TIFR Centre for Interdisciplinary Sciences

Biological Sciences

Measuring cell-cycle related DNA damage responses on a cell-by-cell basis from microscopic image analysis: A microscopy-based assay was developed for determining cell cycle stages over large cell numbers. Upon DNA damage, γH2A.X induction was correlated to nuclear enrichment of p53 on a cell-by-cell basis and in a cell cycle dependent manner. Further imaging-based cell cycle analysis was combined with single molecule tumour suppressor P53 mRNA detection and immunofluorescence for p53 protein in the same cells. 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. (Shivnarayan Dhuppar, Aprotim Mazumder)

Single molecule RNA Fluorescence in situ Hybridization to monitor differential expression of EGFR target genes in primary Drosophila tissue: 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. A modified method of smFISH applicable on various primary whole-mount tissues from the fruit fly *Drosophila melanogaster* was developed. This method is being currently used to investigate the links between EGFR signalling and cell proliferation. (Nikhita Pasnuri, Aprotim Mazumder)

Chromatin compaction changes in response to DNA damage monitored by fluorescence anisotropy: Previously, it was described how fluorescence anisotropy can be used to monitor chromatin compaction states.

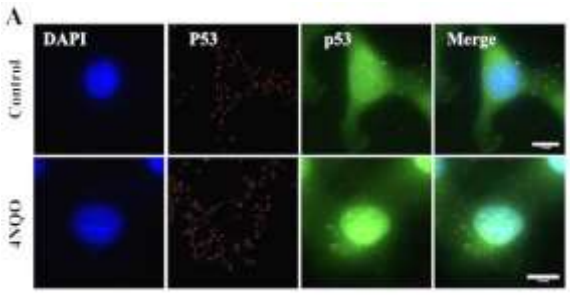

Figure 1: Detecting P53 transcripts (red) and p53 protein (green) in the same cells. The nucleus is in blue.

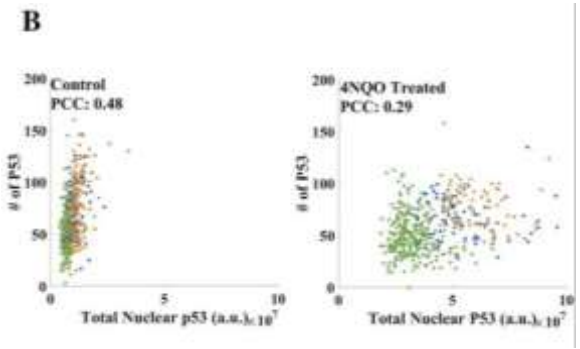

Figure 2: P53 mRNA number plotted against nuclear p53 protein. G1 (green), S (blue) and G2 (orange) cells are shown in control and 4NQO treated cells.

In the current academic year, the aforementioned technique was combined with laser-induced DNA damage to show an unexpected compaction of even undamaged DNA in response to localized double strand breaks. This is concomitant with the spread of damage markers monitored by immunofluorescence. (P. S. Kesavan, Aprotim Mazumder)

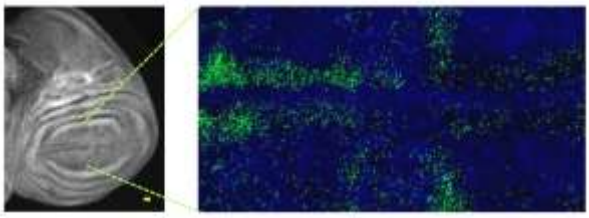

Figure 3: Developing single molecule RNA FISH in tissue. A 3rd instar wing imaginal disc is shown on the left. Single mRNA molecules (green) of Argos, an EGFR target gene, are shown on the zoomed image on the right.

Cellular responses to mitochondrial stress in neuronal health and diseases: To understand the mechanism of mitochondrial quality control and its implications in neuronal health and diseases, a small scale genetic screen was performed in the model organism *Drosophila melanogaster*. The altered mitochondrial abundance was tested, along with the levels of mitochondrial fusion protein Marf in a set of loss-of-function mutants. Through this screen, it was identified that increased mitochondrial biogenesis resulted due to mutations in lrpprc2. An important thing to be noted is that lrppc2 is known to be essential for mitochondrial mtRNA stability. Further, fused mitochondrial phenotype was observed with concomitant degradation of Marf in lrpprc2 mutants. It was found that Pink, Parkin, and Bendless are essential for the degradation of Marf following the mitochondrial fusion to avoid mitochondrial hyperfusion. It is to be noted that human homologs of lrpprc2, pink and parkin genes have been implicated in neurodegenerative diseases. Increased mitochondrial biogenesis and Marf degradation in lrpprc2 appears to be a protective mechanism. (Deepa Balasubramaniam, Arka P. Das, Tanya Singh, Neha Singhal, Manish Jaiswal)

Mechanobiology of cell competition: It remains to be understood how mechanical cues influence the initial stages of cancer development and tumour suppression. It was shown that the stiffening of extracellular matrix (ECM) inhibited the cell competition-mediated removal of Ras-oncogene expressing cells, thus abrogating the primary epithelial defence against cancer. Stiff ECM inhibited the kinetics of the competition-mediated removal of the RasV12-expressing cells. RasV12 expressing cells appeared to be extruding much faster when the competition took place over a 4 kPa ECM than over a 23 kPa or 90 kPa ECM. Upon performing monolayer stress microscopy (MSM), it was found that the homeostatic level of the monolayer stress was higher in the wild-type population than in RasV12 expressing population. Biophysical characterization using Bayesian inverse stress microscopy (BISM) at the collective level revealed that cell competition gave rise to local compressive stress within the loser population. Together, these results showed the implications of forces in cancer biology, especially at the tumour suppression phase. (P. Phani Shilpa, Sanjay Karki, Tamal Das)

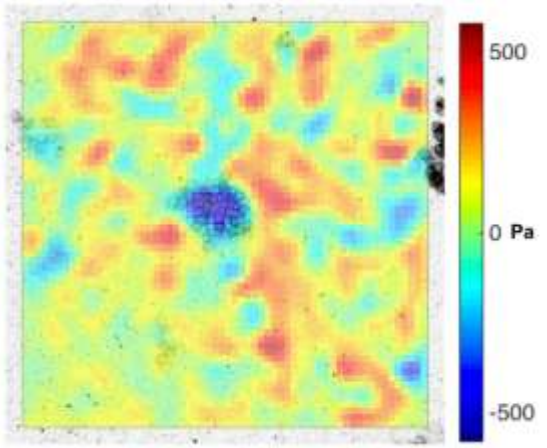

Figure 4: RasV12-expressing cells at the centre (black edges) experience high compressive stress during competition with wild-type cells (illustrated by Bayesian inverse stress microscopy).

Nanoscale analysis of synapses: The localization, transport of mRNA to synapses in neurons of the brain was investigated. Super-resolution microscopy tools were developed to investigate the composition of glutamate receptor ion-channels at ribbon synapses of auditory hair cells with the goal of understanding deafness induced structural rearrangements in these proteins. (Adish Dani)

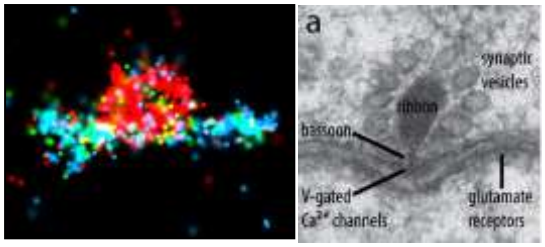

Figure 5: Comparison of a STORM image of single ribbon synapse of the inner ear hair cell, with previously published EM image.

Stoichiometry and dynamics of calcium channels: A novel flexible stoichiometry of calcium ion channel subunits on the plasma membrane was discovered. Insights were gained on how these stoichiometries affect channel function. (Adish Dani)

Molecular Immunology and Cell Signalling: The origin and outcome of cell surface receptor induced ion flux in the signal transmission, gene expression and function of white blood cells, called T cells, is being investigated. Genetic errors in proteins involved in the calcium and magnesium flux inside T cells have been associated with primary immunodeficiencies and cancers in human and mice. In particular, using a multi-disciplinary approach, this work is dissecting the novel and previously unsuspected direct regulation of T cell receptor induced ion flux and signal transmission by SNARE family, a group of proteins thought to be solely involved intracellular trafficking of protein cargo, thus far. Therefore, these studies hold the promise of obtaining paradigm shifting insights into T cell ion flux and moonlighting by SNARE family proteins in the regulation of immune response and cancer progression. (Monika Vig)

Role of cell-death in growing microbial colony: The occurrence of cell-death is an integral phenomenon of any developing multicellular community. Using both, mathematical and agent-based computer simulation modelings, the role of cell-death in a growing colony was investigated. Results show that cell-death can enhance and facilitate branch formation in a growing front. (Pushpita Ghosh and Herbert Levine)

Auto-chemotactic pattern formation in self-propelling bacteria: Bacteria, while forming biofilm-like multicellular complex organization, secrete chemotactic signaling molecules along with various extracellular polymeric substances. These secreted substances, in some cases, can attract or repel cells in the colony. To understand the spatial organization of reproducing bacteria in presence of possible chemo-attractive or chemo-repulsive interaction, a continuum model was invoked using reaction-drift-diffusion framework. The influence of logistic growth on chemotactic pattern formation was investigated. (Mrinmoy Mukherjee and Pushpita Ghosh)

Biological Chemistry and Molecular Biophysics

Structural characterization of α-synuclein oligomers: α-synuclein (α-Syn) aggregation into oligomers and fibrils is associated with Parkinson's disease (PD) pathogenesis. Although the relative role of oligomers versus fibrils in neuronal cell death in PD is not known, recent studies suggest the oligomers are proximate neurotoxin causing the disease. In this study, it was shown that incubation of high concentration of α-Syn in a physiological buffer converts the monomers into a gel state. Structural characterization of the gel revealed simultaneous co-existence of monomers, oligomers and fibrils. Solid-state NMR study of oligomers reveals a structurally heterogeneous population comprising of α-helical and β-sheet rich oligomers while the x-ray diffraction patterns of fibrils indicates cross- β motif morphology. Given the recent evidences of gel-like state of protein aggregation associated with neurodegenerative diseases, the gel-state of α-Syn in this study represents a mechanistic and structural model for in vivo toxicity of α-Syn in PD. (Saayak Halder, Samir Maji (IIT Powai), Vipin Agarwal)

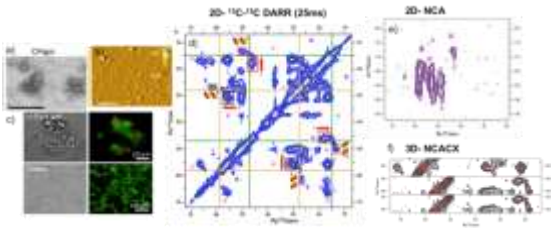

Figure 6: a) TEM & b) AFM picture of α-synuclein Oligomers c) Toxicity studies of human neuroblastoma cells in presence and absence of α-synuclein gels d) e) and f) show different NMR solid-state NMR spectra of α-syn Gel characterizing the structural propensities for different residues.

Understanding Protein Conformational Dynamics: T4 lysozyme (T4L) cavity mutants interconvert between compact conformations on the millisecond (ms) timescale. Although structures of the two compact conformers are available, the mechanistic details are still not available. By studying the interconversion process using CPMG NMR experiments performed as a function of viscosity, it was determined that interactions with water activate the molecules so that they can surmount the activation barrier. (Anusha B. Gopalan, Pramodh Vallurupalli)

New multiquantum (MQ) experiments to study protein conformational dynamics: Protein conformational dynamics occurring on the ms timescale are routinely characterised using CPMG type experiments. However, these experiments cannot be used to study faster process. The double and triple quantum transitions in methyl groups were exploited to investigate the process where the minor state lifetime is just ~50 μs. (Anusha B. Gopalan, Pramodh Vallurupalli)

Ligand binding to solvent inaccessible cavities in proteins: Ligands binding sites in protein molecules can be solvent inaccessible, these include oxygen binding to the heme group in Hemoglobin. Similarly, hydrophobic molecules like benzene bind a solvent inaccesible cavity in T4L cavity mutants rapidly. Using MD simulations, it was shown that tunnels to the cavity from the surface are transiently formed by the displacement of helices in the C-terminal domian of the protein.

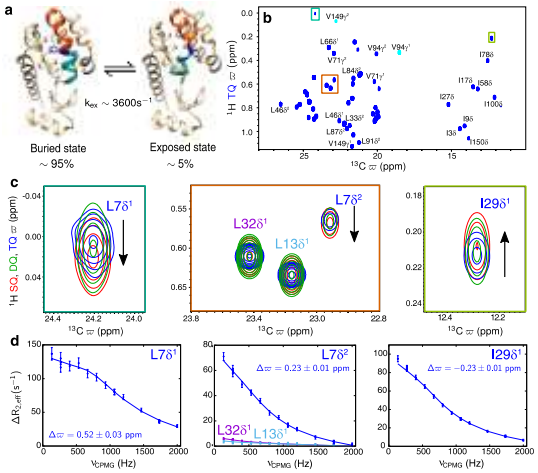

Figure 7: Reconstructing the spectrum of the 'invisible' minor states of proteins.

The fact that paths are created without any distortion in secondary structure shows that activation barrier is modest and hence ligands can bind rapidly. (N. Ahalawat, Subhendu Pandit, L.E. Kay (University of Toronto), Jagannath Mondal, Pramodh Vallurupalli)

Atomistic insights into structural differences among isoforms of Apolipoprotein E: Among various isoforms of Apolipoprotein E (ApoE), the E4 isoform (ApoE4) is considered to be the strongest risk factor for Alzheimer's disease, while E3 isoform (ApoE3) is neutral to the disease. Interestingly, the sequence of ApoE4 differs from its wild type ApoE3 by a single amino acid C112R in the 299 amino acid long sequences. Hence the puzzle remains: how a single-amino- acid difference between ApoE3 and ApoE4 sequence can give rise to structural dissimilarities between the two isoforms, which can potentially lead to functional differences with significant pathological consequences. The major obstacle in addressing this question has been the lack of a three-dimensional atomistic structure of ApoE4 till date. This issue was resolved by computationally modelling plausible atomistic three-dimensional structure of ApoE4. Microsecond-long atomistic simulations elucidated key structural differences between monomeric ApoE3 and ApoE4, which renders

ApoE4 thermodynamically less stable, less structured and topologically less rigid compared to ApoE3. (Angana Ray, Navjeet Ahalawat, Jagannath Mondal)

Kinetic Mechanisms of exit of an anticancer drug dasatinib from the receptor: Obtaining atomistic resolution of drug unbinding from a protein is a much sought-after experimental and computational challenge. The unbinding dynamics of the anticancer drug dasatinib from c-Src kinase in full atomistic resolution was reported using enhanced sampling molecular dynamics simulations. Multiple unbinding trajectories were obtained and a residence time in agreement with experiments was determined. Coupled protein-water movement through multiple metastable intermediates was observed. The water molecules formed a hydrogen bond bridge, elongating a specific, evolutionarily preserved salt bridge and enabling conformation changes essential to ligand unbinding. This water insertion in the salt bridge acted as a molecular switch that controls unbinding. These findings provided a mechanistic rationale for why it might be difficult to engineer drugs targeting certain specific c-Src kinase conformations to have longer residence times. (P.Tiwary, Jagannath Mondal and B. J. Berne (Columbia University))

Insights on mechanical stability of a protein under force at a single molecule level: Single molecule force spectroscopy is a useful technique for investigating mechanically induced protein unfolding and refolding under reduced forces by monitoring the end-to-end distance of the protein. The data is often interpreted via a two-state model based on the assumption that the end-to-end distance alone is a good reaction coordinate and the thermodynamic behaviour is then ascribed to the free energy as a function of this one reaction coordinate. In this study, the free energy surface (PMF) of GB1 protein was determined from atomistic simulations in explicit solvent under different applied forces as a function of two collective variables (the end-to-end-distance, and the fraction of native contacts). Brownian dynamics simulations on the smoothed free energy surface showed that the protein visits a metastable molten globule state and is thus a three state folder, not the two state folder inferred using the end-to-end distance as the sole reaction coordinate. This study lends support to recent experiments that suggest that GB1 is not a two-state folder. (R. Berkovich (Ben-Gurion University), Jagannath Mondal and B. J. Berne (Columbia University))

Solid-state NMR spectroscopy of amyloid fibrils: Aβ peptide continues to be an interesting model for investigating different aspects of amyloid aggregation. Clear evidence was obtained regarding the role of certain structural markers when these transit from monomers to fibrils through oligomers from previous studies by the group. Studies were initiated to understand the binding of these peptides with cell membranes. Initial solid-state NMR experiments suggest a rupture of one of the stable contacts upon binding with the membranes. A similar pattern was also found at the salt-bridge region, although that needs to be quantified. Such studies may lead to a further understanding of the role of these peptides in toxicity. Detailed solid-state NMR and fluorescence correlation spectrorscopy studies were carried out on IAPP, the peptide responsible for type-II diabetes. (P. K. Madhu, Kaustubh Mote, Sudipta Maiti (TIFR Mumbai))

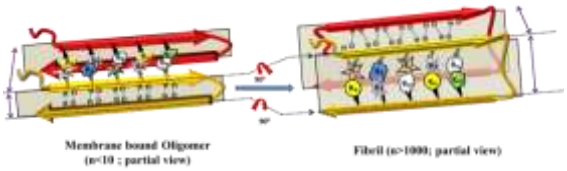

Figure 8: Secondary-structure changes from membrane bound Aβ oligomer to fibrils.

Structural Biology of Actins: In a bid to understand the fibrillization of actins and their regulation a number of proteins, the initial solution NMR experiments were expressed, purified and done. (Kaustubh Mote)

Structural Biology of Membrane proteins: The components of Mitochondrial Pyruvate Carrier Complex, a vital protein involved in the

regulation of the pyruvate flux into mitochondria, were successfully cloned, over-expressed and purified. To address questions in the area of active transport across membranes, the SemiSWEET transporter from bacteria was cloned. (Kaustubh Mote)

Underpinning the mechanistic action of short-chain antimicrobial β-peptides with membrane: Amphiphilic β-peptides are short-chain, rigid synthetic oligomers of β-amino acids which serve as alternatives of natural antimicrobial peptides. It was addressed whether the distinct molecular architecture of these short-chain and rigid β-peptides undergoes a distinct mechanistic action with membrane bilayer. Multi microsecond computer simulations and free-energy calculations were performed which deciphered the interaction of membrane with antimicrobial 10-residue β-peptides at diverse range concentrations. Using specifically developed parameters for β-peptides, this study reveals spontaneous insertion of β-peptides in the membrane interface at a low concentration and identifies partial water leakage in the membrane at a high concentration, without affecting the β-peptides' secondary structure.(Pushpita Ghosh, Jagannath Mondal, Xiao Zhu **(**Purdue University))

Chemical synthesis of novel natural/non-natural protein inhibitors that would interfere with the invasion of human red blood cells by malaria parasite: A new method for the facile cleavage of chemically synthesized peptides from solid support was recently developed. Analogs of malaria parasite proteins were chemically modified and rationally designed using methods developed in the laboratory. These have the potential to prevent formation of tight junction between parasite and erythrocyte, mediated by apical membrane antigen-1 (AMA1) and rhoptry neck protein (RON2), before the process of invasion takes place. These rationally designed protein molecules have the potential to significantly impact the elimination of malaria transmission worldwide. (Puneet Dubey, Sameer Singh, Jamsad Mannuthodikayil, Suman Sinha, Anamika Biswas, Abhisek Kar, Kalyaneshwar Mandal)

Building a super-resolution optical microscope: A super resolution fluorescence microscope was built to monitor growth of amyloid fibrils at single particle level. The data reveal that amyloid growth is highly heterogeneous, and follows a stop and go model. Amyloid fibrils form extensive network via cross-over between the fibrils rather than due to branching. (Kanchan Garai)

Characterization of role of chaperone Hsp70 on aggregation of amylin: It was found that Hsp70 inhibits amyloid aggregation of amylin even in substoichiometric concentrations. Furthermore, Hsp70 interacts with the oligomers but not with the monomers of amylin. (Kanchan Garai)

Characterization of role of apoE on aggregation of Amyloid beta: It was found that apoE interacts with amyloid beta with high affinity. Furthermore, apoE contains multiple independent interaction sites for amyloid beta peptide. (Kanchan Garai)

Fluid Dynamics

Topology of two dimensional flows of dust and gas: Direct numerical simulations (DNS) of passive heavy inertial particles (dust) in homogeneous and isotropic two-dimensional turbulent flows (gas) were performed for a range of Stokes number, St< 1. It was solved for the particles using both a Lagrangian and an Eulerian approach (with a shock-capturing scheme). In the latter, the particles are described by a dust-density field and a dust-velocity field. Using inertial particle velocity gradients and the corresponding flow topology, the density weighted joint distribution shows that converging saddle structures are most probable. (Dhrubaditya Mitra **(**Nordita- KTH Royal Institute of Technology and Stockholm

University), Rahul Pandit (IISc Bangalore), Debarghya Banerjee (Huygens Laboratory), Akshay Bhatnagar (Nordita- KTH Royal Institute of Technology and Stockholm University), Marc Brachet (PSL Research University, Sorbonne Universités), Anupam Gupta (Université de Toulouse) , Nairita Pal (IISc Bangalore), Samriddhi Sankar Ray (ICTS-TIFR), Vishwananth Shukla (CNRS, Universit Paris-Saclay), Dario Vincenzi (Université Côte d'Azur, CNRS) and Prasad Perlekar.

Laser Physics:

Studies on laser-cluster interaction dynamics: Non-linear absorption of intense (>10^15W/cm2), sub-ps pulses by Ar and N2 clusters were observed. When comparatively studied as a function of the pulse width, it allowed distinguishing of field driven ionisation contribution from collective effects. The large difference in absorption trends between Ar and N2 as a function of pulse widths indicated different mechanisms being in play. Small N2 cluster systems provide an ideal model system wherein field ionization dominates, whereas Ar clusters show resonance absorption for long pulses. Till date, it was possible to "switch off" different phenomena which accompany ionisation of clusters only in theory and simulations. The same was demonstrated experimentally, specifically to isolate collective and non-collective effects. The results also indicate that schemes that presume non-uniform electron density wherein different regions of clusters can come into the resonance with the light fields at different times may not always be appropriate. (Soubhik Sarkar, Ram Gopal, M Krishnamurthy)

Intense laser plasmas from matter on mesoscopic scales- Liquid drop experiments: Generation of energetic electrons, as high as 6MeV, has been observed from laser matter interaction in methanol droplets. Two distinct energy regimes, one ranging from 200keV-1MeV and other from 1MeV-6MeV, have been identified. The electron temperatures are found to be 200keV and 900keV respectively. Angular distribution measurements show that the electrons are confined in the laser polarization plane and are emitted mostly at $\pm 50°$ with respect to the laser backward direction. Dependences on intensity and pulse-width have also been studied. Single and double pulse Z-scans of the focussed laser beam on the droplet indicate thermalization effects in presence of a pre-pulse. Protons with energy as high as 560keV have also been detected. X-rays, till 150keV, are found to be emitted directly from the drop. These X-rays have been used to obtain high resolution ~ 50um, images of metallic and biological samples. (Angana Mondal, S. V. Rahul, Debobrata Rajak, Ram Gopal, M Krishnmurthy)

Collaborative experiments in femtosecond dynamics in molecules: A velocity map imaging spectrometer for ions was set up. The dissociative ionization of O2 and CH3I at intensities of 1013-1014 W/cm2 of 30 fs laser pulses was studied. The energy and angle resolved ion fragments from O2 when studied as a function of the incident intensity indicated the role of excited state polarizabilities of the ions and the resultant rotation of the ion under the influence of the electric field post ionization. Further analysis is underway to quantify these mechanisms. In a recently concluded experiment, the dissociation of CH3I, as a function of pulse width of the laser, was studied. The motivation is to look at possible internal conversion events wherein charge transfers from the CH3 to I post ionization. (D Rajak, Ram Gopal, Arnab Sen (IISER Pune), Vandana Sharma (IIT Hyderabad), M. Krishnamurthy)

Figure 9: A methanol drop instantly heated to a billion kelvin emits light (visible and x-rays) like the sun.

Resource generation and innovation activities: In a novel initiative, TIFR Hyderabad and the Central Laser Facility, Rutherford Appleton Lab (RAL), Oxford UK have entered into a collaboration to develop the control systems for next generation Petawatt Laser and particle acceleration systems. The new Innovation Centre was set up with the induction of 5 engineers with software and electronic engineering backgrounds funded by RAL. With support and supervision from members of the Laser Lab and technology and training support from RAL, it envisaged to result in a full self-sustained control system which would be of interest to laser companies and research institutes worldwide. (M. Krishnamurthy)

Material Sciences

Thin film growth of superconducting Magnesium diboride (MgB2): MgB2 is a compound superconducter with the highest transition temperature among other BCS superconductors. Superconducting thin films of this compound were grown using a single tarket sputtering source. Further film optimization and device fabrication is currently underway. (Karthik V. Raman)

Epitaxial growth of topological insulator, Bismuth selenide: Epitaxial growth of Bismuth selenide was possible in our custom designed molecular beam epitaxy system. Complete structural characterization confirmed very high quality of the films grown. Proximity effect with a ferromagnetic insulator such as Europium sulphide is underway. (Karthik V. Raman)

Atomic layers based catalysts: Though graphene technology has reached in to technology readiness level 9 (TRL9), pristine layers are still inactive towards certain important catalytic reactions such as hydrogen evolution reaction (HER), oxygen reduction reaction (ORR), and oxygen evolution reaction (OER). Hydrogen is identified as a futuristic energy resource due to its high energy density, and water splitting as a greener route towards its production. Research efforts were directed at the development of disorderly and orderly arranged atomic heterostructures of graphene, MoS2, and hexagonal boron nitride (hBN), and their activity studies towards various catalytic reactions.

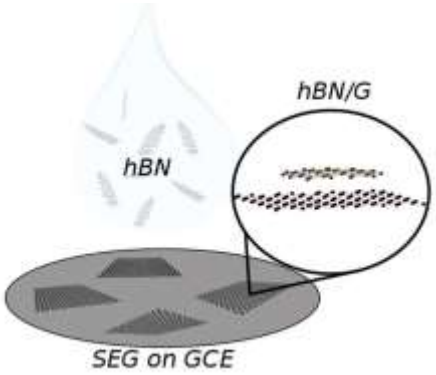

Figure 10: Image showing the assembly of shear exfoliated single layer graphene (SEG) and hBN on glassy carbon electrode (GCE).

Figure 11: A high resolution of transmission electron microscopic image of the same showing two types of atomically thin domains - graphene and hBN.

It was found that such vertical interfaces of two different atomic layers can make the structure active towards HER, where the individual layers are not active at all. A mechanistic picture in to this observed mechanism is given using density functional theory based calculations and molecular dynamics based studies. This heterostructure activity study was extended to other structures such graphene/MoS2, too, where they were also found to be active towards photocatalysis. Further, stacking sequence dependent catalytic activity of layers is also disclosed in these studies. This is a novel aspect of such materials, which was not found in other catalysts and/or reported before on atomic layers.

Ion transport membranes for pure water electrolysis: New type of proton (H+) transport membrane cum separator were designed and developed which was found to be working even in pure water electrolysis. Economically inexpensive, proton transporting solid state polymer membrane (HPEOP) was developed using perchloric acid (HClO4) as proton source with poly(ethylene oxide) (PEO) and polydimethylsiloxane blend as hosting structure. Room temperature (25 oC) low humidity ionic conductivity of HPEOP is found to be 0.0032 S/, and lowering the melting temperature of PEO through HClO4 'salting in' was found to have considerable effect in enhancing the conductivity of solid electrolytes, while this also modifies the microstructure and mechanical strength of the membrane. Water electrolysis cells were constructed with both pure and protonated water using both HPEOP and Nafion separators, and studies showed the possibilities of highly efficient low cost water electrolysis and fuel cells devoid of expensive Nafion membranes.

Figure 12: Photograph of proton conducting membrane developed in the laboratory.

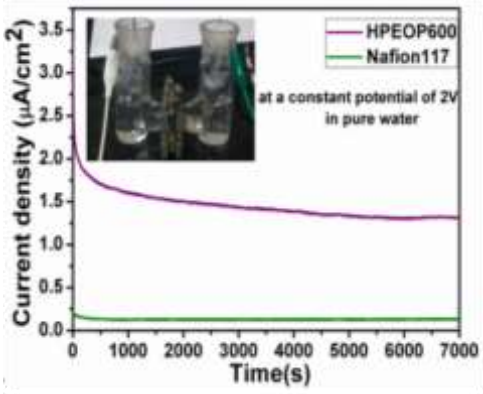

Figure 13: Performance of proton conducting membrane in pure water electrolysis and comparison with Nafion 117 electrolytes.

Chemical vapor deposition assisted synthesis of atomic layers for devices: High quality atomic layers can be developed using chemical vapor or physical vapor deposition assisted methods. Efforts were underway to develop such high quality crystals of graphene, MoS2, and doped graphenes' such as fluorographene (oxide) and boron and/or nitrogen doped graphene. Single step, catalyst free, wafer-scale synthesis of fluorographene oxide (FGO) ultra-thin films synthesis by physical vapour deposition was reported. This FGO, possessing 7% fluorine content, comprises a few nanometer domains of sp2-sp3 carbon with high thermal stability. It was shown that FGO can be utilized as an active hetero-layer on a few-layer MoS2 field effect transistor (FET), significantly improving the performance of MoS2 optoelectronic devices with an

extended spectral response towards the near infrared and responsivity of up to 6A/W. The FGO-MoS2 band alignment as derived from the measured work function of FGO indicated a photoconductive gain mechanism with a fast transit time of holes mediated by FGO quasi-continuous defect states.

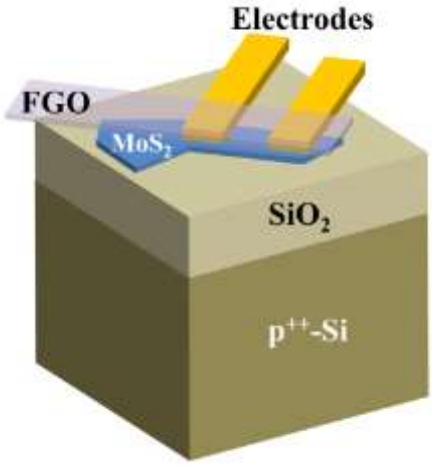

Figure 14: Schematic of the FET device developed using MoS2 atomic layers and FGO.

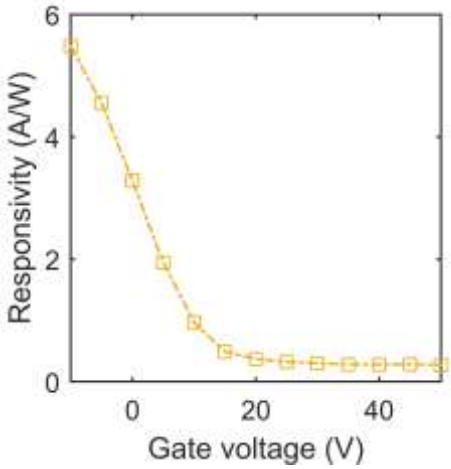

Figure 15: Photoresponsivity of the FET device with different gate voltage.

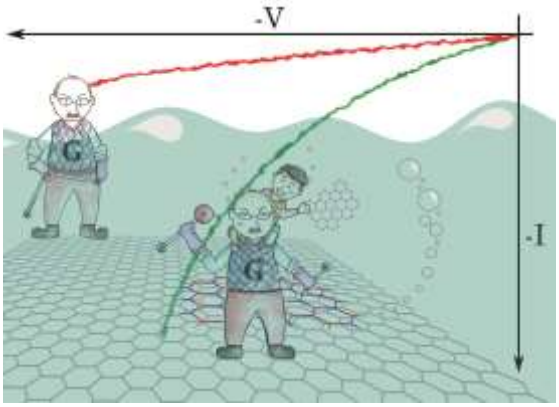

Figure 16: Cover art image (image courtesy: Ms. Anusheela Chatterjee, TIFR-H) describing a work published from the Narayanan's group in collaboration with Dr Jagannath's group, which appears as a cover page image in one of the Phys. Chem. Chem. Phys. issues in 2018.

Nuclear Magnetic Resonance Spectroscopy

Decoupling schemes in solid state NMR: Spin decoupling is essential in solid-state NMR to improve the resolution and sensitivity of the spectra of both rare and abundant spins. In the former case, such as 13C and 15N, heteronuclear dipolar decoupling is used whilst in the latter, such as 1H, homonuclear dipolar decoupling is used. Both these methods were combined in magic-angle spinning (MAS) solid-state NMR experiments. This is important in the observation of high-resolution 1H spectra in samples that are uniformly labelled with either 13C or 15N or both. The homonuclear decoupling scheme was applied to the 1H channel and heteronuclear decoupling on the 13C or 15N channel. Optimal strategies were found to minimise the interference effects between these two time-dependent processes and the MAS. This was the main reason why various attempts in this direction failed in the past and our experiments were able to circumvent this by knowledge of the theory of the interference effects and also with the application of the much robust rotor-synchronised rCW heteronuclear decoupling

scheme developed in our group. This is expected to be useful in the study of biomolecular systems at high MAS and low radiofrequency (RF) amplitude regimes where proton detection can be useful but at the same time one has to encounter the isotopically labelled rare spins. (P. K. Madhu, Kaustubh Mote)

Recoupling pulse schemes and strategies: The standard rotational-echo double resonance (REDOR) experiment used in solid-state NMR has proven to be one of the most useful and robust schemes in distance measurements. Robust variants of this scheme were introduced to measure strong one-bond dipolar couplings with a high precision by shifting the pulses in a way that can be quantified with average Hamiltonian theory and numerical simulations. The proposed methods allow scaling down of the dipolar coupling in the full range of 0-1. The results are also free of any orientational dependence of the crystallites in the sample that plagued similar attempts in the past. The scaling factor is independent of the RF and MAS frequency and can be applied over a wide range of MAS frequencies. (Mukul Jain, G.Rajalakshmi, Kaustubh Mote, Vipin Agarwal, Matthias Ernst (ETH, Zurich), P. K. Madhu)

Towards spin exchange optical pumping of Xe: Spin-exchange optical pumping was set up. This was aimed at hyperpolarising NMR signals, primarily observing NMR signals from noble gases such as Xenon. The aim is mainly investigations in the area of low-field NMR and magnetometry. In this direction, a rubidium magnetometer for the detection of NMR signals was built. (G. Rajalakshmi, Vineeth Francis, P. K. Madhu)

Hydro-dynamics of particle wall interactions: For the first time, it was experimentally established that, as opposed to the common belief of lubrication theory, there is solid-on-solid contact during sphere-wall collision in a viscous fluid. (Sumit Kumar Birwa (ICTS Bangalore), G. Rajalakshmi, Rama Govindarajan (ICTS Bangalore), Narayanan Menon (UMass)

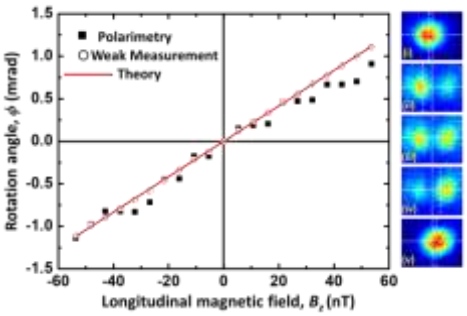

Figure 16: Polarisation rotation angle as a function of longitudinal magnetic field, with images profile change for various rotation angles

Measuring quantitative proton-proton distances in fully protonated solids: The experiments to quantitatively measure proton-proton distances still remain elusive mainly due to the presence of strong and multiple proton-proton dipolar couplings. In this project, a new MAS solid-state NMR method was proposed to selectively measure proton distances in fully protonated samples. The proposed novel sequence generates a homonuclear double quantum dipolar Hamiltonian that is additionally modulated by the sum of the chemical shifts. At certain conditions the chemical shifts modulation can be eliminated which in turn leads to selective recoupling of the dipolar Hamiltonian. It was shown in a small molecule system that quantitative 1H-1H distances of up to few angstroms can be measured despite the presence of other strongly coupled protons. The experiment can also be used for selective first-order proton-proton polarization transfer in macromolecules like proteins. Major applications of this methodology would be in structural characterization of pharmaceutical polymorphs and biomolecules. (Sreejith Kurussi, Yusuke Nishiyama (Jeol, Yokohama Japan), Vipin Agarwal)

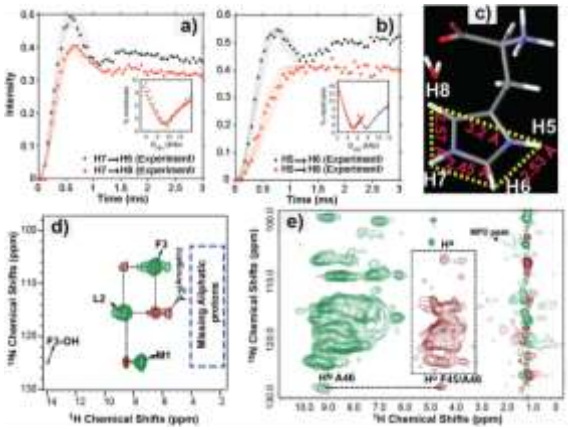

Figure 17: Figure 1 Polarization transfer buildup curves a) H7→ H6 & H8 b) H5→ H6 & H8 using SERP recoupling. The red and black strip show the confidence interval for fitting of the data. The inset highlights the average percentage deviation in intensity per point between experimental and simulated data c) Structure of Histidine and corresponding distances d) Selective HN→HN transfer in MLF tri-peptide and e) Selective HN→ H^{α} transfer in Ubiquitin. Positive contours are depicted in green while negative contours are depicted in brown.

Theoretical description of BASS-SD: In the recent past, the BASS-SD experiment (J. Phys. Chem. Lett., 8, 2399-2405 (2017)) was proposed to obtain long-range selective 1H-1H contacts on the order of 5-6 Å despite the presence of other protons at shorter distances in fully protonated proteins. The BASS-SD experiment is particularly useful in providing 1H-1H structural restraints for structure determination. This year, a theoretical model based on bimodal Floquet theory was proposed to explain these results. The theoretical model can predict the behaviour of magnetization transfer in a homogenously coupled spin system under conditions of weak rf irradiation and ultrafast MAS frequencies. (P.K. Madhu, Vipin Agarwal)

Through bond correlation spectroscopy (TOBSY): Through-bond J-coupling based experiments in solid-state NMR spectroscopy are challenging because the J couplings are typically much smaller than the dipolar couplings. This often leads to a lower transfer efficiency compared to dipolar-based sequences. One of the reasons for the low transfer efficiency is second-order cross terms involving the strong heteronuclear dipolar couplings. In this project, it was shown that by employing a symmetry-based C9 sequence, which was carefully selected to suppress second-order terms, efficient polarization transfers of up to 80% can be achieved without decoupling on fully protonated two-spin model systems at a MAS frequency of 55.5 kHz with rf-field amplitudes of about 25 kHz. In addition, the effects of rf inhomogeneity and crystallites selection due to the polarization preparation method on the TOBSY transfer efficiency was analyzed. It was also demonstrated that on small model substances as well as on the protein ubiquitin (side-chains deuterated, amides fully protonated) that $C9_{1/39}$ and $C9_{1/48}$ are efficient and practical TOBSY sequences, at experimental conditions ranging from proton Larmor frequencies of 400 to 850 MHz and MAS frequencies ranging from 55.5 to 111.1 kHz. (Beat Meier and Matthias Ernst (ETH Zurich, Vipin Agarwal)

Synthetic Chemistry

Preparation of a pentagonal bipyramidal lanthanide complex: The design of the complex was made with the objective of obtaining a weak equatorial crystal field and strong axial field. The challenge in this design was two-fold. One, lanthanide ions prefer large coordination numbers and restricting their coordination to numbers below eight is tricky. Second, the ligand design should be such that a pentagonal bipyramidal geometry is naturally imposed in the resulting complex. These two challenges were met and the complexes (Et3NH)[(H2L)LnIIICl2] (where H4L = 2,6-diacetylpyridine bis-salicylhydrazone and Ln = Tb (1), Dy (2), and Y0.94Dy0.06 (3) could be prepared and characterized. Among these 2 and 3 were shown to be single-molecule magnets. (A. K. Bar, P. Kalita, J. P. Sutter, V. Chandrasekhar)

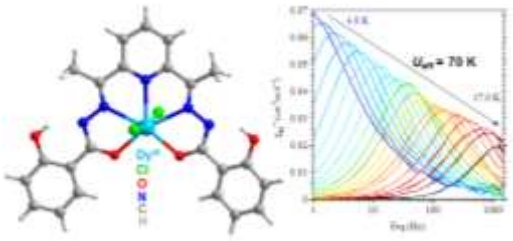

Figure 18: Molecular structure of Et3NH)[(H2L)DyIIICl2] and its ac susceptibility magnetic studies.

Multiple bonded compounds of heavier main group elements: The synthesis of 2-hydroiminosilane and its addition reaction with water was reported. The reactivity of bulky substituted diphosphene, a phosphorus-phosphorus double bonded compound, was enhanced by the reversible coordination of N-heterocyclic carbene with respect to hydrolysis and hydrogenation reactions. (Anukul Jana, Debabrata Dhara, Debdeep Mandal, Avijit Maity, Ramakirushnan Suriya Narayanan)

Low-Valent Main Group Compounds: Electron-rich alkenes considering peralkyl substituted triazaalkenes motif were synthesized. These oxidized reversibly, stepwise and were able to isolate corresponding radical cations and dications of it. The mono and di-coordinated germanium(0) which act as a four electron donor was disclosed. (Anukul Jana, Debdeep Mandal, Ramapada Dolai, Debabrata Dhara, Avijit Maity, Ramakrishnan Suriya Narayanan)

Molecular Phosphates: Bulky aryl substituted neutral and anionic phosphatemonoesters have been synthesized and solid state molecular structure resembles with that of carboxylic acids. (Biswajit Santra, Debdeep Mandal, Ramakirushnan Suriya Narayanan, Anukul Jana)

Soft Matter

Characterising solid-solid transitions in colloids: A framework to segregate the roles of elastic and non-elastic deformations in the examination of real-space experiments of solid-solid transitions was presented. The Martensitic transformation of a body-centred-tetragonal (BCT) to a body-centred-orthorhombic (BCO) crystal structure has been studied in a model system of micron-scale ionic microgel colloids. Non-affine fluctuations, i.e., displacement fluctuations that do not arise from purely elastic (affine) deformations, are detected in particle configurations acquired from the experiment. Tracking these fluctuations serves as a highly sensitive tool in signaling the onset of the Martensitic transition and precisely locating particle rearrangements occurring at length scales of a few particle diameters. Particle rearrangements associated with non-affine displacement modes become increasingly favorable during the transformation process. The nature of the displacement fluctuation modes that govern the transformation are shown to be different from those predominant in an equilibrium crystal. It was shown that BCO crystallites formed through shear may, remarkably, co-exist with those resulting from local rearrangements within the same sample. (Saswati Ganguly, Priti S. Mohanty (KIIT University, Lund University), Peter Schurtenberger (Lund University), Surajit Sengupta and Anand Yethiraj (Memorial University, St. John's Newfoundland Labrador))

Dynamical, feedback controlled laser traps for stabilising colloidal crystals of any given symmetry: It was shown that dynamic, feed-back controlled optical traps, whose positions depend on the instantaneous local configuration of particles in a pre-determined way, can stabilise colloidal particles in finite lattices of any given symmetry. Unlike in a static template, the crystal so formed is invariant under uniform translations and retains all possible zero energy modes. This was demonstrated in silico by stabilising the unstable two-dimensional square lattice in a model soft solid with isotropic interactions. (Pankaj Popli, Saswati Ganguly and Surajit Sengupta)

Theoretical Physics

Spreading of non-motile bacterial colonies on a hard agar plate: The spreading of a non-motile bacterial colony on a hard agar plate was studied using agent-based and continuum models. It was shown that the spreading dynamics depends on the initial nutrient concentration, the motility, and the inherent demographic noise. Population fluctuations are inherent in an agent-based model, whereas for the continuum model we model them by using a stochastic Langevin equation. It was shown that the intrinsic population fluctuations coupled with nonlinear diffusivity lead to a transition from a diffusion limited aggregation type of morphology to an Eden-like morphology on decreasing the initial nutrient concentration. (Navdeep Rana, Pushpita Ghosh, Prasad Perlekar)

A novel method to study growth of amorphous order in glass-forming liquids: Existence and growth of amorphous order in supercooled liquids approaching glass transition is a subject of intense research. Even after decades of research, there is still no clear consensus on the molecular mechanisms that lead to a rapid slowing down of liquid dynamics approaching this putative transition. The existence of a correlation length associated with amorphous order has recently been postulated and this has been estimated using multi-point correlation functions, which cannot be calculated easily in experiments. Thus the study of growing amorphous order remains mostly restricted to systems like colloidal glasses and simulations of model glass-forming liquids. An experimentally realizable yet simple correlation function was proposed to study the growth of amorphous order. The validity of this approach was then demonstrated for a few well-studied model supercooled liquids and the results obtained were consistent with other conventional methods. (Rajshekhar Das, Saurish Chakrabarty (ICTS Bangalore), Smarajit Karmakar)

Block analysis for the calculation of dynamic and static length scales in glass-forming liquids: Block analysis is an efficient method of performing finite-size scaling for obtaining the length scale of dynamic heterogeneity and the point-to-set length scale for generic glass-forming liquids. This method involves considering blocks of varying sizes embedded in a system of a fixed (large) size. The length scale associated with dynamic heterogeneity is obtained from a finite-size scaling analysis of the dependence of the four-point dynamic susceptibility on the block size. The block size dependence of the variance of the α relaxation time yields the static point-to-set length scale. The values of the obtained length scales agree quantitatively with those obtained from other conventional methods. This method provides an efficient experimental tool for studying the growth of length scales in systems such as colloidal glasses for which performing finite-size scaling by carrying out experiments for varying system sizes may not be feasible. (Saurish Chakrabarty, Indrajit Tah, Smarajit Karmakar, and Chandan Dasgupta (IISc Bangalore))

Glass transition in supercooled liquids with medium range crystalline order: The origins of rapid dynamical slow-down in glass forming liquids in the growth of static length scales, possibly associated with identifiable structural ordering, is a much-debated issue. Growth of medium range crystalline order (MRCO) has been observed in various model systems to be associated with glassy behaviour. Such observations raise the question about the eventual state reached by a glass former, if allowed to relax for sufficiently long times. Is a slowly growing crystalline order responsible for slow dynamics? Are the molecular mechanisms for glass transition in liquids with and without medium range crystalline order the same? If yes, glass formers with MRCO provide a paradigm for understanding glassy behaviour generically. If not, systems with MRCO form a new class of glass forming materials whose molecular mechanism for slow dynamics may be easier to understand in terms of growing crystalline order, and should be approached in that manner, even while they will not provide generic insights. In

this study, extensive molecular dynamics simulations of a number of glass forming liquids in two dimensions were performed. It was shown that the static and dynamics of glasses with MRCO are different from other glass forming liquids with no predominant local order. An important issue regarding the so-called Point-to-set method for determining static length scales was resolved, it was demonstrated to be a robust, order agnostic, method for determining static correlation lengths in glass formers. (Indrajit Tah, S. Sengupta, S. Sastry, C. Dasgupta, Smarajit Karmakar)

Role of α and β relaxations in collapsing dynamics of a polymer chain in supercooled glass-forming liquid: Understanding the effect of glassy dynamics on the stability of bio-macromolecules and investigating the underlying relaxation processes governing degradation processes of these macromolecules are of immense importance in the context of bio-preservation. The stability of a model polymer chain in a supercooled glass-forming liquid at different amount of supercooling was studied in order to understand how dynamics of supercooled liquids influence the collapse behavior of the polymer. Our systematic computer simulation studies find 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. This is in agreement with some recent experimental findings. These observations are in stark contrast with the common belief that only long time relaxation processes are the sole player. Convincing evidence was found that suggest that one might 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. Our results may potentially lead to the understanding of primary factors in protein stabilization in the context of bio-preservation. **(**Mrinmoy Mukherjee, Jagannath Mondal, and Smarajit Karmakar)

Possible universal relation between short time β-relaxation and long time α-relaxation in glass-forming liquids: Relaxation processes in supercooled liquids are known to exhibit interesting as well as complex behavior. One of the hallmarks of this relaxation process observed in the measured auto correlation function is occurrence of multiple steps of relaxation. The shorter time relaxation is known as the β-relaxation which is believed to be due to the motion of particles in the cage formed by their neighbors. On the other hand, longer time relaxation, the α-relaxation is believed to be the main relaxation process in the liquids. The timescales of these two relaxations processes dramatically separate out with supercooling. In spite of decades of researches, it is still not clearly known how these relaxation processes are related to each other. It was shown that there is a possible universal relation between short time β-relaxation and the long time α-relaxation. This relation is found to be quite robust across many different model systems. Finally it was shown that length scale obtained from the finite size scaling analysis of β timescale is same as that of length scale associated with the dynamic heterogeneity in both two and three dimensions. **(**Rajsekhar Das, Indrajit Tah, and Smarajit Karmakar)

Inductive and Deductive Modelling of Matter

Development of a big data repository of molecular and materials properties: The main components of a web-based data-mining platform has been implemented and hosted at TCIS. Molecular datasets from various sources has been injected into this repository. A new dataset of substituted poly-aromatic hydrocarbons with over several billion molecular structures and desirable opto-electronic properties has been generated at TIFR Hyderabad. (Raghunathan Ramakrishnan)

Science Education:

Outreach was initiatiated in schools of the Telangana Social Welfare Residential Educational Institutions Society (TSWREIS). This sustained program of interaction included 73 mainly weekend visits to three neighbouring TSWREIS schools, each by an average of 4-5 volunteers from TCIS and University of Hyderabad. The volunteers conducted sessions with secondary and intermediate students aimed to support meaningful, laboratory-based science learning. Low-cost paper microscopes called 'Foldscopes' were introduced in these schools on a pilot basis. A 'Meet a Scientist' program was conducted in face-to-face mode a local TSWREIS school and, in distance mode over the T-SAT Nipuna channel reaching remote schools in Telangana State. Interactions with TSWREIS are leading into an R&D project on curiosity and questioning.

Implementation of the 'Homi Bhabha Curriculum for Primary Science' (developed at HBCSE 15-20 years ago) was followed up with teachers in a few schools around the country. This community of progressive and innovative teachers was supported to document and share their experiences on the 'Small Science' website of HBCSE. (Jayashree Ramadas)

Faculty Members

Surajit Sengupta, V. Chandrasekhar (from Jun 19, 2017) Smarajit Karmakar, Prasad Perlekar, Anukul Jana, Kanchan Garai, Pramodh Vallurupalli, T.N. Narayanan, Aprotim Mazumder, Karthik V. Raman, M. Krishnamurthy, P.K. Madhu, Vipin Agarwal, Jagannath Mondal, Raghunathan Ramakrishnan, Kalyaneswar Mandal, Tamal Das, Manish Jaiswal, Jayashree Ramadas, Monika Vig (from Jul 10, 2017), Adish Dani (from Jul 17, 2017), Pranav R. Shirhatti (from Jul 17, 2017), N. D Haridass (till Jun 30, 2017), Mustansir Barma, Kaustubh R. Mote, Pushpita Ghosh, Subodh R Shenoy, N.D. Haridass (from Jul 11, 2017)

Research Scholars

Anshul Deep Singh Parmar (till Jul 31, 2017), Vinutha H A (till Jul 31, 2017), Shivnarayan T Dhuppar, Pankaj Popli, Rashmi Ramadugu, Shubhadeep Pal, Rayan Chatterjee, Debabrata Dhara, Debdeep Mandal, Timir Baran Sil, Rahul K Gupta, Rajsekhar Das, Saurabh Chaudhary, Sudeshna Patra, Mrinmoy Mucherjee, Bhanu Prasad Bhowmik, Pappu Acharya, Subhrajyoti Dolai, Mukul G Jain, Indrajit Tah, Subhendu Pandit, Khandekar Jishan Bari, Dheeraj P Dube, Sripati V Rahul, Lokrshi Prawar Dadhichi, Navdeep Rana, Keerthan Subramanian (till Sep 30, 2017), Archit Bhardwaj, Vikash Pandey, Shashank Yadav (till Sep 29, 2017), K. Jaya Krishna, Kallol Paul, Janeka, Kshama Sharma, Debankur Das, Anusha Bargavi Gopalan, P. S Kesavan, Shamasree Ghosh, Rahul Sharma, Nikhita Pasnuri, Avijit Maiti, Sumit Bawari, Vishnu V Krishnan, Bhupendra R Dandekar, Mithun Maddheshiya Subinoy Adhikari, Abhisek Kar, Suman, Soham Mukhopadhyay, Satyabrata Bandyopadhyay, Anamika Biswas, Pravin Pralhad Taware, Mithilesh Kumar Nayak, Sabyasachi Chakraborty, Anku Guha, Phani Shilpa Pothapragada, Paswa Nath, Geetika, Satyaki Sasmal, Anoop Mutneja, Krishna Rani Sahoo, Pallavi, Sarawata B Sharanwala (from Aug 1, 2017), Sahil (from Aug 1, 2017), Rajit Narayanan C (from Aug 1, 2017), Purnati Khuntia (from Aug 1, 2017), Piyush Daga (from Aug 1, 2017), Mohammad (from Aug 16, 2017), Basil Thurakkal (from Aug 1, 2017), Sourav Das Adhikari (from Aug 1, 2017), Md Alamgir (from Aug 1, 2017

to Feb 13, 2018), Avinash Kumar (from Aug 1, 2017), Olivia Basu (from Aug 1, 2017 till Nov 15, 2017), Sourav Bhakta (from Aug 1, 2017), Ved Prakash Tiwari (from Aug 1, 2017), George Kurian K.K. (from Aug 1, 2017), Aishwayra Mandya (from Aug 7, 2017)

Post-Doctoral Fellows

C. Neeraja(till Dec 31, 2017), Deepa Jaiswal, Sitara Roy (till Apr 04, 2017), Biswajit Santra, S. Mathimalar (till May 31, 2017), Guntupalli Gopi Krishna, Ravi Kumar Biroju (till Apr 28, 2017), Laxman Mahadev Alakonda, Chandrakala M Gowda, Venkata Subbarao R (till Nov 30, 2017), Bankanidhi Sahoo, Anand Puthirath Balan (till Nov 20, 2017), Naddi Shankaraiah, Tapas Singha, Navjeet Ahalawat , Jamad Mannuthodikayil, Shrikanth Sharma (till Jul 31, 2017), Ronald Benjamin (till Feb 23, 2018)), Atul Singh Bharadwaj (till Sep 13, 2017), Rajasekhar Pothala (from February 15, 2017), Angana Roy (till Feb 02, 2018), Vivek Gupta (till Sep 20, 2017), Rahul Kumar (till Mar 22, 2018), Sreekanth N (from Apr 04, 2017), Sitara Roy (from Apr 17, 2017), Subas Chandra Bera (from Apr 28, 2017), Ravi Kumar Biroju (from May 01, 2017), Suman Sinha (from May 03, 2017) Krishnendu Gope (from May 16, 2017 to Oct 20, 2017), Vineesh T. Veettil (from Jun 01, 2017), S. Mathimalar (from Jun 02, 2017), Pankaj Kumar Rastogi (from Jun 05, 2017), R Suriya Narayanan (Jul 03, 2017), Shrikant Sharma (from Aug 01, 2017), Prabhakar Eeka (from Sep 01, 2017), Atul Singh Bhardwaj (from Sep 14, 2017), Vivek Gupta (from Sep 21, 2017), Atanu Dey (from Aug 30, 2017), Neha Singhal (from Oct 25, 2017), Baljeet Singh (from Oct 31, 2017), Amit Chakraborty (from Nov 03, 2017), Ravi Shankar Palani (from Jan 25, 2018 – Mar 15, 2018), Sai Ram Turaga (from Jan 25, 2018), Munaiah Yeddala (from Mar 05, 2018), Joynarayan Mukherjee (from Mar 15, 2018), Sourav Ganguly (from Mar 16, 2018).

Junior / Senior Research Fellows

Sarika Kumari (till May 25, 2017), Akshi Gupta (till Jun 30, 2017), Sambit Mohapatra (till Jun 03, 2017), Ramapada Dolai, Naresh Kumar(till May 17, 2017), Saayak Halder (till July 14, 2017), Vineeth Francis, Syed Muhammed Muazzam Kamil (till Dec 05, 2017)), Rakesh Kumar Y, Arka Provo Das, Nisheal Michael Kaley (from May 05, 2017), Deepa Balasubramanian (from May 22, 2017), Sanjay Karki (from Aug 17, 2017), Puneet Kumar Dubey (from Jul 21, 2017), Debpbrata Rajak (from Aug 01, 2017), Bhaskar P Soman (from Aug 01, 2017), Dipanjana Saha (from Aug 24, 2017 to Dec 29, 2017), Badal Mondal (from Sep 01, 2017), Sameer Singh (from Sep 01, 2017), Naresh Kumar (from Sep 19, 2017), Greeshama Jain (from Oct 03, 2017), Abhirath Batra (from Nov 03, 2017), Anusheela Chatterjee (from Nov 16, 2017), Dipanjana Saha (from Jan 01, 2018), Chhabi Pal (from Jan 12, 2018)

Visiting Student/Project Assistant & Scientist/Project Associate/Short Term Visiting Fellows

Nikhil Jaisinghani (till Jun 30, 2017), Swapneel A Pathak (from Apr 03, 2017 to Jul 13, 2017), Samvit Mohapatra (from May 09, 2017 to Nov 30, 2017), Abhirath Batra (from May 01, 2017 to Oct 31, 2017), Apeksha Madhukar Chipade (from Jan 01, 2018), Subindev (from Jan 01, 2018), C. Neeraja (from Jan 02, 2018 to Feb 01, 2018), Vandna Gokhroo (from Jan 05, 2018, Mar 04, 2018), Ramita Anand (from Jan 17, 2018), Adyasha Panda (from Mar 15, 2018), Rajvi Chandrakanth Dhimar (from Mar 26, 2018)

Scientific/Technical staff

Ram Gopal, Rajalakshmi G, N. Kalyan Kumar, Krishnarao Doddapuneni, Suman Saurav, Deepa S, Velmurugan G.V. (till Jan 25, 2018), Sreejith Raran-Kurussi, Rajasekhar Rajapurmath, N. Srenaiah, Krishna A Elipilli

Administrative Staff

D. Hariprasad, J. Ratna, Mruduta R. Barde (till Jul 20, 2017), Vivek Baban Hadawale, D. Raghuram Dathu, M. Varalakshmi, Roopashri R Prasad, Hemalatha P, Hanumanth Rao , T. Srinu Babu (from Apr 04, 2017)

Project Staff

Pittala Kumar, P. Kasiviswanath, Rajdip Das, Lalitha Minocha (till Jun 01, 2017), Nakkireddy Swapna (till Dec 29, 2017), , Pemberla Rajitha (till Dec 29, 2017), Mallikarjun S. (till Jan 04, 2018), K. Archana (till Aug 07, 2017), Vikas Kumar Arandker, T. Srinu Babu (till Apr 03, 2017)), Narsimulu (till September 18, 2017), Anil Kumar Mora (from Apr 17, 2017), Sripal Sulgae (from May 02, 2017 to Jul 24, 2017), Srinidhi K.S. (from May 29, 2017), Tanya Singh (from Jul 03, 2017), Mahender Allam (from Sep 01, 2017 to Dec 13, 2017), Swarnalatha S (from Nov 30, 2017)

National and International involvement

Mazumder, Aprotim: Reviewer for scientific articles in Cell Cycle, Biology Open, Current Science; Member of the Subject Board of Biology of TIFR; Member of the Subject Board of Chemistry of TIFR; Member of the Academic Advisory Committee of TCIS; Chairperson of the Institutional Biosafety Committee of TIFR Hyderabad.

Mondal, Jagannath: Associate of Indian Academy of Sciences, Member of Biophysical Society, Member of the American Physical Society, Member of the American Chemical Society.

Ramadas, Jayashree: Member, International Commission on Physics Education, 2011-17, (ICPE, or IUPAP Commission 14)

Mandal, Kalyaneshwar: Member of the American Peptide Society, Reviewer at Nature Communications

Raman, K. V.: International advisory board member, SPINOS conference, 2018

Krishnamurthy, M: Editorial board member of High Power Laser Science and Engineering Cambridge university press Journal (2017) , Editorial board member of Scientific Reports (a Nature group Journal), Secretary of the Asian committee on ultra-intense laser (ACUIL), Technical program committee for the 2nd Asia Pacific conference held by Association of Asia Pacific Physical Societies, Division of Plasma Physics (2018), Member of the Swarnajathi Felloship selection committee for the Physics section (2017), Member of the Expert committee for faculty recruitment and promotions in IIT Palakkad, NISER Bhubaneswar.

Madhu, P. K.: Head of Research, finance, and administration at TCIS-TIFR Hyderabad, Fellow of the National Academy of Science, Member secretary of the TIFR H management board, Convener of the MagRes academic advisory body (MRAAB) TIFR- Hyderabad, Editorial board member of Journal of Magnetic Resonance, Editorial board member of Solid State Nuclear Magnetic Resonance, Editorial board member of Journal of Biomolecular NMR, International advisor of the European School on Solid-State NMR, Member of MAC, National Facility for High-Field NMR at TIFR, Scientific programme committee member of ISMAR at Quebec, Canada 2017, ISMAR (International Society for Magnetic Resonance) council member, Member of the National Magnetic Resonance Society of India, Member of the LTF in TIFR Mumbai committee, Member in various TIFR Hyderabad campus committees, such as

research committee, project implementation team, academic core committee, master plan committee, and detailed plan report committee.

Ramakrishnan, Raghunathan: Editorial board member of Scientific Reports.

Sengupta, Surajit: Fellow of the Indian Academy of Sciences, Fellow of the National Academy of Sciences.

Narayanan, T. N.: Member of the Materials Research Society (2018), Member of the American chemical Society (July 2015-July 2018), Fellow of the Royal Society of Chemistry, Associate at the Indian Academy of Sciences (July 2015 –December 2018), Guest Editor of a special issue of MRS Communications (2D Nanomaterials for Healthcare and Lab-on-a-Chip Devices), Fellow of the Royal Society of Chemistry (FRSC), Organizer of Materials Research Society Fall Symposium Tutorial on "Future Perspective of 3D Graphene & Beyond" (November 26, 2017, Boston, USA), Reviewed articles from the following international journals: Science Advances, ACS Catalysis ACS Nano, Carbon, Optical Materials, Journal of Energy Storage, European Physics Letters, Physical Chemistry Chemical Physics, Electrochimica Acta.

Chandrasekhar, V: Member of the Editorial Board at Dalton Transactions (Published by Royal Society of Chemistry, Cambridge, UK), Chairman of the Project Advisory Committee of Inorganic and Physical Chemistry (Science and Engineering Research Board).

Agarwal, Vipin: Member of the National Magnetic Resonance Society of India.

Rajalakshmi, G: MOU agreement with Indian and UK groups under the Newton Bhabha Fund Collaboration Agreement (along with Dr. Karthik Raman)

Awards and Distinctions:

Mandal, Kalyaneswar: 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 year, successfully renewed to its 2nd year term in the year 2017.

Jaiswal, Manish: Ramalingaswami Re-entry Fellowship for the year 2016-17 by Department of Biotechnology, India. Fellowship duration - 5 years.

Madhu, P. K.: Elected as ISMAR (International Society for Magnetic Resonance) Council Member.

Narayanan, T. N.: Materials Research Society Membership Award (with MRS-2017 Travel Grant) - 2018 January - December.

Das, Tamal: Max Planck Partner Group award, Intermediate Fellowship by Wellcome Trust / DBT India Alliance.

Visits

Jana, Anukul:

- Saarland University, Germany as a part of Research Group Linkage Programme, Alexander von Humboldt Foundation, Germany, May, July, October, 2017

Mazumder, Aprotim:

- Visited institutes within India (Presidency University, University of Hyderabad)

Madhu, P. K.:

- EUROMAR meeting, Warsaw, Poland, July 2-6, 2017
- University of Leipzig, Leipzig, Germany, September 3-8, 2017
- University of Leipzig, Leipzig, February 24- March 9, 2018
- University of Bayreuth, Bayreuth, Germany, March 5-6, 2018

Ghosh, Pushpita:

- Indian Association for the Cultivation of Science and S. N. Bose National Centre for Basic Sciences, Kolkata, March 7-8, 2018

Ramakrishnan, Raghunathan:

- HiPC conference on high-performance computing, Le Meridien, Jaipur, December, 2017.

Narayanan, T.N

- Materials Research Society, Fall symposium, Boston, USA, November-December, 2017.
- Rice University, USA, December, 2017.
- Industry visit: M/s SCOGEN, Mysore, India.
- Various colleges in India for talks - BITS Pilani Hyderabad, Govt. Arts & Science College, Calicut, Govt. Victoria College, Palakkad, Mar Thoma College for Women, Perumbavoor, and KKTM Govt. College, Kodungallur, and Cochin University of Science and Technology, Kerala.

Das, Tamal:

- Stuttgart, Germany to strengthen the collaboration between our group and that of Prof. Joachim P. Spatz, Max Planck Institute of Medical Research, as a part of the Max Planck Partner Group award, 29th May – 11th June, 2017.
- Bengaluru, India to attend Workshop on Physical and Systems Biology (WPSB) at International Centre for Theoretical Sciences (ICTS), 12th June – 13th June, 2017.

Agarwal, Vipin:

- JSPS Invitational Fellow, Riken NMR Centre, Japan, October-November 2017.
- NMR meets Biology III Meeting, Leipzig, September 2017.
- 11th Alpine conference on solid-state NMR, Chamonix, France, September 2017.

Rajalakshmi, G:

- Summer school on "Theory in NMR" at Windischleuba, Germany, 25 Feb -04 Mar 2018.
- Visit to Xe NMR Lab of Prof. Senker at University of Bayreuth, Germany, 5 -9 Mar 2018.

Invited Talks

Jana, Anukul:

1. "Coordination Chemistry of Germanium(0): Syntheses of Molecular Complexes Containing Formally Neutral Iron Germanide Motifs", Anorganisch-Chemisches Kolloquium in Goettingen, University of Goettingen, Germany, October, 2017.
2. "Reactivity Enhancement of a Diphosphene by Reversible N-Heterocyclic Carbene Coordination", Chemistry and Physics of Materials Unit, JNCASR Bangalore, November, 2017.
3. "Coordination Chemistry of Molecular Mono - and Dicoordinated Germanium(0)", Department of Chemical Sciences Annual Talks 2017, TIFR Mumbai, November, 2017.

4. "Heterodimer of N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC): Influence of Substituents", School of Chemistry, University of Hyderabad as a part of UH-TIFRH Seminar Series (Lecture 4), December, 2017.
5. "N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC) Heterodimers: Influence of N-Substituents", MTIC-XVII, Pune, December 2017.
6. "Reactivity Enhancement of a Diphosphene by Reversible NHC-Coordination: Influence of N-Substituents", Department of Inorganic Chemistry, IACS Kolkata, December, 2017.
7. "Recent Advances in Chemistry of Carbenes: Compounds Involving Low-valent Carbon", Department of Chemistry, Prabhat Kumar College, Contai, West Bengal, December, 2017.
8. "Mono- and Dicoordinate Germanium(0) as Four Electron Donor", Department of Chemistry, IISER Kolkata, January, 2018.
9. "Recent Advances in Main Group Chemistry: Compounds Involving Low-valent Low-coordinate Elements" Ramakrishna Mission Vidyamandira, Belur Math, Howrah, January, 2018.
10. "Recent Advances in Main Group Chemistry: Efforts to Mimics with Transition Metal Chemistry", R. K. M. Residential College, Narendrapur, Kolkata, January, 2018.
11. "Mono- and Dicoordinate Germanium(0) as a Four Electron Donor", Department of Chemistry, IIT Kanpur, March, 2018.
12. "Mono- and Dicoordinate Germanium(0) as a Four Electron Donor", Department of Chemistry, IIT Madras, March, 2018.

Mazumder, Aprotim:

1. Panelist, Presision 2017 (an undergraduate research conference), Kolkata, April, 2017.
2. "Measuring cell-cycle dependent DNA damage responses on a cell-by-cell basis from image analysis", Bioquest 2017, University of Hyderabad, October, 2017.
3. "Measuring cell-cycle related DNA damage responses on a cell-by-cell basis from microscopic image analysis", ICCB2018, Leonia Resort Hyderabad, January, 2018.

Mondal, Jagannath:

1. "Force spectroscopy of GB1 protein",Current Trends in Computational Natural Sciences, IIIT Hyderabad, March, 2017.
2. "Mechanistic pathways of recognition of a solvent-inaccessible cavity of protein by a ligand", American Physical Society March meeting, New Orleans, LA, USA, March, 2017.
3. "Mechanistic pathways of recognition of a solvent-inaccessible cavity of protein by a ligand", American Chemical Society Fall meeting, Washington DC, USA, August, 2017.
4. "Atomistic resolution mechanism of ligand recognition in L99A T4 Lysozyme", RARE, Agra, India, December, 2017.
5. "Self-organization inside E. Coli.", IIT Gandhinagar, India, February, 2018
6. "Atomistic resolution mechanism of ligand recognition in L99A T4 Lysozyme", BITS Hyderabad, India, February, 2018.

Ramadas, Jayashree:

1. "The textbook as motivator of teacher discourse", RVEC Conference for Elementary School Science Teachers, RV Educational Consortium, Bangalore, 2-3 June, 2017.
2. "Supporting science in local schools - An outreach initiative of TIFR Hyderabad", College for Integrated Studies, University of Hyderabad, 2 August, 2017.
3. "Curiosity and Questioning, The CogTalk", Centre for Neural and Cognitive Sciences, University of Hyderabad, 25 January, 2018.

Garai, Kanchan:

1. Visit to Washington University in St. Louis and gave a talk.

Mandal, Kalyaneshwar:

1. "A Mirror Image Protein Antagonist of VEGF-A Function", Dr. Reddy's Institute of Life Sciences (DRILS), Hyderabad, April, 2017.
2. "Systematic development of novel therapeutics against malaria", Wellcome Trust/DBT India Alliance annual Fellows' meeting, May, 2017.
3. Attended Meditech Conclave, Conference on Advanced Medical Technologies for better Health Care, Hyderabad, June, 2017.
4. Participated in the '24th Congress and General Assembly of the International Union of Crystallography', Hyderabad International Convention Centre, August, Hyderabad, 2017.
5. "Designing Nonnatural Proteins to Inhibit Natural Protein-protein Interactions", Department of Chemical Sciences Annual Talk, TIFR Mumbai, November, 2017.

Raman, K. V.:

"Emerging trends in condensed matter physics", IACS Kolkata, January, 2018

Mote, Kaustubh, R.:

"Multiple Sequential Acquisition Strategies to speed up experiments in solid state NMR", Grossbothen, Germany, September, 2017

Jaiswal, Manish:

1. "Bidirectional synergism between fly and human genetics in health and diseases", Departmental seminar at Dr. Reddy's Institute of Life Sciences, Hyderabad, May, 2017.
2. "Mito-dysfunction and retrograde signaling: lessons learned from forward genetic screen in flies", Mitochondria & Metabolism Network Meeting, IISER, Pune, November, 2017.
3. "Regulation of mitochondrial dynamics under metabolic stress", Indian Drosophila Research Conference, IISER, Bhopal, December, 2017.

Krishnamurthy, M:

1. "Building a compact neutral atom accelerator", IISER Pune, 2018.
2. "Acceleration of neutral atoms in intense laser fields", Special lecture on DPS day, IISER Kolkata, 2018.
3. "Bringing stars down to a lab", National Science Day, RGUKT, Basra, 2018.
4. "Extreme Light: a window to extreme matter", Science day lecture held by the Indian Physics Associate at Hyderabad Central University Hyderabad, 2018.
5. "Neutral atom generation in intense laser plasma", IISER Tirupati, 2017.
6. "Acceleration of neutral atoms in intense laser fields", Conference on High intensity Lasers, Israel, 2017.
7. "Acceleration of neutral atoms in laser produced plasmas", 1st Asia-Pacific Conference on Plasma Physics, China, 2017.

Vig, Monika:

1. "CRAC Channels: The molecular basis and immunological benefits of being selective", Dr. Reddy's Institute of Life Sciences, Hyderabad.
2. "High affinity interactions governing the optimal assembly and selectivity of CRAC channels", Annual Symposium, Department of Chemical Science, TIFR, Mumbai, India.

Ghosh, Pushpita:

1. "Spreading of non-motile bacteria on hard surface" in "Nonequilibrium Dynamics: Diffusion, Populations and Aging" at TIFR-TCIS Hyderabad, June, 2017.
2. "Spatiotemporal ordering in growing bacterial colony" at S.N. Bose National Centre for Basic Sciences, Kolkata, March, 2018.

Karmakar, Smarajit:

1. Plasticity, Rheology and Nonlinear response in Driven Amorphous Solids, Grenoble, France, June 2017.

Sengupta, Surajit:

1. "The equilibrium transitionunderlying irreversible deformation of solids", French-Indian meeting on plasticity and rheology in amorphous solids, in connection with glassy dynamics, Grenoble, France, June, 2017.
2. "The equilibrium transition underlying irreversible deformation of solids", Correlation and disorder in classical and quantum systems, ICTS Bangalore, May, 2017.
3. "Modelling of plastic response of solids", Fracmeet School, The Institute for Mathematical Sciences, Chennai, February, 2018.

Narayanan, T.N:

1. "Combining Theory & Experiment in 2D Electrocatalysis" (Plenary Talk), DAE-BRNS sponsored International Conference on Electrochemistry in Advanced Materials, Corrosion, and Radiopharmaceuticals, DAE Convention Centre, Anushaktinagar, BARC, Mumbai, India, February, 2018
2. "Hybrid Nanostructured Electrodes for Heterogeneous Catalysis", Conference on Advances in Catalysis for Energy and Environment (CACEE-2018), TIFR Mumbai, India, January, 2018.
3. "Fluorographene Sensing Platform", Materials Research Society (MRS) Fall Symposium, Boston, USA, November, 2017.
4. "Carbon Nanotube Junctions & Their Aftereffects", International Conference & XXXVIII Annual Meeting of Electron Microscopy Society of India (EMSI), July, 2017.

Das, Tamal:

1. "Mechanobiology of Collective Cell Migration", 5th Heidelberg Forum for Young Life Scientists, Heidelberg, June, 2017.
2. "Mechanobiology of Collective Cell Migration", Workshop on Physical and Systems Biology (WPSB) at International Centre for Theoretical Sciences (ICTS), Bengaluru, June, 2017.
3. "Mechanobiology of Collective Cell Migration", TCIS-UoH collaboration program at Dr. Reddy's Institute of Life Sciences, Hyderabad, July, 2017.
4. "Mechanobiology of Collective Cell Dynamics: Migration and Competition", Soft and Active Matter Workshop, School of Physics, University of Hyderabad, Hyderabad, February, 2018.

Chandrasekhar, V:

"NHC-stabilized Hydrosilaimines and –Phosphasilenes", Indo-German Meeting- Elementary Reactions in Functional Materials: From Biophysics to Technological Applications", University of Heidelberg, Germany, November, 2017.

Agarwal, Vipin:

1. "Characterization of protein structures and transient species of α-Synuclein with MAS solid-state NMR techniques", Indo-German meeting on structural Biology (NMR meets Biology III), University of Leipzig, September, 2017.
2. "New developments of in fast MAS Solid-state NMR methodology of protein samples", Department of chemistry, Kyoto University, Japan, November, 2017.

3. "Solid-state NMR methods to characterize transients' species of protein and development of optimisation independent heteronuclear decoupling sequences for MAS solid-state NMR", Jeol Riken NMR Centre, Yokohama, Japan, November, 2017.
4. "Novel solid-state NMR methods for protein structure determination of crystalline and non-crystalline solids at nanomolar concentrations", Indian Biophysical Society Meeting, Indian Institute of Education and Research, Pune, India, March, 2018.

Rajalakshmi, G:
1. "Low field NMR using optical magnetometry", Emerging Trends in NMR One-Day Symposium, TIFR Hyderabad, 25 August 2017.
2. "Low field NMR using optical magnetometry", TIFR Hyderabad High Field NMR Facility: Inaugural Symposium, TIFR Hyderabad, 13-14 February 2018.

Conferences organized by the Department

- "TIFR-UoH Life Sciences seminar series" with colleagues from the University of Hyderabad.
- "EMBO Global Exchange Lecture Series" talks by Professors William Earnshaw (University of Edinburgh), Anne Spang (University of Basel), Sandra Schmid (UT Southwestern) and Thomas Lecuit (Institute of Developmental Biology) who had been invited by the ICCB2018 organizers.
- "NMR Meets Materials", TIFR Hyderabad, May 5-6, 2017 (An exploratory meeting that explored the NMR materials science connections and collaborative research possibilities in India.)
- "Emerging Trends in NMR: One-Day International Symposium", TIFR Hyderabad, August 25, 2017. An international symposium that focussed on the recent methods, materials and biomolecular applications of NMR, and hyperpolarisation methods.
- "NMR Meets Biology", Grossbothen, Leipzig, Germany, September 3-8, 2017. An international meeting focussing on the methods mainly in solid-state NMR in the investigation of biomolecular systems.
- TIFR Hyderabad High Field NMR Facility: Inaugural International Symposium, TIFR Hyderabad, February 13-14, 2018. An international meeting to mark the inauguration of the National Facility for High Field NMR in TIFR Hyderabad along with talks on recent developments in NMR together with a session on Prof. Dharmatti to mark the 60th year of NMR in India.
- Teacher workshop 'Atoms to Amoeba', TCIS, Hyderabad, 12 October, 2017.

Non-DAE Research Projects

Dani, Adish:

- Investigators: Adish Dani (Co-Investigator), Mark Rutherford (PI), Title: Excitation and excitotoxicity in cochlear afferents: synaptic structure and function, Funding Agency: NIH, USA (National Institute of Deafness and Communication Disorders -NIDCD), Duration: Mar-01-2016 to Feb-28-2021.
- Investigators: Adish Dani (Co-Investigator), Monika Vig (PI), Funding Agency: NIH, USA (National Institute of Allergy, Immunology, Infectious Diseases -NIAID).

Jana, Anukul:

- Investigator: Anukul Jana, Title: Rational design for the syntheses of multiple bonded compounds involving heavier Group 14 elements and their reactivity, File No: EMR/2014/001237, Funding Agency: DST-SERB, India, Duration: 2015-2018

- Investigator: Anukul Jana, Title: Syntheses and Reactivities of Compounds Involving Formal Zero Oxidation State of Mono- and Di-Nuclear Group 14 Elements, File No: NS/5747, Funding Agency: CSIR, India, Duration: 2016-2019
- Investigator: Anukul Jana, Title: Molecular Manifestations of Transition Metal Tetrelides MxEy (M = Cr, Mn, and Fe; E = Si and Ge) for Thin Film Deposition, Funding Agency: AvH Foundation, Germany, Duration: 2017-2019

Mazumder, Aprotim:
Investigator: Aprotim Mazumder, Title: "Developing novel methods for single cell detection of transcripts and proteins in primary cells and tissue to explain variable sensitivities of body cells to DNA-damaging chemotherapeutic agents", Funding agency: SERB Early Career Research Grant, Duration: 3 years

Mondal, Jagannath:
Investigators: Jagannath Mondal, Xiao Zhu, Title: "Mechanistic Investigation anti-microbial peptides in action using large-scale computer simulations", Funding Agency: Extreme Science and Engineering Discovery Environment (XSEDE), USA for Computational allocation (allocation provided in San Diego Supercomputer), Duration: September 2016 - August 2017

Garai, Kanchan:
Investigator: Kanchan Garai, Funding agency: DST ECR Grant 2015

Mandal, Kalyaneshwar:
Investigator: Kalyaneswar Mandal, Title: "Systematic development of novel therapeutics against malaria", Funding Agency: Wellcome Trust/ DBT India Alliance, Duration: 60 months (project activated in June 2016)

Raman, K. V.:
- Investigator: Karthik. V. Raman, Funding agency: Ramanujan Fellowship, Duration: 2013-2018
- Investigator: Karthik. V. Raman, Funding agency: SERB Early Career research grant

Mote, Kaustubh R.:
Investigator: Kaustubh R. Mote, Title: Inspire Faculty Award (DST): Continuation of the Project entitled "Structural and mechanistic characterization of the Mitochondrial Pyruvate Carrier Complex", Duration: 2015-2020

Krishnamurthy, M.:
Investigator: M. Krishnamurthy, Title: "Developing control systems for Laser based accelerators", a TIFR-RAL collaboration project funded by RAL UK. Duration: Three years.

Vig, Monika:
Investigator: Monika Vig, Title: "CRAC channel components and molecular basis of store-operated calcium entry", 1 R01 AI108636-01 (Vig), Funding Agency: NIH/NIAID, Duration: 2018 – 2019.

Madhu, P.K.:
- Investigator: P. K. Madhu, Title: "Transiently formed non-native conformers of transthyretin: Structure, function and their roles in formation of amyloid fibril", Funding agency: DBT.

- Investigator: P. K. Madhu, Title: "Novel nanocatalysts synthesis guided by DNP NMR", Funding agency: IFCPAR/CEFIPRA.

Narayanan, T. N.

- Investigator: T. N. Narayanan, Title: "Development of Graphene & MoS2 based van der Waals Solids for Smart Sensors", Funding Agency: DST-Extra Mural Research Grant (Individual Centric) DST-SERB, Duration: 3 years (2017-2020).
- Investigator: T. N. Narayanan, Title: "Development of Graphene based Functional Coatings for Possible STP and ETP Technologies", Funding Agency: Private Sponsored Research - M/s Southern Cogen Systems Pvt. Ltd. (SCOGEN), Mysore-571302, Karnataka, India, Duration: One year (2018-2019).

Das, Tamal:

- Investigator: Tamal Das, Funding Agency: Max Planck Partner Group award, Max Planck Society Germany, Duration: March, 2017 –February, 2020.
- Investigator: Tamal Das, Title: Mechanobiology of cell competition: Elucidating the role of mechanical forces in cell-cell sensing and collective fitness measurement towards tumor suppression in epithelial tissues, Funding Agency: Wellcome Trust / DBT India Alliance, Duration: January, 2018 –December, 2022.

Chandrasekhar, V.:

Investigator: V. Chandrasekhar, Funding Agency: J. C. Bose Research Fellowship, SERB, Duration: 2017-22

Agarwal, Vipin:

Investigators: Vipin Agarwal, Yusuke Nishiyama, Title: Selective recoupling of Protons in fully protonated molecules, Funding Agency: Japan Society for the Promotion of Science, fellowship titled "FY2017 JSPS Invitational Fellowship for Research in Japan", Duration: 1 month.

Lectures given elsewhere

Dani, Adish:

University of Hyderabad, School of Life Sciences, Seminar, March 2018

Mote, Kaustubh R.:

Taught basics of NMR lectures at a workshop titled 'Insights into Biomolecular Interactions: A Biophysical Perspective', Centre for Data Analytics and Research Guru Nanak Dev University, Amritsar, Punjab February, 2018

Madhu, P. K.:

- "Observing Ab transition from monomers to oligomers to fibrils through the solid-state NMR looking glass", CCMB, Hyderabad, November, 2017.
- Winter school on hyperpolarisation, Two lectures on NV centres, Schloss Windischleuba, Leipzig, Germany, February, 2017.
- "Robust magic-angle solid-state NMR methods for structure elucidation", University of Bayreuth, Germany, March, 2018.

Karmaker, Smarajit:

Workshop Lecturer, Soft and Active Matter Workshop, University of Hyderabad, Hyderabad, February, 2018.

Narayanan, T. N.:

- Combining theory and experiment in electrochemistry, BITS Pilani Hyderabad Campus, 21st February 2018.
- Combining Theory and Experiment in 2D Electrochemistry, National Seminar on "Theoretical and Experimental Approaches for Exploring Advanced Materials" (TEAM2017), 13th December 2017, Govt. Arts & Science College, Calicut, Kerala, India.
- Atomic Layers: Advances in the Science & Engineering of Ultra-Thin Films, National Seminar at KKTM Govt. College, Kodungallur, Kerala, 14th November 2017.
- Novel Nanostructured Electrodes for Energy Technologies, National Seminar on Frontiers & Developments in Materials Science, Govt. Victoria College, Palakkad, Kerala 13th November 2017.
- Novel Nanostructured Electrodes for Energy Technologies, University of Hyderabad - TIFR-H Meeting held on 04th October 2017.
- Mesoscale Interfaces – A New Era of Materials Engineering, National seminar on Frontiers of Nanotechnlogy, Mar Thoma College for Women, Perumbavoor, Kerala, 8-9 August, 2017.
- Nanoscale Interfaces – A New Era of Materials Engineering, one day seminar on "Magnetic Research Advancements – 2017 (MRA-2K17)", Department of Physics, Cochin University of Science and Technology, Kochi, India.

Lectures at TIFR

Mohinish Shukla: University of Massachusetts, Boston, "Language learning as a constrained computation" January 2018.

Dr. Ravi Gutti, Dr. Bramanandam Manavathi, Dr. Krishnaveni Mishra, Dr. Sharmistha Banerjee, "TIFR-UoH Life Sciences seminar series", University of Hyderabad

Professors William Earnshaw (University of Edinburgh), *Anne Spang* (University of Basel), *Sandra Schmid (*UT Southwestern) *and Thomas Lecuit* (Institute of Developmental Biology), EMBO Global Exchange Lecture Series talks, February 2018

Dr. R. S. Praveen Kumar, Secretary, Telangana Social Welfare Residential Educational Institutions Society: Scientists and Neglected Generations, Cultural Colloquium, TIFR Centre for Interdisciplinary Sciences, Hyderabad, March, 2018

Dr. Subhojit Sen, Centre for Excellence in Basic Sciences, Mumbai, Epigenetics, September, 2017.

Michael Sattler, Helmholtz Zentrum, Munich, Germany, Dynamics in biomolecular recognition studied by NMR and integrative structural biology, October, 2017.

Kevin Gardner, The City College of New York, USA, Controlling biochemical function via environmentally-modulated protein/protein interactions: Using biophysics to turn Nature's switches into our tools, October, 2017.

Harald Schwalbe, University of Frankfurt, Germany, RNA-based regulation-Insights from NMR, February, 2018.

Dieter Suter, University of Dortmund, Germany, Velocity fields of non-Newtonian liquids from magnetic resonance microscopy, February, 2018.

Ph.D Theses:

- Ravi Shankar Palani (joint student of P. K. Madhu and N. C. Nielsen, Univ. of Aarhus, Denmark), 2017.
- Bappaditya Chandra (joint student of P. K. Madhu and Sudipta Maiti, TIFR, Mumbai), 2017.

Publications

1. D. Dhara, T. Vijayakanth, M. K. Barman, K. P. Kumar Naik, N. Chrysochos, C. B. Yildiz, R. Boomishankar, C. Schulzke, V. Chandrasekhar, and A. Jana; "NHC-Stabilized 1-Hydrosilaimine: Synthesis, Structure and Reactivity", Chem. Comm. 2017, 53, 8592−8595.
2. D. Mandal, R. Dolai, N. Chrysochos, P. Kalita, R. Kumar, D. Dhara, A. Maiti, R. S. Narayanan, G. Rajaraman, C. Schulzke, V. Chandrasekhar, and A. Jana, "Stepwise Reversible Oxidation of N-Peralkyl-Substituted NHCCAAC Derived Triazaalkenes: Isolation of Radical Cations and Dications", Org. Lett. 2017, 19, 5605–5608.
3. D. Mandal, B. Santra, P. Kalita, N. Chrysochos, A. Malakar, R. S. Narayanan, S. Biswas, C. Schulzke, V. Chandrasekhar, and A. Jana, "2,6-(Diphenylmethyl)-Aryl-Substituted Neutral and Anionic Phosphates: Approaches to H-Bonded Dimeric Molecular Structures", ChemistrySelect, 2017, 2, 8898–8910.
4. D. Mandal, D. Dhara, A. Maiti, L. Klemmer, V. Huch, M. Zimmer, H. S. Rzepa, D. Scheschkewitz, and A. Jana, "Mono- and Dicoordinate Germanium(0) as Four Electron Donor", Chem. Eur. J. 2018, 24, 2873−2878.
5. D. Dhara, V. Huch, D. Scheschkewitz, and A. Jana, "Synthesis of a α Chlorosilyl Functionalized Donor-Stabilized Chlorogermylene", Inorganics, 2018, 6, 6.
6. 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", Chemical Science, 2018, DOI: 10.1039/C8SC00348C.
7. C.M Margulies, I. A. Chaim, A. Mazumder, J. Criscione, and L. D. Samson; "Alkylation induced cerebellar degeneration dependent on Aag and Parp1 does not occur via previously established cell death mechanisms", PLoS One, 2017, 12, e0184619.
8. P. Tiwary, J. Mondal, and B. J. Berne "How and when does an anticancer drug leave its binding site?" Science Advances, 2017, 3, e1700014.
9. R. Berkovich, J. Mondal, I. Paster and B. J. Berne "Simulated Force Quench Dynamics Shows GB1 Protein Is Not a Two State Folder" J. Phys. Chem. B, 2017, 121, 5162.
10. S. Ray, A. Maitra, A. Biswas, S. Panjikar, J. Mondal and R. Anand "Functional Insights into the Mode of DNA and Ligand Binding of the TetR Family Regulator TylP from Streptomyces fradiae", J. Biol. Chem. 2017, 292, 15301.
11. A. Ray, N. Ahalawat and J. Mondal, "Atomistic Insights into structural differences between E3 and E4 isoforms of Apolipoprotein E", Biophys. J. 2017, 113, 2682-2694.
12. S. Bawari, N. M Kaley, S. Pal, T. V. Vineesh, S. Ghosh, J. Mondal, T. N. Narayanan, "On the Hydrogen Evolution Reaction of Activity of Graphene-hBN van der Waals heterostructures", Phys. Chem. Chem. Soc. (in press) 2018, DOI: 10.1039/C8CP01020J.
13. Y. Lyu, N. Xiang, J. Mondal, X. Zhu, G. Narasimhan, "Characterization of interaction between curcurmin and different types of lipid bilayers using Molecular Dynamics simulation", J.Phys.Chem. B, 2018, 122, 2341-2354.
14. N. Deshmukh, S. Bhide, V. Sonawane, S. Chunawala and J. Ramadas, "Experiences and learning from 'Participatory Action Research' with a local school, In S. Ladage & S. Narvekar (Eds.)", Proceedings of epiSTEME 7 , An International Conference to Review Research on Science, Technology and Mathematics Education, 204-13, 2018. India: Cinnamon Teal
15. 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.

16. F. Hoffmann, J. Adler, B. Chandra, K. R. Mote, G. Bekioglu-Neff, D. Sebastiani and D. Huster, "Perturbation of the F19-L34 Contact in Amyloid β (1-40) Fibrils Induces Only Local Structural Changes but Abolishes Cytotoxicity", J. Phys. Chem. Lett. 2017, 8(19):4740–4745.
17. B. Chandra, D. Bhowmik, B. K. Maity, K. R. Mote, D. Dhara, R. Venkatramani, S. Maiti and P. K. Madhu, "Major reaction coordinates linking transient amyloid-β oligomers to fibrils measured at atomic level", Biophys. J. 2017, 113(4):805–816
18. M. G. Jain, G. Rajalakshmi, A. Equbal, K. R. Mote, V. Agarwal and P. K. Madhu, "Sine-squared shifted pulses for recoupling interactions in solid-state", NMR. J. Chem. Phys. 2017, 146(24):244, 201.
19. 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", App. Phys. Lett. 2018.
20. M. Dalui, M. Kundu, S. Tata, A. D. Lad, J. Jha, K. Ray, and M. Krishnamurthy, "Novel target design for enhanced laser driven proton acceleration", AIP Advances, 2017, 7, 095018.
21. S. Tata, A. Mondal, S. Sarkar, A. D. Lad, and M. Krishnamurthy, "Gated Thomson parabola spectrometer for improving energetic particle measurements in intense laser plasmas", Rev. Sci. Instrum. 2017.
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Popular Science Articles/Lectures:

Mazumder, Aprotim: Was an invited panelist at Presision 2017, a first undergraduate research meeting of Presidency University, Kolkata, and was mentioned in a newspaper article (The Telegraph) in April 2017 about the event: https://www.telegraphindia.com/1170410/jsp/calcutta/story_145546.jsp

Ramadas, Jayashree: Feluda Science Mission, Aparna Sarovar, Hyderabad, September 2017; Learning with 'Small Science', Vivekananda School, Hyderabad, 12 February 2018.

Jaiswal Manish:

Popular lecture on science activities at TCIS to the group of students and teachers visited at TCIS, organised by Dr. K.V.Rao Scientific Society and TCIS outreach committee, May 2017; Introductory lecture on science activities, workshop on "Atoms to Amoeba", organized by TCIS outreach committee at TCIS, Oct 2017; Sawaal Jawaab: Tales of the fly and the human: understanding biology and diseases, Lamakaan, Hyderabad, March 2018.

Agarwal, Vipin:

Lecture on "NMR Spectroscopy: Introduction and Perspectives", at IEEE local chapter, Shri Ramdeobaba College of Engineering and Management, Nagpur, March, 2018.

Rajalakshmi, G.:

"Seeing and hearing Black Holes: opening a new era in Astronomy", 1 Nov 2017, ETHER Talks at Hyderbad Central University.

Conferences in TIFR Hyderabad:

- TIFR Hyderabad High Field NMR Facility: Inaugural Symposium, February 13 – 14, 2018.
- EMBO Global Exchange Lecture Series, February 01, 2018.
- TIFRH-UH Joint Discussion Meet in Experimental Physics, October 04, 2017.
- Emerging Trends in NMR One-Day Symposium, August 25, 2017.

- Summer Research Symposium, July 14, 2017
- Nonequilibrium Dynamics: Diffusion, Populations and Aging, June 30 – July 1, 2017.
- NMR Meets Materials, May 5-6, 2017.

Science Popularisation and Public Outreach

- Sawaal-Jawaab: "Tales of a fly and a human: understanding of biology and diseases", Dr. Manish Jaiswal, TIFR, Hyderabad, March, 17, 2018.
- District Institute of Education and Training (DIET), New Tihari visits TIFR-H (~10 members), February, 21, 2018
- Sawaal-Jawaab: "The Big and Small of the Universe", Prof. Mayank Vahia, TIFR, Mumbai, February, 3, 2018.
- Interaction with TSWREIS school students, Prof. Mayank Vahia, TIFR, Mumbai, February, 2, 2018.
- Broadcast of Interaction with TSWREIS school students, Prof. Mayank Vahia, TIFR, Mumbai, February, 3, 2018 over T-SAT Nipuna, in order to reach out to remote TSWREIS schools in Telangana.
- Madras Christian College visits TIFR-H (43 students + 3 faculty members), January 5. 2018.
- G. Pulla Reddy Degree & P.G college visits TIFR-H (50 Students + 5 Faculty members), December, 18, 2017.
- Students and Faculty members from the Department of Physics, Mar Thoma College visits TIFR-H, October 26, 2017.
- Workshop on "Atoms to Amoeba" for secondary and higher secondary science teachers of TSWREIS, October 12, 2017.
- Feluda Science Mission, vacation activity designed for an urban gated community at Aparna Sarovar, September 15, 2017 and September 22, 2017.
- B.Tech. ECE, IV Semester Students (5 Students) CBIT, Hyderabad visit TIFR-H, September 16, 2017.
- K.V.R. Society visits TIFR-H, May 27, 2018.