & P. Vallurupalli, "Exchangeable deuterons introduce artifacts in amide 15 N CEST experiments used to study protein conformational exchange", J. Biomol. NMR, 2019, 1-6.

33) D. Mitra and P. Perlekar, *"Topology of two-dimensional turbulent flows of dust and gas",* Phys. Rev. Fluids, 2018, 3, 044303.

34) D. Tahchieva, D. Bakowies, R. Ramakrishnan, O. Anatole von Lilienfeld, *"Torsional potentials of glyoxal, oxalyl halides and their thiocarbonyl derivatives: Challenges for DFT"*, J. Chem. Theory Comput, 2018, 14, 4806-4817.

35) A. R. Kammath, R. Ramakrishnan*, "Exact separation of radial and angular correlation energies in two-electron atoms",* Chem. Phys. Lett. 2019, 720, 93–96.

36) S. Chakraborty, P. Kayastha, R. Ramakrishnan, *"The Chemical Space of B, N-substituted Polycyclic Aromatic Hydrocarbons: Combinatorial Enumeration and High-Throughput First-Principles Modeling"*, J. Chem. Phys. 2019, 150, 114106 (1-14).

37) R. V. Bhavsar, R. Ramakrishnan, *"Machine learning modeling of Wigner intracule functionals for two electrons in one dimension"*, J. Chem. Phys. 2019, 150, 144114 (1-9).

38) M. Allocca, J. Corrigan, A. Mazumder, K. R. Fake, and L. D. Samson, *"Inflammation, necrosis, and the kinase RIP3 are key mediators of AAG-dependent alkylation-induced retinal degeneration",* 2019, Science Signaling, 12, eaau9216

39) N. Pasnuri, P. Khuntia, and A. Mazumder, *"Single transcript imaging to assay gene expression in wholemount Drosophila melanogaster tissues",* Mech Dev, 2018, 153, 10-16.

40) S. Dhuppar, and A. Mazumder, *"Measuring cell cycle-dependent DNA damage responses and p53 regulation on a cell-by-cell basis from image analysis"*, 2018, Cell Cycle, 17, 1358-1371.

41) I. Tah, S. Sengupta, S. Sastry, C. Dasgupta and S. Karmakar, *"Glass Transition in Supercooled Liquids with Medium Range Crystalline Order",* Phys. Rev. Lett. 2018, 121, 085703.

42) R. Das, I. Tah, and S. Karmakar, *"Possible Universal Relation Between Short time β-relaxation and long time α-relaxation in Glass-forming Liquids*", J. Chem. Phys. 2018, 149, 024501.

43) P. Nath, S. Ganguly, J. Horbach, P. Sollich, S. Karmakar and S. Sengupta,Do Thermodynamically Stable rigid solids exist? –PNAS, 115, E4322 (2018).

44) B. P. Bhowmik, I. Tah, and S. Karmakar, *"Non-Gaussianity of van Hove Function and Dynamic Heterogeneity Length Scale",* Phys. Rev. E, 2018, 98, 022122.

45) M. Mukherjee, J. Mondal, and S. Karmakar, *"Role of α and β relaxations in Collapsing Dynamics of a Polymer Chain in Supercooled Glass-forming Liquid*", J. Chem. Phys. 2019, 150.11 (2019): 114503.

46) S. Ganguly, D. Das, J. Horbach, P. Sollich, S. Karmakar and S. Sengupta, *"Plastic deformation of a permanently bonded network: Stress relaxation by pleats",* J. Chem. Phys. 2018, 149, 184503.

47) A. Srivastava, S. Karmakar, A. Debnath, *"Slow Relaxations of Chemically Confined Hydration Layers near Lipid Bilayers: Dynamical Heterogeneities above Supercooling*", (under review Phys. Rev. Lett), arXiv:1808.03933, 2018.

48) B. P. Bhowmik, P. Chaudhuri and S. Karmakar, *"Effect of random pinning on the yielding transition of amorphous solids"*, (under review in Phys. Rev. Lett.), arXiv:1808.09723, 2018.

49) B. P. Bhowmik, S. Karmakar, I. Procaccia and C. Rainone, *"Particle pinning suppresses spinodal criticality in the shear banding instability*", (under review in PRE 2019), arxiv:1909.03020, 2019.

50) M. Vishwakarma, J. D. Russo, D. Probst, U. S. Schwarz, T. Das, and J. P. Spatz, *"Mechanical interactions among followers determine the emergence of leaders in migrating epithelial cell collectives*", Nature Communications, 2018, 9, 3469.

51) P. K. Rastogi, K. R. Sahoo, P. Thakur, R. Sharma, S. Bawari, R. Podila, and T. N. Narayanan, *"Graphene-hBN non-van der Waals Vertical Heterostructures for Four Electron Oxygen Reduction Reaction",* Phys. Chem. Chem. Phys. 2019, 21, 3942-3953.

52) A. Guha, N. Sreekanth, and T. N. Narayanan, *"Tuning the Hydrogen Evolution Reaction Activity on Metals by Lithium Salt*", ACS Appl. Energy Mater. 2018, 1, 7116-7122.

53) Y. Dong, P. Parajuli, A. M. Rao, W. Thielemans, S. Eylely, K. R. Sahoo, T. N. Narayanan , and R. Podila, *"Intrinsic five-photon non-linear absorption of two-dimensional BN and its conversion to two-photon absorption in the presence of photo-induced defects",* Opt. Mater. 2018, 86, 414-420.

54) K. K. Paul, N. Sreekanth, R. K. Biroju, A. J. Pattison, E. L. Daniel, A. Guha, T. N. Narayanan , N. V. Rees, W. Theis, and P. K. Giri, *"Strongly Enhanced Visible Light Photoelectrocatalytic Hydrogen Evolution Reaction in n-doped MoS2/TiO2(B) Heterojunction by Selective Decoration of Platinum Nanoparticles at the MoS2 Edge Sites",* J. Mater. Chem. 2018, A 6, 22681-22696.

55) S. Pal, N. Sreekanth, B. Kundu, M. Sahoo, S. Bawari, D. K. Rao, S. Nayak, A. J. Pal, and T. N. Narayanan, *"Mechanistic Insight into Formate Production via CO2 Reduction in C-C Coupled Carbon Nanotube Molecular Junctions",* J. Phys. Chem. C, 2018, 122, 23385−23392.

56) A. Guha, T. V. Vineesh, A. Sekar, N. Sreekanth, M. Sahoo, S. Nayak, S. Chakraborty, and T. N. Narayanan, *"Mechanistic Insight in to Enhanced Hydrogen Evolution Reaction Activity of Ultra-Thin h-BN Modified Pt Electrodes",* ACS Catal. 2018, 8, 6636-6644.

57) (Chapter) New Advances in 2D Electrochemistry - Catalysis & Sensing, T N Narayanan,* Ravi Kumar Biroju, and T V Vineesh, (Book) "2D Materials - Characterization, Production, and Applications" Editors: Prof Craig E. Banks, and Dr Dale. A. C. Brownson, CRC Press (Taylor & Francis Group), USA (2018). (*Communicating/Corresponding Author) ISBN: 13: 978-1-4987-4739-4.

58) (Chapter) Phosphazenes. Chandrasekhar, V.; Narayanan, R. S.; Mamidala, R.; Venkatasubbaiah, K. In "Organophosphorus Chemistry" Volume 47, Eds. David W. Allen, David Loakes and John C. Tebby. Royal Society of Chemistry, Cambridge, U. K. 2018, 363-424.

59) A. K. Bar, P. Kalita, J. P. Sutter, V. Chandrasekhar, *"Pentagonal-bipyramid Ln(III) complexes exhibiting single-ion magnet behavior: a rational synthetic approach for a rigid equatorial plane",* Inorg. Chem. 2018, 57, 2398-2401.

60) V. Chandrasekhar, B. Mahanti, M. D. Pandey, R. S. Narayanan, *"Cyclometalated Ir(III) complex as a metalloligand and a selective Cu(II) sensor: synthesis and structural characterization of a heterometallic tetranuclear Ir(III)/Cu(II) complex",* ACS Omega, 2018, 3, 2786-2792.

61) A. Dey, S. Das, M. A. Palacios, E. Colacio, V. Chandrasekhar, *"Single-molecule magnet and magnetothermal properties of two dimensional polymers containing heterometallic [Cu5Ln2] (Ln = GdIII and DyIII) motifs",* Eur. J. Inorg. Chem. 2018, 1645-54.

62) A. S. Singh, A. Ali, J. N. Behera, S. S. Sun, V. Chandrasekhar, R. K. Tiwari, *"Thermal induced 1D to 2D polymer conversion accompanied by major packing changes in a single-crystal- to-single-crystal transformation*", CrystEngCommun. 2018, 20, 2346-50.

63) A. K. Bar, P. Kalita, M. K. Singh, G. Rajaraman, V. Chandrasekhar, *"Low-coordinate mononuclear lanthanide complexes as molecular nanomagnets",* Coord. Chem. Rev. 2018, 367, 163-216.

64) P. Kalita, J. Goura, J. M. Herrera, E. Colacio, V. Chandrasekhar, *"Heterometallic octanuclear NiII4LnIII4(Ln = Gd, Tb, Dy, Ho, Er) complexes containing NiII2LnIII2O4 distorted cubane motifs: synthesis, structure and magnetic properties",* ACS Omega, 2018, 3, 5202-11.

65) A. Dey, P. Kalita, V. Chandrasekhar, *"Lanthanide(III)-based single-ion magnets",* ACS Omega, 2018, 3, 9462-9475.

66) A. Chakraborty, J. Goura, P. Kalita, A. Swain, G. Rajaraman, V. Chandrasekhar, *"Heterometallic 3d-4f single molecule magnets containing diamagnetic metal ions",* Dalton. Trans. 2018, 47, 8841-64.

67) J. Acharya, S. Biswas, J. van Leusen, P. Kumar, Vierendra, R. S. Narayanan, P. Kögerler, V. Chandrasekhar*, "Exploring tuning of structural and magnetic properties of modification of ancillary β-diketonate co-ligands in a family of near-linear tetranuclear Dy(III) complexes",* Cryst. Growth. Des. 2018, 18, 4004-16.

68) R. Kumar, S. Das, S. K. Rout, S. Halder, G. M. Mohite, N. N. Jha, S. Mehra, V. Agarwal, and S. K. Maji, *"Neurotoxic oligomers and fibrils of α-synuclein gel assemblies*", Angew. Chem. Int. Ed. 2018, 57, 19, 5262-5266.

69) N. T. Duong, S. RaranKurussi, Y. Nishiyama and V. Agarwal, *"Quantitative 1H-1H Distances in Protonated Solids by Frequency Selective Recoupling at Fast Magic Angle Spinning NMR",* J. Phys. Chem. Lett., 2018, 9, 5948-5954.

70) M. G. Jain, K. R. Mote, J. Hellwagner, G. Rajalakshmi, M. Ernst, P. K. Madhu, and V. Agarwal, *"Measuring strong one-bond dipolar couplings using REDOR in MAS solid-state NMR"* J. Chem. Phys. 2019, (In press).

71) B. Sahoo, T. B. Sil, B. Karmakar, and K. Garai, *"A fluorescence correlation spectrometer for measurements in cuvettes"*, 2018, Biophys. J. 115(3), 455-466.

72) N. Singhal and M. Jaiswal*, "Pathways to Neurodegeneration: Lessons learnt from unbiased genetic screens in Drosophila",* J. Genet. 2018, 97(3):773-781.

73) A. Mondal, S. V. Rahul, R. Gopal, D. Rajak, M. Anand, J. Jha, S. Tata, A. K. Dharmadhikari, A. K. Gupta, and M. Krishnamurthy, "Misjudging negative ions for electrons in intense laser plasma diagnostics", AIP Adv. 2019, 9, 025115.

74) R. Gopal, A. Sen, S. R. Sahu, A. S. Venkatachalam, M. Anand, and V. Sharma, “An ion imaging spectrometer for studying photo-induced fragmentation in small molecules”, Rev. Sci. Instrum. 2018, 89, 086107.

75) S. Tata, A. Mondal, S. Sarkar, Y. Ved, A. D. Lad, J. Colgan, J. Pasley and M. Krishnamurthy, “Recombination of protons accelerated by a high intensity high contrast laser”, Phys. Rev. Lett. 2018, 121, 134801.

76) M. J. V. Streeter, S. J. D. Dann, J. D. E. Scott, C. Baird, C. D. Murphy, S. Eardley, R. A. Smith, S. Rozario, J.-N. Gruse, S. P. D. Mangles, Z. Najmudin, S. Tata, M. Krishnamurthy, S.V. Rahul, D. Hazra, P. Pourmoussavi, J. Osterhoff, J. Hah, N. Bourgeois, C. Thornton, C. D. Gregory, C. J. Hooker, O. Chekhlov, S. J. Hawkes, B. Parry, V. Marshall, Y. Tang, E. Springate, P. P. Rajeev, A. G. R. Thomas, and D. R. Symes, “Temporal feedback control of high-intensity laser pulses to optimize ultrafast heating of atomic clusters”, Appl. Phys. Lett. 2018, 112, 244101.

6. Conferences organised:

1. “4th NMR Meets Biology Meeting”, 16 December -21 December 2018, Khajuraho, Madhya Pradesh. This conference was organised by the NMR group in TIFR Hyderabad.

2. “International Symposium on Malaria Biology and 29th National Congress of Parasitology on Basic and Applied Aspects”, 01 November - 03 November 2018, School of Life Sciences, University of Hyderabad, Telangana, India. The conference was jointly organized by five leading institutions located at Hyderabad (University of Hyderabad, TIFRH, CCMB, NIAB and CDFD) and the Indian Society for Parasitology. Kalyaneswar Mandal was a part of the organizing committee.
3. “1st India-Japan NMR workshop”, Riken Yokohama Campus, June 2018, Yokohama Japan. This is a joint effort by TIFR NMR group and the Riken NMR group (one of the largest NMR centres in the world) to boost bilateral exchange in advanced magnetic resonance spectroscopy.
4. “Entropy, Information and Order in Soft Matter”, 27 August – 02 November 2018, ICTS, TIFR, Bangalore. Smarajit Karmakar was a part of the organising committee.
5. “Science Academies Refresher Course on Statistical Physics (for College Teachers and Students),) 09 – 24 December 2018, Department of Physics, Ramakrishna Mission Vivekananda Educational and Research Institute (RKMVERI), Kolkata. This course was organized jointly by Mustansir Barma and Shamik Gupta (RKMVU).
6. "TIFR-University of Hyderabad Life Sciences Seminar Series", 2018. Aprotim Mazumder was one of the organizers of this series.
7. “Pan-TIFR Biologists' Meeting” April 24 – April 26, 2018, TIFR Hyderabad, organised by Aprotim Mazumder.
8. -“Pan-TIFR Chemistry Meeting, 30 November-2 December 2018, TIFR Hyderabad, organised by Raghunathan Ramakrishnan.
9. “Genome Organization and Cell Fate Regulation (GACFR) meeting, 2018, University of Hyderabad”. Aprotim Mazumder was listed as a local organizer for the meeting.

10. -“Workshop on Plasticity”, Polytechnico de Milan, Milan, Italy 03 September – 04 September 2018. Surajit Sengupta was one of the organizers of this workshop.

7. Invited talks/ lectures given:

1. Anukul Jana, "Convenient Access to Pyrrolinium Cations: A Synthon for Carbon Based Radicals" at Department of Chemical Sciences, IISER Kolkata, India, March 2019.
2. Anukul Jana,"Heterodimer of N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC)" at Department of Chemistry, Vidyasagar University, India, January 2019.
3. Anukul Jana,"Heterodimer of N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC)" at Department of Chemistry, University of Calcutta, India, December 2018.
4. Anukul Jana, "Rational Design for Carbon Centre Based Open-Shell Compounds" at PAN-TIFR Chemistry Meet, TIFR Hyderabad, India, December 2018.
5. Anukul Jana, "Synthesis of Carbon Centre Based Open-Shell Compounds" at 1st Int. Symposium on Main Group Molecules to Materials, IISc Bangalore, India, December 2018.
6. Anukul Jana, "Heterodimer of N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC)" at Department of Chemistry, IISER Berhampur, India, December 2018.
7. Anukul Jana, "Mono- and Dicoordinate Germanium(0) as a Four Electron Donor" at Department of Chemistry, IISER Bhopal, India, December 2018.
8. Anukul Jana, "Influence of N-Heterocyclic Carbene (NHC) on Reactivity Enhancement of a Diphosphene" at Department of Inorganic Chemistry, Freie Universität Berlin, Germany, July 2018.
9. Anukul Jana, "Influence of N-Heterocyclic Carbene (NHC) on Reactivity Enhancement of a Diphosphene" as a GDCH Lecture, Grieswald, Universität Greifswald, Germany, July 2018.
10. Anukul Jana, "Mono- and Dicoordinate Germanium(0) as a Four Electron Donor" at Department of Chemistry, IISER Tirupati, India, April 2018.
11. Anukul Jana, "Mono- and Dicoordinate Germanium(0) as a Four Electron Donor" at Department of Chemistry, IIT Hyderabad, India, April 2018.
12. Jagannath Mondal, " Computer simulation of protein-ligand recognition in real time", OpenTox symposium , IICT Hyderabad, March, 2019.
13. Jagannath Mondal, "Quantifying protein-ligand binding pathways", at American Chemical Society March meeting, Orlando, LA, USA, March, 2019.
14. Jagannath Mondal, “Optimization of Collective variable for biomolecular processes", at ASM 2019, IIT Delhi, March, 2019.
15. Jagannath Mondal, “Optimization of collective variables for biomolecular processes”, at the Workshop on free energy simulations, IIT Kanpur, India, March, 2019.
16. Jagannath Mondal, “Computer simulations of protein ligand binding”, at Kaleidoscope, Goa, July, 2018.
17. G. Rajalakshmi, “Low field NMR using optical magnetometry", University of Nottingham, UK, August 2018.
18. Kalyaneswar Mandal, “Designing D-proteins to inhibit red blood cell invasion by malaria parasites” at School of Life Sciences, University of Hyderabad, August 2018.

19. Kalyaneswar Mandal, “Systematic development of novel protein inhibitors to prevent red blood cell invasion by Plasmodium falciparum merozoites", at the University of Chicago, Chicago, IL, USA, 20 October 2018.
20. Kalyaneswar Mandal, "Towards the development of novel D-protein inhibitors to prevent red blood cell invasion by Plasmodium falciparum merozoites", at the “International Symposium on Malaria Biology and 29th National Congress of Parasitology on Basic and Applied Aspects”, School of Life Sciences, University of Hyderabad, November 2018.
21. Kalyaneswar Mandal, “Exploring the D-space: A mirror image protein that has potential to inhibit AMA1-RON2 interactions", at the "PAN TIFR Chemistry meeting", TIFR Hyderabad, December 2018.
22. Kalyaneswar Mandal, “Mirror-image protein based drug discovery against cancer and other Diseases”, at the "Cancer Drug Discovery Conference", School of Life Sciences, University of Hyderabad, 23 February 2019.
23. Kalyaneswar Mandal, “A mirror-image protein that has potential to inhibit red blood cell invasion by malaria parasites”, at the "National Conference on Synthetic and Biological Peptides: Structures and Strategies for the Development of Drugs, Biologics and Materials”, Bangalore University, March 2019.
24. Karthik V. Raman, “Probing magnetic anisotropy at molecule-transition metal interface”, ICCFM 2018, Kolkata.
25. Kaustubh R. Mote, “A link between DIPSHIFT and REDOR experiments”, at the 4th NMR Meets Biology Meeting, Khajuraho, India, December 2018
26. Kaustubh R. Mote “Solid state NMR methods for material sciences”, at the First Indian Materials Conclave and the 30th Annual General Meeting of MRSI, IISc Bangalore, India, February 2019.
27. Manish Jaiswal, “Roles of Mito-nuclear crosstalk in neuronal survival and degeneration”, at the International Conference on Genome Architecture and Cell Fate Regulation, University of Hyderabad, December 2018.
28. Manish Jaiswal, “Aftermath of mitochondrial dysfunction in neuronal activity and maintenance” at the 2nd Asian Pacific Drosophila Neuroscience Conference (APDNC) Taipei, Taiwan, January 2019.
29. Manish Jaiswal, “Identification of novel genes linked to human neurological diseases through fly genetic screens” at the International Conference on Chemical Biology & Biologics”, CSIR-Indian Institute of Chemical Technology, Hyderabad, February -March 2019.
30. Mustansir Barma, “Stochastic Evolution of Interacting Particle Systems”, at the Workshop on Long-range Interactions and Synchronization, International Centre for Theoretical Physics - South American Institute for Fundamental Research, Sao Paulo, Brazil, May 2018.
31. Mustansir Barma, “Phase transitions in two-component nonequilibrium systems”, at the Workshop on Soft and Active Matter, University of Hyderabad, May 2018.
32. Mustansir Barma, “Bose Statistics”, at the Mumbai Area Complex Systems Conference, Pillai College of Engineering, New Panvel, November 2018.
33. P. K. Madhu, “Biomolecular studies with solid-state NMR”, at the PAN-TIFR Biologists’ Meet, TIFR Hyderabad, April 2018.
34. P. K. Madhu, “Improving recoupling efficiency in solid-state NMR”, First India-Japan NMR Workshop (JEOL and TIFR Hyderabad), June 2018.
35. P. K. Madhu, “Sensing magnetic fields optically”, at the Spin Physics, Spin Chemistry and Spin Technology, Novosibirsk, Russia, September 2018.

36. P. K. Madhu, “Sensing magnetic fields optically”, at the 8th National Symposium on Advances in Chemical Sciences, GNDU, Amritsar, Punjab, February 2019.
37. Pramodh Vallurupalli, “Studying Protein Conformational Dynamics Using NMR Spectroscopy”, at the 1st Indo Japan NMR coference, Yokohama, June 2018.
38. Pramodh Vallurupalli, “Studying Protein Conformational Dynamics” at I-DEC 2018, IISER Bhopal, December 2018
39. Pramodh Vallurupalli, “Methyl 1H Multi-Quantum experiments to study µs-millisecond Protein Dynamics” at ‘NMR meets biology’, Khajuraho, December 2018.
40. Pramodh Vallurupalli, “Studying Protein Conformational Dynamics Using Methyl 1H CPMG Experiments”, at 25th NMRs, Feburuary 2019.
41. Pranav R. Shirhatti, “Using atom/molecule scattering as a soft and universal probe for surfaces” at Kaliedoscope 2018, International Center, Goa, July 2018.
42. Pranav R. Shirhatti, “Understanding elementary processes in surface chemistry using state resolved molecular beam – surface scattering experiments”, at Physical Research Laboratories, Ahmedabad, Photonics Research Laboratory, August 2018.
43. Pranav R. Shirhatti, “Understanding elementary processes in surface chemistry using quantum state resolved molecular beam – surface scattering experiments”, at the Quantum Measurement Lab, Physics Department, IIT Kanpur, January 2019.
44. Pranav R. Shirhatti, “Gas – surface scattering experiments: A tool for understanding elementary steps in surface chemistry and probing surfaces” at the Inorganic and Physical Chemistry department, IISc Bagalore, March 2019.
45. Pranav R. Shirhatti, “Vibrational energy dissipation in molecule – surface collisions” at the National Conference on Atomic and Molecular Physics 2019, Physics Department, IIT Kanpur, March 2019.
46. Prasad Perlekar, “Energy spectra of 2D buoyancy driven bubbly flows”, at COMPFLU2018, IIT-Roorkee, December 2018.
47. Prasad Perlekar, “Turbulence in active polar fluids”, at SMYIM2018, Shimla, May, 2018.
48. Pushpita Ghosh, “Spatiotemporal ordering in growing bacterial colony”, at S.N. Bose National Centre for Basic Sciences, Kolkata, March 2018.
49. Raghunathan Ramakrishnan, Sessions chair of the conference: “Spectroscopy and Dynamics of Molecules and Clusters” at Koti, Shimla, 21-24 February 2017.
50. Aprotim Mazumder, Instructor at the 'Bioscopy 2019' workshop following the 43rd Indian Biophysical Society Meeting at IISER Kolkata, March 2019.
51. Aprotim Mazumder, Instructor at the 'National Level Workshop on Microscopy Image Analysis' organized by NCCS, Pune, March 2019.
52. Aprotim Mazumder, Instructor and Resource person at the 'Refresher course on - Recent advances in Cell and Molecular Biology' organized by the University of Hyderabad, March 2019.
53. Aprotim Mazumder, scientific seminar at the 'Cancer Drug Discovery Conference' , Transcell Biologics, University of Hyderabad, February 2019.
54. Aprotim Mazumder, scientific seminar at the TIFR-Weizmann Interaction Meeting, TIFR Mumbai, January 2019.
55. Aprotim Mazumder, Sawaal-Jawaab - popular science talk on 'Microscopy', Hyderabad, January 2019.
56. Aprotim Mazumder, scientific seminar at the Indian Society for Developmental Biologists Meeting, IIT Kanpur, December 2018.

57. Aprotim Mazumder, scientific seminar at the Genome Organization and Cell Fate Regulation (GACFR) meeting, University of Hyderabad, December 2018.
58. Aprotim Mazumder, seminar on cancer research in TIFR Hyderabad, Research and Innovation Centre of Hyderabad (RICH) Cancer Conference, IICT, Hyderabad, August 2018.
59. Aprotim Mazumder, Infrastructure description at the Regional Young Investigators' Meeting (RYIM), SLS, University of Hyderabad, Hyderabad, August 2018.
60. Aprotim Mazumder, scientific seminar to commemorate Prof. BJ Rao, TIFR Mumbai, August 2018.
61. Aprotim Mazumder, scientific seminar in the Pan-TIFR Biologists' Meet, TIFR Hyderabad, April 2018.
62. Tamal Das, “Mechanobiology of Collective Cell Dynamics: Cells in the Epithelium”, at the Biophysical controls and Quantitative interpretation in Medicine, IIEST, Shibpur, September 2018.
63. Tamal Das, “Mechanobiology of Collective Cell Dynamics: Cells in the Epithelium”, at the Center For BioSystems Science And Engineering, Indian Institute of Science (IISc) Bengaluru, January 2019.
64. Tamal Das,” Mechanobiology of Collective Cell Dynamics: How Forces Dictate Cell Migration and Competition”, at the Cancer Drug Discovery Meeting, University of Hyderabad, Hyderabad, February, 2019.
65. T. N. Narayanan, “Engineering the Interfaces for Future Energy Technologies”, at the India Annual Physics Symposium APS 2019, St. Theresa's College Ernakulam, Kerala, January 2019.
66. T. N. Narayanan, “Molecular Junctions - Catalysis to Electronics”, at the International Conference on Optoelectronic and Nano Materials for Advanced Technology (iCONMAT 2019), CUSAT. Kochi, January 2019.
67. T. N. Narayanan, “Physics and Chemistry of Atomic Layers”, at the Workshop of International Conference on Optoelectronic and Nano Materials for Advanced Technology (iCONMAT 2019), Department of Physics, CUSAT, Kochi, January 2019.
68. T. N. Narayanan, “Engineered Mesoscopic Interfaces for Energy Conversion”, at the 7th Interdisciplinary Symposium on Materials Chemistry (ISMC-2018), DAE Convention Centre, BARC Mumbai, December 2018.
69. T. N. Narayanan, “Engineering the Interfaces for Catalysis”, Pan TIFR Chemistry Meeting 2018, TIFR-Hyderabad, 30th November 2018. [Talk]
70. T. N. Narayanan, “Mesoscopic Interfaces - A New Era of Materials Science”, at the Erudite Lecture Series, Department of Chemistry, Mercy College Palakkad, September 2018.
71. T. N. Narayanan, “Experiments with Mesoscopic Interfaces”, Refresher Course in Frontiers in Materials Chemistry in the Human Resource Development Centre (HRDC), UoH, Hyderabad September 2018.
72. T. N. Narayanan, “Novel Mesoscopic Interfaces for Energy Technology”, International Conference on Microscope and XXXIX Annual Meeting of Electron Microscope Society of India - EMSI 2018, Bhubaneswar, July 2018.
73. T. N. Narayanan, “Molecular Junctions for Energy Technology”, at the Indo-US Joint Centre kickoff meeting, IISER - Thiruvananthapuram, Kerala, July 2018.
74. T. N. Narayanan, “Introduction to Nanomaterials & 3D Graphene”, at the Faculty Development Program, Adi Shankara Institute of Engineering and Technology, Kalady, Kerala, April 2018.
75. V. Chandrasekhar, “Homo-(4f) and Heteronuclear(3d/4f) Complexes as Molecular Magnets”, at Main-group Molecules to Materials, IISc Bangalore, October 2018.

76. V. Chandrasekhar, “Single Molecule Magnets Containing Lanthanide- and Transition Metal Ions”, at the Indo-French Conference: Magnetism of Molecular Systems, SSCU, IISc, Bangalore, November 2018.
77. V. Chandrasekhar, “Molecular Magnets”, at the School of Chemistry, University of Hyderabad, September 2018.
78. V. Chandrasekhar, “Single Molecule Magnets Containing Transition- and Lanthanide Metal Ions”, at the Department of Chemistry, Institute of Science, NSETCS-18, Banaras Hindu University, November 2018.
79. V. Chandrasekhar, “Periodic Table @150”. Lectures given at NISER Bhubaneswar January 5, 2019; IIT Kanpur January 7, 2019; TIFR Hyderabad January 23, 2019; IISER Kolkata March 6, 2019; IISER Bhopal, March 14, 2019; IISER Pune, March 18, 2019.
80. Vipin Agarwal, “NMR based Structural Biophysics”, at the Pan-TIFR Biology Meet, TIFRHyderabad, April 2018.
81. Vipin Agarwal, “An attempt to measure quantitative proton-proton distances in fully protonated solids”, at Expanding Horizons of NMR, DCS, TIFR Mumbai, May 2018.
82. Vipin Agarwal, “Quantitative proton-proton distances in fully protonated solids at fast Magic angle spinning”, at the 1st India-Japan NMR workshop, Riken Yokohama Campus, June 2018.
83. Vipin Agarwal, “Novel Proton-Proton Coherence Transfer Pathways in fully protonated solids at Fast Magic Angle Spinning NMR”, at the Pan-TIFR Chemistry Meet, TIFR Hyderabad, 30 November-2 December 2018.
84. Vipin Agarwal, “Quantitative and Qualitative 1H-1H distances in fully protonated solids at fast magic spinning NMR: A Theoretical Perspective”, at NMRS meeting, New Delhi, February 2019.
85. Ram Gopal, “Intense Laser Plasma interactions with kHz, mJ class lasers”, at the 2nd Asia-Pacific Conference on Plasma Physics, Japan, November 2018.
86. Ram Gopal, “Taaren Zameen Pe: the Sun on Earth”, Popular talk on Intense Lasers, on National Science Day, RGUKT, Basara, February 2019.
87. M. Krishnamurthy, “Dynamic structures enable relativistic electron generation in Microdroplets,” High energy density science (HEDS), Yokohoma, Japan, 2019.
88. M. Krishnamurthy, “Nano particles in intense laser matter interaction”, SERB summer school, RRCAT, Indore, 2019.
89. M. Krishnamurthy, “How to convert a dazzling drop to a micro-accelerator”, IIT Hyderabad, Dept of Physics, Annual day colloquium, 2019.
90. M. Krishnamurthy, “Building a compact neutral atom accelerator”, IISER Pune Colloquium, 2018.
91. M. Krishnamurthy, “Relativistic electron generation with mJ class lasers ELI workshop” at IIT Delhi, 2018.
92. M. Krishnamurthy, “Lasers in modern days science”, National Science day Celebrations, Raman Auditorium HCU Hyderabad, 2018.

8. New Initiatives

- T. N. Narayanan has initiated a project with a Mysore-based company that works on water treatment technologies. The goal is to improve the efficiency of the existing effluent treatment and sewage treatment plants by adopting the concepts of nanomaterials and catalysis.

-The NMR group has initiated collaborations with RIKEN, Japan, to conduct high frequency magic-angle spinning studies in solid-state NMR.

- G. Rajalakshmi and colleagues have built a facility to detect changes in local magnetic field with a sensitivity of 1nT by a new technique based on the concept of weak measurement and Faraday effect. In addition to local field changes, the same system can also detect optical activity and the corresponding polarisation rotation sensitivity is 12µrad. By moving to spin exchange relaxation free regime of atomic interaction and tuning the experimental parameters, one can reach fT sensitivity.

- TIFR Hyderabad actively participates in the Gachibowli Research Cluster Lecture Series. This lecture series is aimed at promoting scientific discussions between the three institutions- University of Hyderabad, TIFR Hyderabad and National Institute of Animal Biotechnology.

- TIFR Hyderabad aims to establish a 'Centre for Quantum Computing' that would serve as an intersection for researchers with complimentary specializations in mathematics, condensed matter theory and experiments, physics and material science. This initiative aims to develop broad expertise in established quantum computing techniques. Research efforts will be directed at developing new concepts of topological quantum computing as well.

-TIFR Hyderabad and Rutherford Appleton Laboratories (RAL), UK have entered into an active collaboration funded by the Newton-Bhabha funds for developing novel sources of ionizing radiation based on next-generation laser technology. In the first step towards this collaboration, an innovation centre was set up at the Laser Lab in TIFRH, dedicated to development of control systems for intense laser particle accelerators. The project was initiated with the hiring of four engineers whose training was completed at RAL between April and September 2018.

-TIFR is hosting a one-day science communication workshop 'SciComm101' on August 26, 2019. This workshop will be conducted by the Wellcome Trust- DBT India Alliance and is open to students belonging to educational institutions in Hyderabad.

9. Significant Achievements

- The planning, indenting, construction, instrument installation and validation of the specific pathogen free (SPF) mouse facility at TIFR Hyderabad was initiated and successfully completed. Further, the Committee for Purpose and Control and Supervision of Experiments on Animals (CPCSEA), Ministry of Environment, Forest and Climate Change (MOeF), Government of India, has registered our facility for housing, breeding and experimentation on small animals, following inspection. The Institutional Animal Ethics committee (IAEC) conducted its first meeting where multiple experimentation protocols to be pursued for Basic Research in the institute were reviewed and approved. As a result of these developments, we are now set to commence experiments on transgenic/knockout mice that are geared towards deciphering functions of genes involved in T cell ion flux and immune signalling as well as the molecular and synaptic organization of mouse sensory systems.

- The current high performance computation (HPC) facility in TIFR Hyderabad has a total capacity of 300 TF (6 clusters). Two of the clusters have been included in the list of 'India's top 500 supercomputers', maintained by CDAC, India.

- TIFR Hyderabad houses the world's first custom integrated cryogen free scanning tunnelling microscope (STM) with a cryogen free superconducting magnet. With a base temperature of 13K, this setup allows probing spin-resolved surface electronic density of states, with atomic resolution, of various surfaces ranging from molecular adsorption on magnetic surfaces to superconductors and topological insulators. One of the main technical challenges in the integration of the system was to effectively decouple the vibrational and acoustic noises created by the cold heads at the microscope stage.

- Kanchan Garai's lab has built a novel fluorescence correlation spectroscopy (FCS) setup for measurements inside cuvettes. This cuvette-FCS setup can detect and characterize the early intermediates of amyloid aggregation. This technique can extend the applications of FCS on various experiments, which are regularly performed in Spectrofluorometers. In addition, TIFR Hyderabad has signed a MoU with Dr. Reddy's Laboratory for "evaluation of stability of peptides using cuvette-FCS".

- Jagannath Mondal's group published exciting insights about the substrate recognition pathway in cytochrome P450. Unbiased molecular dynamic simulations show that there is no major opening in cytochrome P450 when camphor binds to it.

- Surajit Sengupta's group provideed novel insights into the thermodynamics of solid rigidity. They found that every crystalline solid comes in two forms, which are identical in crystal structure but differ in the way they respond to changes of shape. While the first one is rigid and resists changes of shape the second variant always eliminates stress from its bulk and rearranges atoms to conform to shape changes. Further, they are connected by a "first order phase transition" similar to commonly observed liquid-gas or liquid-solid phase changes. When deformed by any amount, howsoever small, the rigid solid goes into a meta-stable state analogous to superheated water. Eventually, this meta-stable state always decays by nucleating bubbles of the stable, stress-free, solid by a process very similar to how bubbles of steam appear in a kettle of boiling water.