Annual Report 2015 -16
TIFR Centre for Interdisciplinary Sciences

Agarwal Vipin, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

In the current year, the group worked primarily in the field of developing solid-state nuclear magnetic resonance theory and methods. The following are the key points of the research work:

- A generalized theoretical framework to analyze the performance of any heteronuclear decoupling condition under MAS.
- Interference of decoupling with R^3 conditions can be minimized by appropriate choice of rf fields in the fast MAS regime.
- Experimental demonstration of selective proton-proton distance restraints in fully protonated solids.
- Dipolar coupling based polarization methods were shown to be superior compared to scalar coupling based methods at 90-100 kHz MAS frequency.

A theoretical description of heteronuclear decoupling sequences: We have developed a generalized theoretical framework, that allows rapid analysis of residual couplings of arbitrary decoupling sequences in solid-state NMR under magic-angle spinning conditions. The generalization relies on the tri-modal Floquet theory, where three characteristic frequencies are used to describe the pulse sequence. This approach can be used to describe arbitrary periodic decoupling sequences that differ only in magnitude of the Fourier coefficients of the interaction-frame transformation. We have exemplified the usefulness of this framework by analyzing the performance of commonly used high-power and low-power decoupling sequences such as amplitude-modulated XiX and TPPM. The theory also rationalizes why some sequences are better offset compensated than others. (Vipin Agarwal with Kong O. Tan, Beat Meier and Matthias Ernst, ETH, Zurich)

Where to decouple in the fast MAS regime? The performance of heteronuclear spin decoupling sequences severely degrades when the proton radiofrequency (RF) nutation frequencies are close to or at multiples of magic-angle spinning (MAS) frequency, referred to as rotary-resonance recoupling conditions in literature. Recently, PISSARRO and rCW^{AiA} decoupling sequences have been shown to be less affected by the problem of MAS and RF interference, specifically at *n=2* condition, in the fast MAS regime. We systematically evaluated the loss in intensity of several heteronuclear decoupling sequences at *n=1,2* rotary resonance conditions compared to high-power decoupling in the fast-MAS regime. We have experimentally demonstrated that in the fast-MAS regime (above 40 kHz) the entire discussion about RF and MAS interference can be avoided by using appropriate low-power decoupling sequences which give comparable performance to decoupling sequences with 200kHz of ^{1}H irradiation. (Vipin Agarwal, Kshama Sharma, P.K. Madhu, TCIS, TIFR, Hyderabad.)

^{1}H-^{1}H distance restraints in immobile peptide and proteins at fast MAS: The structure determination of perdeuterated proteins by solid-state NMR has become routine using a large set of ^{1}H-^{1}H distance restraints at fast magic angle spinning. However, not all proteins can be deuterated so the approach has limited applications. The progress in magic-angle spinning (MAS) technology now provides a possibility to record meaningfully resolved proton spectrum of fully protonated proteins. Fast MAS (~ 100 kHz) combined with high static fields has enabled proton-detected correlation spectroscopy in fully protonated samples with sufficient resolution, primarily for the purpose of assignment. Here, we propose a new experimental method to obtain long-range **^{1}H-^{1}H** contacts, in fully protonated proteins, at fast MAS using selective spin diffusion. The novel method demonstrates that ^{1}H-^{1}H contacts on the order of 6-7 Å can be obtained in fully protonated proteins. A systematic comparison of the experimental ^{1}H-^{1}H contacts was performed with the expected ^{1}H-^{1}H contacts at a distance of 7 Å based on the X-ray structure.

A quantitative comparison of J-coupling and dipolar- coupling-based polarization transfer methods: Spin identification in NMR is the first step to perform any further analysis. In case of biomolecules, spin identification is primarily achieved through assignment experiments. In solid-state, NMR assignments can be achieved by experiments that rely on dipolar or scaling based polarization transfer method. We compared

experiments based on both polarization transfer method and showed that dipolar coupling based polarization transfer methods outperform scalar coupling transfer methods under most circumstances. Scalar coupling methods primarily work better where proton density is low or regions where biomolecules are highly mobile. (Vipin Agarwal , Beat Meier, Matthias Ernst, ETH, Zurich, Ago Samoson , University of Technology , Tallin, Estona and Anja Bockmann , CNRS/Universite´ de Lyon, France)

Barma Mustansir, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Fluctuation-dominated Order

In a class of nonequilibrium systems, fluctuations are anomalously strong but coexist with long-range order, leading to fluctuation-dominated phase ordering (FDPO). The signature of FDPO, a singularity in the scaled two-point function, was earlier observed in a variety of systems, ranging from models of active biological systems and granular media to experiments on vibrated rods. It has now been shown that a single order parameter does not suffice to characterize the order; a larger, infinite, set is required. This set is built from long-wavelength Fourier components of the density profile, and captures an essential aspect of the state, namely the continuous breakup and re-emergence of particle-rich regions. For a system of passive particles sliding on a fluctuating surface and for a related coarse-grained depth model, simulations revealed that each mode is populated for a finite fraction of time, in strong contrast to customary phase separation. The corresponding probability distributions remain broad in the thermodynamic limit and are described by simple scaling laws. Further, the temporal behavior of the principal mode shows an interesting property in some cases: the flatness, which is related to dynamical structure functions, was found to exhibit a divergence at a small argument, indicating that the behavior in time is intermittent. [M. Barma with R. Kapri (IISER, Mohali) and M. Bandyopadhyay (IIT Bhubaneswar)]

Chary KVR, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

An unusual calcium binding protein from *E. Histolytica* that binds and hydrolyzes guanosine triphosphate has been structurally characterized. In an in-cell NMR study, differential accumulation and mobilization of starch or/and lipids in *Chlamydomonas reinhardtii* has been studied. In continuing the structural characterization of an UV inducible protein (UVI31+) from *C. reinhardtii,* the study uncovered first structural description of a plant chloroplast endonuclease that is regulated by UV-stress response in *C.reinhardtii* cells.

Structure, dynamics and interaction of Ca^{2+}-binding proteins

The protozoan parasite *E. histolytica* encodes twenty-seven Ca^{2+}-binding proteins (CaBPs) suggesting that the organism has an intricate and extensive Ca^{2+}-signaling system. The structural and functional characterization of some of these CaBPs studied so far reveals their predominant role in phagocytosis and endocytosis. However, not all amoebic CaBPs are involved in phagocytosis and endocytosis.

An unusual calcium binding protein from *E. Histolytica* that binds and hydrolyzes adenosine and guanosine triphosphates: A calcium binding protein (abbreviated as EhCaBP6) is mainly localized in the nucleus and present at the microtubule end and at the intercellular bridge with the microtubules during cytokinesis. Hence, it is supposed to be involved in cell division. In other organisms, calmodulin (CaM) plays a role of a major signal-transducing factor, through which Ca^{2+} concentrations are regulated during the cell cycles. In an attempt to understand the structural and functional similarity of EhCaBP6 with CaM, we have determined the 3D solution structure of EhCaBP6 using NMR. The protein EhCaBP6 has one unusual (EF-I), one canonical (EF-III) and two non-canonical (cryptic) (EF-II and EF-IV), EF-hands. The cryptic EF-II and EF-IV pair with Ca^{2+}-binding EF-I and EF-III, respectively, to form a two-domain structure similar to CaM. The structural similarity between EhCaBP6 and CaM, despite their low sequence similarity, suggests towards their similar functions during the cell cycle. Intriguingly, the EhCaBP6 binds and hydrolyzes adenosine triphosphate. This is the first known instance of a CaBP that hydrolyzes guanosine triphosphate. (Deepshikha Verma, and A. Bhattacharya (JNU, New Delhi)

Biomolecular Interaction

Structure and Dynamics of a putative UV inducible protein (UVI31+) from *C. reinhardtii* that exhibits RNA and DNA endonuclease activity: C. reinhardtii is a single celled alga, which undergoes apoptosis in response to UV-irradiation. UVI31+ in C. reinhardtii

exhibits DNA and RNA endonuclease activity, induced upon UV-stress. UVI31+ that normally localizes to cell wall and pyrenoid regions gets redistributed into punctate foci within the whole chloroplast, away from the pyrenoid, upon UV-stress. The structure, dynamics and the putative function of UVI31+ have been studied. The 3D structure of UVI31+ has $\alpha_1\beta_1\beta_2\alpha_2\alpha_3\beta_3$ fold very similar to BolA family of proteins, which in turn is similar to the well-described K-Homology Class-II (KH) domain that contains RNA and DNA binding motif. KH domains bind RNA or ssDNA, and are found in proteins associated with transcriptional and translational regulation, along with other cellular processes. Further, UVI31+ is found to recognize DNA primarily by its sheet domain with a dissociation constant of 52 nM. Point mutation at S114 of UVI31+ to Ala residue (S114A) reduced the endonuclease activity 10 fold. (Himanshu Singh, Sunita Patel, B.J. Rao (DBS))

Towards Tailoring Plant Protease Inhibitors for Control of the Crop Pest *Helicoverpa armigera*
Developing a peptide based eco-friendly insecticidal agents to control insect pests that adversely affect the agricultural production by destroying the crops or infesting the livestock is a major challenge. The most common Lepidoptera species, that cause damage to agriculture sector is *Helicoverpa.* Recently, it has been reported that peptide based protease inhibitors (PIs) from *Capsicum annuum* potently inhibit *H. armigera* gut proteases and also show a significant effect on its larval growth. However, very little information is currently available about the three-dimensional (3D) structure of these PIs or information about the residues that mediate their interaction with insect gut proteases. Recently, three recombinant PIs (IRD7, IRD9, IRD12) have been found to be very potent inhibitors with specific reference to their (i) stability in proteolytic environment (ii) proteinase inhibition specificities and (iii) inhibitory activity against insect proteinases. Thus, we set out to overexpress these three recombinant PIs, compare their activity *in-vitro* and *in-vivo*, and determine their 3D structure with a view to selecting the best candidate for future development as bioinsecticide proteases. As a prelude to the determination of 3D structures, we have carried out complete sequence specific ^{1}H, ^{13}C and ^{15}N resonance assignments for IRD7 and IRD12 and studied their dynamics using ^{15}N-relaxation data. The chemical shift index and the relaxation data show that ITD7 and IRD12 are well folded and highly stabilized with four disulphide bridges. (This project is being undertaken under DST-DIISRTE joint research project (*Australia-India Strategic Research Fund (AISRF*)). (Janeka Gartia, Glenn King, The Queen'sland University, Brisbane, Australia and Dr. Ashok Giri, NCL Pune)

Differential accumulation and mobilization of starch and lipid in *Chlamydomonas reinhardtii*
Chlamydomonas reinhardtii has recently emerged as a viable alternative source of fossil fuel. However, the metabolic flow of carbon in *C. reinhardtii* for making the carbon reserve is not yet understood. In addressing this issue, we have grown the wild-type (cw15) and the starch deficient (sta6) strains of *C. reinhardtii* with a singly or doubly ^{13}C-labelled acetate as the sole source of carbon to monitor its assimilation by ^{13}C-NMR under nitrogen starvation and study the dynamics of starch and lipid reserves formed as dominant sinks of carbon. During such growth condition, the starch was found to accumulate and mobilize faster than TAG. This study describes different growth conditions for acetate carbon flow into formation of either starch or/and TAG and their re-mobilization during nitrogen replenishment condition, thus establishing a system for probing the cellular nitrogen sensing, uptake mediated changes in carbon flux. *(Himanshu Singh, Manish Shukla, B.J. Rao (DBS))*

Garai Kanchan, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Aggregation of proteins are involved in several neurodegenerative diseases such as Alzheimer's, Parkinson's diseases and type 2 diabetes. In the current year we have worked primarily on biophysical characterization of protein aggregation in presence and absence of indigenous proteins apoliroprotein E and chaperone protein Hsp70. We have observed that both these proteins strongly affect aggregation of amyloid proteins such as amyloid beta, alpha-synuclein and amylin. Additionally, we are exploring the possibility of application of our knowledge of protein self-assembly to prepare smart bionanomaterials such as peptide hydrogels. Important highlights of our work in the last year are listed below.

Development of a highly sensitive Fluorescence Correlation Spectrometer (FCS). Last year, we built a fluorescence correlation spectroscopy (FCS) set up in house for characterization of protein dynamics and

protein-protein interactions. However the sensitivity of the instrument was less than satisfactory. We identified several problems with different optical components mainly with the dichroic mirrors and one of the lenses. This year, we rectified those problems to build one of the most sensitive FCS instrument in the world. The counts per molecules (CPM) obtained is about 400 kHz which is one of highest, reported in the literature.

Determination of solubility of amyloid peptides. We have established a new methodology for measurement of solubility of amyloid beta peptide using fluorescence of tetramethylrhodamine (TMR). We have found that amyloid fibrils are extremely insoluble in native buffer and their solubility is controlled by the folding-unfolding behaviour of the peptide monomers.

Characterization of interactions of apoE and Hsp70 with amyloid proteins. We have used FCS, ensemble fluorescence and atomic force microscopy (AFM) to establish that the proteins such as apoE and Hsp70 strongly influence amyloid aggregation. We are now collaborating with Prof. P K Madhu to understand the molecular basis of these interactions.

***Understanding the structure-function differences between the apoE isoforms*.** We have used tryptophan fluorescence and secondary structure of the apoE proteins to find presence of intermediates in folding-unfolding pathway. We hypothesize that these intermediates may have strong functional consequences. We are currently collaborating with Dr. P Vallurupalli to characterize the structural properties of the intermediates. We are collaborating with Dr. J Mondal to identify the structural differences between apoE3 and apoE4.

Preparation of switchable peptide hydrogels. We have synthesized a new 18 residue peptide named MAX2 which forms hydrogel in native buffer and at physiological temperature 37 degree Celsius. The hydrogel formation can be reversed by altering the temperature and pH of the media. We think that this hydrogel can have useful applications in bionanotechnology.

Developing single molecule techniques for characterization of oligomers of amyloid proteins. We are working to setup a microfluidic based single molecule detection setup for quantitative characterization of the amyloid oligomers. Additionally, we are working to build a super resolution optical microscopy setup. Currently its sensitivity and the resolution are not good. We are working to improve it. This will be used for characterization of amyloid aggregates and their interactions with proteins such apolipoprotein E and the chaperones.

Govindarajan Rama, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Particulate flows

Our studies on inertial particles in turbulent flows had revealed that caustics, i.e., regions of the flow where particle dynamics does not constitute a field, are an important contributor to clustering. We took this finding further to examine water droplets in a vortical flow, and showed that caustics droplets are far more likely to collide with other droplets repeatedly, coalesce, and grow much bigger than other droplets. This could mean that caustics droplets in clouds are far more likely to become rain drops.

Flow of foam:

We have shown that attractive interactions in the flow of foam change flow characteristics in a fundamental way. An unjamming driving force depends linearly on the attractive potential, and a stick-slip and a steady flow regime occur at higher forcing.

Rotating flows

In a collaboration with Prof. Benoit Pier under an Indo-French grant, we have shown that flow past a rotating cylinder can be described a similarity flow which includes a wall-jet and a boundary layer. This has consequences for the stability of such a flow, which we are studying now. We have found several features in the transition to turbulence in a rotating channel. In particular, a non-monotonic response to rotation is found. Flow is far more likely to go into turbulence at moderate rotation rates than at low rotation rates, with coherent structures distributed very asymmetrically in the channel. At higher rotation rates, the stability operator becomes close to self-adjoint, leading to the strong suppression of algebraically growing perturbations.

Jana Anukul, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

- Rational design for the syntheses of N-Heterocyclic Carbene (NHC) coordinated 2-hydrophosphasilenes.

- Reversible coordination of NHC's with 2-hydrophosphasilenes.

- Imidazolidine derived NHC-coordinated phosphorous trichloride for the syntheses of multiple bonded phosphorus compounds.

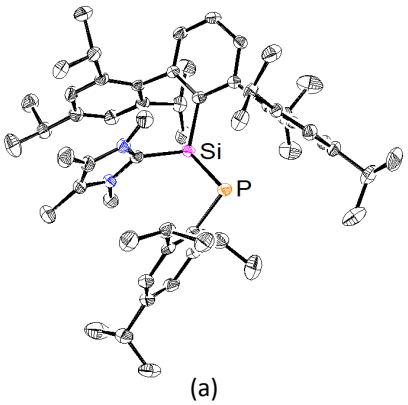
- Syntheses of mono-aryl phosphates for the design of chiral phosphates.

❖ **Rational design for the syntheses of N-Heterocyclic Carbene (NHC) coordinated 2-hydrophosphasilenes** - Compounds with a heteroleptic multiple bond between heavier main-group elements, in particular those between group 14 and 15 elements, have attracted considerable attention, because of their unique reactivity and electronic properties. We have synthesised 2-hydrophosphasilene **(figure a)** stabilized by bulky terphenyl substituent along with N-Heterocyclic Carbene (NHC) and characterized by solution state NMR (^{1}H, ^{29}Si, ^{31}P,) spectroscopy and single crystal x-ray diffraction study.

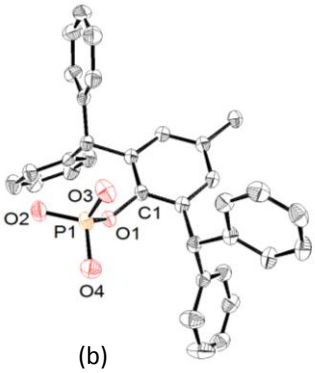
❖ **Reversible coordination of NHC's with 2-hydrophosphasilenes.** We have synthesized different NHC's substituted 2-hydrophosphasilenes and we have observed reversible coordination of NHC with it.

❖ **Imidazolidine derived NHC-coordinated phosphorous trichloride for the syntheses of multiple bonded phosphorus compounds**. We have synthesized imidazolidine derived N-heterocyclic carbene, SIdipp in modified way with better yield and successfully isolated its PCl_3 adduct. The purity of these adducts were characterized through solution state NMR.

❖ **Syntheses of mono-aryl phosphates for the design of zwitterionic phosphates.**
We have successfully prepared various phosphate monoesters of bulky aryl groups **(figure b)** and subsequently, we were able to form zwitterionic phosphates when these aryl groups react- with triethyl amine.



(a)



(b)

Karmakar Smarajit, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Dynamics of Supercooled Liquids with Random Pinning:
Extensive molecular dynamics simulations are performed to determine the phase diagram of two model glass forming liquids in the presence of external quenched disorder. The quenched disorder is introduced in the system by randomly choosing a fraction ρ_{pin} of particles from an equilibrium configuration of the supercooled liquids at temperature T and freezing them in space. The study of the dynamics of supercooled liquids with this type of quenched disorder has drawn a lot of attention in recent years due to theoretical predictions of the possibility of observing the ideal thermodynamic glass transition in such systems. In this Letter, we numerically examine this possibility by determining the phase diagram of the systems in the $\rho_{pin}T$ plane. We find that the phase diagram differs considerably from existing theoretical predictions and show that a rapid decrease in the kinetic fragility of the system with increasing $\rho_{pin}T$ concentration is a probable reason for this difference.

The Static Length scale in the Glass Transition
The existence of a static length scale that grows in accordance with the dramatic slowing down observed at the glass transition, is a subject of intense interest. We showed how one can reach a typical length scale that grows in accordance with at least 15 orders of magnitude increase in the relaxation time, competing with the best experimental conditions. We also proposed a new susceptibility, "Pinning Susceptibility" which directly extract this static length scale and will be easily implementable in experiments. Possible correlation between static and dynamics length scales are also looked at, to understand some of the puzzling phenomena of glass transition.

Glass-Like Slow Dynamics in a Colloidal Solid with Multiple Ground States
We study the phase-ordering dynamics of a 2D model colloidal solid using molecular dynamics simulations. The colloid particles interact with each other with a Hamaker potential, modified by the presence of equatorial patches of attractive and repulsive regions. The total interaction potential between two such colloids is, therefore, strongly directional and has a 3-fold symmetry. Working in the canonical ensemble, we determine the phase diagram in the density temperature plane. We obtain three distinct crystalline ground states, viz., a low density honeycomb solid, a rectangular solid at intermediate density, and finally a high-density triangular structure. We show that when cooled rapidly from the liquid phase along iso-chores, the system undergoes a transition to a strong glass, while slow cooling gives rise to crystalline phases. We claim that geometrical frustration arising from the presence of many competing crystalline ground states causes glassy ordering and dynamics in this solid. Our results may be easily confirmed by suitable experiments on patchy colloids.

Short-Time Beta Relaxation in Glass-Forming Liquids Is Cooperative in Nature
Temporal relaxation of density fluctuations in supercooled liquids near the glass transition occurs in multiple steps. Using molecular dynamics simulations for three model glass-forming liquids, we show that the short-time *β*-relaxation is cooperative in nature. Using finite-size scaling analysis, we extract a growing length scale associated with beta relaxation from the observed dependence of the beta relaxation time on the system size. We find, in qualitative agreement with the prediction of the inhomogeneous mode coupling theory, that the temperature dependence of this length scale is the same as that of the length scale, that describes the spatial heterogeneity of local dynamics in the long-time α-relaxation regime.

Elasto-plasticity in Amorphous Solids The conditions which determine whether a material behaves in a brittle or ductile fashion on mechanical loading are still elusive and comprise a topic of active research among Materials physicists and engineers. In this study, we present the results of in silico mechanical deformation experiments from two very different model solids in two and three dimensions. The first consists of particles interacting with isotropic potentials and the other has strongly direction dependent interactions. We show that in both cases, the excess vibrational density of states is one of the fundamental quantities which characterizes the ductility of the material. Our results can be checked using careful experiments on colloidal solids.

Krishnamurthy M., TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Laser Installation
After overcoming all the technical related issues with the pump lasers etc, the new 7 fs, 1 kHz, 1.5 mJ laser system with Carrier Envelope Phase (CEP) control has been installed. The CEP stability of the amplifier was demonstrated to be <250 mrad over a period of 4 hours, testimony to the environmental stability in the laser cabin. Optical parametric amplified (TOPAS) is also installed and demonstrated to generate a combined Signal (S) + Idler (I) power of a maximum of 1.7 mJ at 1300 nm (S) +1700 nm (I). The wavelength spans from 1140 nm to 1640 nm (S) and 1560 nm to 2600 nm (I). A low dispersive pump probe set up for broad band wavelengths from 650 nm to 2600 nm and short pulse widths upto 7 fs, was set up and installed within the laser cabin to have environmental stability for the two arms of the pump probe and a resolution of 0.1 um, allows ultra precise time resolution of ~ 1 fs over time delays of 1ns.
(*Ram Gopal, M. Anand and M. Krishnamurthy)*

A new set up for high-density gas phase experiments
With the success of using CH4 clusters in improving features of electron acceleration in 2014-15, the study of laser plasmas generated from a plume of clusters becomes imperative. We have designed and

completed the set up of a new chamber to this end. The 6-way CF 150 cross chamber is pumped by a 3200 L/s turbomolecular pump. The laser beam is focused at the centre of the chamber with a 150 mm focal length off-axis parabolic mirror. The cluster beam is presently generated by a pulsed commercial Parker Valve nozzle (series 90), which crosses the laser focus at the centre. The nozzle can be moved in vacuum using a UHV manipulator. In line with the requirement to have the set up to be mobile, an innovative mobile pumping station housing the turbo pump and a large bellow was designed and commissioned. The first set of experiments to characterize the cluster beam using Rayleigh scattering have been completed. A new nozzle with ~ 30 um opening has been designed and is being fabricated presently. This nozzle will also be cryogenically cooled to 170-200 K, for generating large clusters.
(*Ram Gopal, M.Anand, Soubhik Sarkar and M. Krishnamurthy)*

Ultra short electron pulses
An independent project was taken up to develop a source for generating ultrashort electron electron pulses. The rich collective physics of the generation of such electron beams apart, the possible application of electron pulses to study time resolved electron attachment processes or as a diagnostic probe for magnetic fields in plasmas etc. In collaboration with Dr Vandana Sharma and Ms Shilpa Rani (IITH) a chamber has been designed, fabricated and installed on the laser beam line to generate ultrashort electrons pulses from nanotips, using laser assisted field emission. Initial results showed the generation of ultrashort electron beams and developments to do pump probe experiments are designed.
(*Dr Vandana Sharma, Ms Shilpa Rani and Ram Gopal)*

Hard X rays from mesoscopic particles
We had taken up to built an experiment, where in mesoscopic particles of any size, shape and composition can be used as an isolated, replenishable target for laser matter studies. Though we had success in developing the experiments, we had to redesign the experimental strategy to enhance the particle density and temporal stability. An innovative particle flux concentrator is designed to enhance the particle density at interaction region. Our first experiments with the microcrystalline boric acid particle exposed to 3 mJ 30 fs laser pulses (Intensity: 3e15 W/cm^2) showed electron temperatures greater than 25 keV as measured from bremsstrahlung X ray spectra obtained by a NaI (Tl) detector. The maximum absorption of the laser as measured by the transmitted flux on a photodiode shows absorption of greater than 75%. We are pursuing to study the processes involved and the responsible absorption mechanisms. Preliminary results indicate the effect of the carrier gas on the yield of the X-rays, which would suggest either self focussing in the gas to play a role, or additional heating of the plasma from background low energy electrons through ionization of carrier gas.
(*Ram Gopal, M. Anand, Rakesh Sharma, M. Krishnamurthy)*

Madhu P.K. , DCS, TIFR, and TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Notable advances have been made in developing methods in solid-state nuclear magnetic resonance and its applications to materials, especially, amyloid beta peptides. A unified theoretical and experimental understanding of heteronuclear spin decoupling in solid-state NMR has lead to unifying many decoupling schemes under a single classification. Rotary-resonance recoupling leading to decoupling deterioration has been shown to be insignificant by working at very high radiofrequency regimes and slow magic-angle spinning conditions or vice-versa. Efficient recoupling methods have been introduced for geometry elucidation that are robust with respect to crystal orientations and experimental parameters which are also ideally suited for application in strongly coupled spin systems. Unique structural features have been observed in the transition of A peptidefrom its oligomer stage to fibril stage. Insights have been obtained regarding the intramolecular antiparallel beta sheet transition to intermolecular parallel bets sheet arrangement during the conformation change from oligomers to fibrils.

Unification of heteronuclear dipolar decoupling schemes: Heteronuclear spin decoupling is very essential in magic-angle spinning solid-state NMR experiments for resolution and sensitivity enhancement. We have refined rCW^{A} decoupling method extensively by incorporating supercycling strategy. A unification of various schemes in vogue has been attempted under the general framework of phase and time modulation of radiofrequency

pulses. This has clearly brought out common features among many schemes that were not obvious earlier. This has also pointed to several good decoupling conditions which are being currently exploited. (P. K. Madhu with Niels Nielsen and Asif Equbal, Univ. of Aarhus, Denmark.)

Theoretical understanding of heteronuclear dipolar decoupling schemes: Multi-mode Floquet theory has been used to obtain several key features of the rCW^A scheme, both in the non-supercycled and supercycled version. This has also established interesting symmetry properties of the various spin operators and their role in achieving good decoupling. A Floquet analysis was also performed on the performance of the rCW^A scheme under fast magic-angle spinning conditions and low radiofrequency regime. This has clearly established the conditions under which the rCW^A decoupling scheme can be applied under these regimes for efficient performance. (P. K. Madhu with Niels Nielsen and Asif Equbal, Univ. of Aarhus, Denmark, Michal Leskes and Shimon Vega, Weizmann Institute of Science, Israel, and Vipin Agarwal, TCIS, TIFR, Hyderabad.)

Quenching of rotary-resonance conditions during decoupling: Rotary resonance recoupling, R3, leads to deterioration of decoupling efficiency when the radiofrequency field matches magic-angle spinning frequency. There has been some debate in the literature regarding design of schemes that can quench these conditions. We have suggested strategies to overcome the R3 conditions by performing experiments at high magic-angle spinning conditions and low radiofrequency regime. This completely avoids any discussion regarding R3 quenching and routine experiments can be performed without optimising yet another decoupling scheme. (P.K. Madhu, Kshama Sharma ,Vipin Agarwal, TCIS, TIFR, Hyderabad.)

Recoupling pulse schemes and strategies: We have introduced non-linearly spaced pulses with regard to the rotor period for recoupling dipolar interactions under magic-angle spinning in rotational-echo double-resonance experiments. These experiments are useful to obtain distance constraints. The new strategy leads to a scaling of the dipolar coupling, however, it is independent of crystallite orientation dependence and other experimental parameters. The scaling factor is robust with regard to spinning frequency and radiofrequency amplitude. The scaling property will be useful in the measurement of strong dipolar couplings and this experiment is currently underway. Experiments to measure order parameter under very fast spinning are also underway. We have further improved our theoretical and experimental understanding in performing symmetry-based pulse schemes in an asynchronous way. Such a strategy has been extended to various symmetry-based schemes with higher efficiency in recoupling. (P. K. Madhu with Matthias Ernst, ETH, Zurich, and Mukul Jain, Kshama Sharma and Vipin Agarwal, TCIS, TIFR Hyderabad.)

Solid-state NMR spectroscopy of amyloid fibrils: Aβ peptide continues to be an interesting model for investigating different aspects of amyloid aggregation. The link between toxicity and size of Alzheimer's amyloid-β (Aβ) aggregates likely has a structural origin. However, the major structural features of Aβ peptide (dominated by β-sheets) appear to be conserved across sizes from small oligomers onwards, presenting an unsolved puzzle. We have probed Aβ aggregates of increasing size from the mesoscopic to the atomic scale with a combination of spectroscopic and imaging tools. We found that the apparently conserved beta sheet character hides a major secondary structure transition, where an intramolecular anti-parallel beta sheet structure (containing a beta turn) in the small oligomers evolves to a intermolecular in-register parallel beta sheet structure in the mature fibrils. At the atomic level, the salt bridge between D23 and K28, a key inter-residue contact in fibrillar Aβ which is frequently altered in early onset AD mutations, emerges in parallel. Our findings regarding the anti-parallel to parallel transition and the salt bridge are mirrored by molecular dynamics simulations. Notably, structural signatures for the soluble oligomers resemble the porin-like features of membrane bound oligomers. This suggests a mechanism of toxicity for the small soluble oligomers, and a reason why the mature aggregates may have lower toxicity. (P. K. Madhu with Baapaditya Chandra and Prof. Sudipta Maiti, TIFR, Mumbai, and Kaustubh Mote, TCIS, TIFR, Hyderabad.)

Mazumder Aprotim, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

This year saw the start of Biological programmes at TCIS. In addition to recruiting students and setting up academic programmes, actual biological research

has now taken off Dr. Aprotim Mazumder investigates DNA damage responses in cells for its relevance to the emergence of cancers. To support such research, in addition to standard laboratory workspaces and equipment, a cell culture facility has been set up with incubators, biosafety cabinets, inspection microscopes, liquid nitrogen storage etc. Two widefield epifluorescence imaging systems with live-cell chambers have been set up, and a flow cytometer for evaluating high number statistics of fluorescence across large cell populations is operational too. Methods have been optimized for performing single molecule RNA fluorescence in situ hybridization in cells, steady-state anisotropy measurements and quantitative image analysis, and these tools are being applied to a variety of biological questions, most notably in the study of cell-cycle dependent DNA damage responses.

Mondal Jagannath, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

- Deciphering the binding and unbinding pathways of the ligand approach to protein by computer simulations.

- Delineating role of mutation in the drug resistance of kinase using computer simulation.

- Key insights on role of solvent and steric effects on hydrophobic cavity-ligand unbinding.

- Understanding role of osmolytes in conformations of hydrophobic polymer.

Mote Kaustubh R, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

We were able to show that high resolution proton-detected NMR of proteins is possible under slow magic angle conditions and that these experiments can be very useful for a diverse range of samples such as nanoparticles. Solid state NMR was also used to understand the interaction of amyloid-beta oligomers with membranes and we were able to show, for the first time, the secondary structure of the amyloid-beta oligomers, interacting with the membranes.

My research group works on understanding the metabolite transport across membranes. The current work focuses on the mitochondrial pyruvate carrier, which transports pyruvate from the cytoplasm into the mitochondria. This system is at the edge of what can be possibly studied by solid state NMR spectroscopy and as such, warrants the development of new techniques for its characterization. Towards this aim, I have developed several new techniques in solid state NMR over the past year, focusing on how these can be applied. This work has resulted in three high impact publications and has been highlighted in popular press as well.

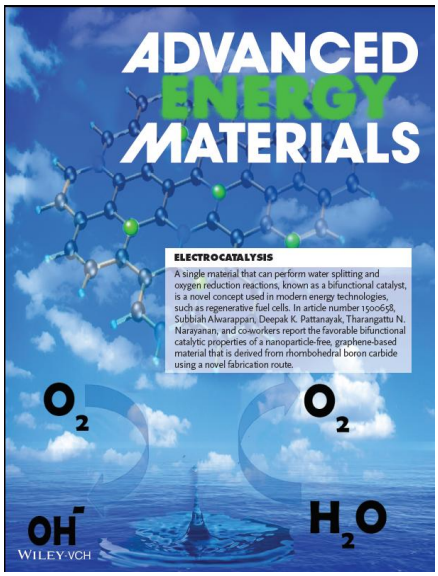
High resolution 1H detection at moderate MAS frequencies: One of the big challenges in solid state NMR is to achieve high resolution detection of protons. We used windowed 1H detection with phase-modulated Lee-Goldberg homonuclear decoupling technique to obtain resolution in the 1H dimension that is comparable to that achieved under much higher magic angle spinning frequencies. This method will be of tremendous use for cases where sample availability is not a limiting factor, particularly membrane proteins and fibrils Together with Prof. V. Polshettiwar and Prof. P.K. Madhu, we used this method to look at catalytically active nitridated silicon nanoparticles in an effort to understand their catalytic activity as a base. We were able to determine, that the catalytic activity is primarily as result of primary amines -

In collaboration with Prof. Sudipta Maiti and Pro. P.K. Madhu, we were able to determine that amyloid-beta oligomers maintain a beta-sheet conformation when attached to membranes. interestingly, we were also able to determine that the membrane bound species contains a contains a beta-turn, which possibly indicates the presence of an antiparallel beta-sheet structure when bound to the membrane This work received wide press coverage in Eureka Alert as well as popular press

Narayanan TN, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Synthesis and assembly of atomic layers:
The discovery of atomically thin layers (also called 2-dimensional (2D) materials/layers) with a variety of intrinsic properties has spawned a new field of materials science research. Recent research on nanomaterials proved that new classes of engineered materials/solids can be designed by the combinatorial stacking or arrangements of various atomic layers. Hence, atomic layers are not only

interesting in their pristine form, but are intriguing in their stacked form too. One of the main focus of my research at TCIS is the study of interface induced properties in the stacked forms of atomic layers. This includes the controlled synthesis and systematic assembly of atomic layers, and probing their interface induced properties. Further, this research also includes theoretical understanding of the junction formation - from statistical to atomistic calculations, where we will try to model the system with potential in classical regime. Controlling and manipulating these junctions and assemblies can control the electronic, optical and electrochemical properties of resultant solids. The interfacial charge separation, heterogeneous electron transfer process etc. will also be studied. A chemical vapor deposition (CVD) set up is also developed at TCIS for the synthesis of individual atomic layers and layer by layer deposition of various layers. (T N Narayanan, Shubhadeep Pal, Ravi Kumar Biroju, Vineesh T V and Rahul Sharma)



Small molecule detection and development of bio-sensors:

Biosensing is receiving enormous attention from the scientific community due to its importance in the development of point-of-care devices. Various platforms were used in the recent past for the detection of ppm/ppb levels of small molecules, and electronic and electrochemical bio-sensing are important classes among them. In our present research, we are trying to develop engineered graphene based small molecules, such as ammonia, sensors. A first principle study on the interaction possibilities of graphene and ammonia is conducted using Density Functional Theory calculations. The bio-sensing possibilities of engineered graphene materials are also being studied experimentally. An impedance spectroscopy based electrochemical sensing possibilities are being explored. (T N Narayanan, Kiran Kumar Tadi, Shubhadeep Pal, Ravi Kumar Biroju, Ananth Puthirath)

Viscoelastic Studies on Self/forced assembled 3-dimensional structures:

Controlled assembly of 1D or 2D nanomaterials to form macroscopic 3D structures is another intriguing field where these high surface area 3D structures can find applications in energy storage devices (3D batteries) and sensors (high diffusion electrodes). But the stable assembly of individual nanomaterials is a challenge. We are trying to make those controlled structures by solution self-assembly process and using external cross-linking agents. The interconnected structures need to have high mechanical strength for their further applications, and covalent linkage among nano blocks is highly demanding for ensuring the mechanical sturdiness of these 3D macroscopic structures. In my past studies it was revealed that microscopic characterization are not sufficient to prove the covalent linkage of individual nano blocks, and only a systematic viscoelastic measurement can render information about the covalent linkage. We are studying the viscoelastic properties of 3D graphene and 3D CNT assemblies to understand the fundamental mechanism underlying in the reinforcement of these 3D structures. (T N Narayanan, Sudeshna Patra)

Perlekar Prasad, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Impact of the Peterlin approximation on polymer dynamics in turbulent flows

We study the impact of the Peterlin approximation on the statistics of the end-to-end separation of polymers in a turbulent flow. The finitely extensible nonlinear elastic (FENE) model and the FENE model with the Peterlin approximation (FENE-P) are numerically integrated along a large number of Lagrangian trajectories resulting from a direct numerical simulation of three-dimensional homogeneous isotropic turbulence. Although the FENE-P model yields results in qualitative agreement with those of the FENE model, quantitative differences emerge. The steady-state probability of

large extensions is overestimated by the FENE-P model. The alignment of polymers with the eigenvectors of the rate-of-strain tensor and with the direction of vorticity is weaker when the Peterlin approximation is used. At large Weissenberg numbers, the correlation times of both the extension and of the orientation of polymers are underestimated by the FENE-P model.

Clustering of vertically constrained passive particles in homogeneous, isotropic turbulence.
We analyze the dynamics of small particles vertically confined, by means of a linear restoring force, to move within a horizontal fluid slab in a three-dimensional (3D) homogeneous isotropic turbulent velocity field. The model that we introduce and study is possibly the simplest description for the dynamics of small aquatic organisms that, due to swimming, active regulation of their buoyancy, or any other mechanism, maintain themselves in a shallow horizontal layer below the free surface of oceans or lakes. We have quantified the compressibility, the preferential concentration of the particles, and the correlation dimension by changing the strength of the restoring force. The main result is that there exists a particular value of the force constant, corresponding to a mean slab depth approximately equal to a few times the Kolmogorov length scale η, that maximizes the clustering of the particles.

Inertial particle acceleration in strained turbulence

The dynamics of inertial particles in turbulence is modelled and investigated by means of direct numerical simulation of an axisymmetrically expanding homogeneous turbulent strained flow. This flow can mimic the dynamics of particles close to stagnation points. We report results relative to the acceleration variances and probability density functions for both passive and inertial particles. A high mean strain is found to have a significant effect on the acceleration variance both directly by an increase in the frequency of the turbulence and indirectly through the coupling of the fluctuating velocity and the mean flow field. The influence of the strain on the normalized particle acceleration probability distribution functions is more subtle. The magnitude changes in the inertial particle acceleration variance and the effect on the probability density function, are then discussed in a wider context for comparable flows, where the effects of the mean flow geometry and of the anisotropy at small scales are present.

Raman Karthik V, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Thin film spintronics An ultra high vacuum system was setup demonstrating the capability to grow thin films of ferromagnets and oxides with a sensitivity of less than 1 Angstrom per second. Capability to grow devices in-situ was also achieved for growing vertical junction devices. Further installations are ongoing to start performing research and produce new experimental findings. This unique system, which is still in its early stage of development, is expected to become a sophisticated world class tool to perform cutting edge experimental research in spintronic and nanoelectronics.

Figure: Setting up of a thin film cluster vacuum system with the capability evaporate ultra clean thin films of metal and oxides (As shown in the inset)

Ramaswamy Sriram, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Silent Flocks: Constraints on Signal Propagation Across Biological Groups, Phys Rev Lett *114*, 218101 (2015), highlighted with a Physics Synopsis and selected as Editor's Choice.

In collaboration with the group of A Cavagna (Rome), S Ramaswamy co-authored theoretical work

showing that the collective dynamics of bird flocks was characterized by a long-wavelength regime displaying travelling density waves, and -- for large orientational inertia -- a short-wavelength regime with propagating spin waves. For large enough inertia they predicted the existence of a range of length scales over which neither density nor spin was propagative, compromising coherent information transfer and coordination for mid-sized flocks. This finding is of potential importance for flock size selection.

Sengupta Surajit, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

A new perspective on lattice defects

Understanding plastic deformation is essential from both technological and fundamental viewpoints. In crystalline solids, deformation is mediated by lattice defects which begin to flow in response to stress when the solid yields. Yielding in disordered solids is much less understood and there is no universal language which can describe deformation in crystalline and disordered solids alike. In our group we have been working towards such a description. We have found that certain special displacements of atoms, called non-affine displacements, are related to lattice defects. Indeed, in a crystal, dislocation pairs appear as lowest energy non-affine modes. Defect densities can be tailored by external fields which couple to non-affine displacements. Since non-affine displacements may be defined in both crystalline and disordered matter, our work raises the hope that a unified understanding of deformation may be possible.

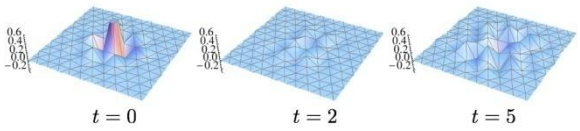


Figure: Decay of defect correlations with time ***t*** of a two dimensional triangular lattice in a non-affine field.

Vallurupalli Pramodh, TIFR Centre for Interdisciplinary Sciences, Hyderabad.

Using a combination of experimental and computational techniques, we have determined how the cavity mutant of the protein T4 lysozyme (T4L L99A/G113A/R119P) interconverts between two compact conformations. We find that the barrier is just ~6 k_BT.

i) The lab is now functional: a) The 700 MHz solution NMR spectrometer equipped with a cryoprobe has been installed successfully. b) The biochemistry/molecular biology wet lab has also been setup.

ii) Using a combination of experimental and computational techniques, we have determined how the cavity mutant of the protein T4L interconverts between two compact conformations. We find that the barrier is just ~5 k_BT.

iii) We have shown using NMR experiments that the activation energy required for the cavity mutant of T4L to interconvert between two compact subtle conformations is obtained due to interactions of the protein with the solvent water. (Anusha B Gopalan ,Mukul Jain)

iv) Using a combination of computational (in collaboration with J. Mondal at TCIS) and experimental techniques, we have determined how T4 lysozyme L99A binds hydrophobic molecules like benzene in a buried cavity. (BR Dandekar, S Pandit, J Mondal)

4. Figure / Photograph Captions

5. Staff List

Agarwal Vipin:

TCIS/TIFR students:

- Subhajit Dey (Feb-April 2016)→ Semester student

Post-doctoral fellows:

- Satya Prakash (September 2015-Present)
- Laxman Alakonda (March 2016- Present)

External Students/Visitors:

- Bharti Kumari (July-November 2015)→ JRF
- Arpita Sundaria (October 2015-June 2016) → M.Tech student, Rajasthan University

Govindarajan Rama:

Project assistants

- Karthik Menon (OMM grant)

- Arthi Appathurai (Indo-French grant)

Students
- Mamta Jotkar (graduated)
- Sharath Jose
- S Ravichandran
- Sumit Birwa
- S Ganga Prasath
- Ritabrata Thakur
- Rashmi Ramadugu (shared with Prasad Perlekar)

Jana Anukul:

Graduate Students
- Debabrata Dhara (April 2015-)
- Debdeep Mandal (April 2015-)

Post-doctoral fellows:
- Biswajit Santra (Sept 2015-)
- K. Praveen Kumar (Oct 2015-)

Project-A Students (Graduate Students of TCIS Hyderabad)
- Avijit Maiti (Jan 2016-April 2016)

Project Students (JRF)
- Subrata Kuliya (Aug 2015-July 2016)
- Ramapada Dolai (Feb 2016-)

Garai Kanchan:

TCIS/TIFR students

- Timir Sil
- Subhrajyoti Dolai
- Shamasree Ghosh
- Aslamuddin

Post-doctoral fellows:
- C Neeraja
- Bankanidhi Sahoo

Karmakar Smarajit:

- Indrajit Tah, PhD Student (2015 -)
- Rajshekher Das, PhD Student (2015 -)
- Bhanu Prasad Bhowmik, PhD Student (2015 -)
- Kallol Paul, PhD Student (2015 -)

Krishnamurthy M:

- Ram Gopal
- M . Anand

Madhu P.K:

- G. Rajalakshmi, Scientific Officer E
- Krishna Rao, Scientific Officer D (NMR Facility Manager)

Mazumder Aprotim:

Post-doctoral fellows:
- Sitara Roy

Graduate Students:
- Shiv Narayan Dhuppar
- Nikhita Pasnuri
- Kesavan P.S.

Narayanan T.N:

Post-doctoral fellows:
- Kiran Kumar Tadi
- P. M. Sudeep
- Santosh Bikkarolla

Graduate Students:
- Shubhadeep Pal
- Sudeshna Patra

Visiting Students/Scientists:
- Anil Palve (Mahatma Phule College, 2015, May, November)
- Sathyavathi Ravulapalli (Visiting Post-Doctoral Fellow, 2015 August-November)
- Agnish Dev Prusty (Visiting Student from IIT Bhubaneswar
- Kapil K. Bhorkar
- Vineesh T V (CSIR-CECRI)

Project Students:
- Sourabh (Project A, Chemistry)
- Pappu Acharya (Project A, Physics)
- Rahul (Project A, Physics)

Summer Students:
- Preethi S. Mathew (TIFR Summer Student, IISER, TVM, 2015, May-July)
- Narayan Kunchur (NIT, Calicut, 2015 May-July, 2016 May-July)
- Anish H. Verma (TIFR Summer student, UPES, Dehradun, 2015 May-July)

Raman Karthik V:

Post-doctoral fellow:

- Mathimalar

Graduate Student:

- Saurabh Chaudhary

JRFs:

- Sambit Mahopatra
- Swapneel Pathak

Ramaswamy Sriram

Post-doctoral fellows:

- Sarada Seetharaman
- Abhijeet Joshi

Graduate Students

- Rayan Chatterjee
- Rahul Chajwa
- Lokrishi Prawar Dadhichi
- Rahul Gupta

6. National and International Involvement (Professional and Academic) Memberships of editorial, academic and national committees, Office bearership of professional societies, etc.

Agarwal Vipin:

Member, National Magnetic Resonance Society, India

Chary KVR:

- Elected Council Member of The National Academy of Sciences, India (2016-2018).
- Member of Fellowship Scrutinizing Group of The National Academy of Sciences, India (2016-
- Elected as Treasurer and Steering Committee Member, Asian Biophysics Association (2013-present).
- Elected as Member, International Advisory Board, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2014-2016).
- Member, IUPAB National Committee of INSA (2012-16).
- Executive Council Member (2008-present) and Advisor (2012-present), Royal Society of Chemistry, West India Section.
- Member, Editorial Advisory Board, of the Journal Current Bioinformatics, launched by Bentham Science Publishers, The Netherlands and U.S.A. (2005-present); Member, Editorial Board, of "The Open Magnetic Resonance Journal", launched by Bentham Science Publishers, The Netherlands and U.S.A., (2007- Present).
- Fellow of Royal Society in Chemistry (FRSC) (2004-present).
- Convenor, Indian Science Congress Association, Mumbai Chapter, Mumbai (2010-2015).
- Member, J.N. Tata Endowment Selection Committee, Mumbai (2005-Present).
- Member, Management Advisory Committee for the "National Facility for High Field NMR", TIFR.
- Member, National Magnetic Resonance Society, India; Chemical Research Society of India, India; Indian Biophysical Society, India; Indian Chemical Society, India; and Member, Society of Biological Chemists.

Govindarajan Rama:

- Editorial Board of Physical Review Fluids (from 2016 Jan)
- Editorial Advisory Board of the Physics of Fluids (till 2015 Dec)

Krishnamurthy M:

- Elected as Secretary of the Asian committee on ultra intense laser (ACUIL), Busan Sept 2015.

Madhu P.K:

Convener, MagRes academic advisory body (MRAAB), TIFR, Hyderabad.

- Head: Research, finance, and administration, TCIS, 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, European School on Solid-State NMR.
- Member, MAC, National Facility for High-Field NMR, TIFR.
- Member, Board of Trustees of EUROMAR, European Magnetic Resonance Meeting.
- Scientific programme committee member, EUROMAR, Prague, July 1-5, 2015.
- Member, National Magnetic Resonance Society, India.

Narayanan T.N:

- Editorial Board Member of American Journal of Engineering and Applied Sciences (2015).

- Associate Editor of Carbon-Based Materials – Frontiers in Materials (2015).
- National Organizing Committee member of 4th International Conference, COCHIN NANO-2016, to be held at Kochi during February 20-23, 2016. (International Program Committee Member of EMN Meeting on Electrocatalysis, Energy Materials Nanotechnology, February 15-19, 2016 Orlando, USA

Raman Karthik V:

- International Advisory member, SPIN-OS 2016

Ramaswamy Sriram:

- Member, Editorial Committee, Annual Review of Condensed Matter Physics, 2011-2015.
- Member, Editorial Board, Advances in Physics, since June 2007.
- Member, Editorial Board, European Physical Journal E, since Dec 2009
- Member, Editorial Board, Journal of Statistical Mechanics: Theory and Experiment, since January 2004. Member, Editorial Advisory Board, Soft Matter, since May 2008
- Member, Editorial Committee, Annual Review of Condensed Matter Physics, 2011-2015.
- Higgs Centre Associate, University of Edinburgh, 2012- present

Research Grants:

- J C Bose Fellowship of the Department of Science and Technology, India; Research grant: Rs 10,00000 per year; 2007-2017 (renewed 2012)

Vallurupalli Pramodh:

- Reviewed articles for: Proceedings of the National Academy of Sciences (USA), Journal of Bimolecular NMR

7. Visits:

Agarwal Vipin:

- Monthly visits to TIFR Mumbai for experimental measurements.

Barma Mustansir:

- Visited Rudolf Peierls Centre for Theoretical Physics, University of Oxford for a month (May 2015)

Chary KVR:

- SP Pune University, Pune held on February 26, 2015 to deliver an invited talk.
- State Key Laboratory of Bio-organic and Natural Product Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Science on Friday, May 8, 2015 to deliver an invited talk.
- Hongzhou, China, from May 9-12, 2015 to attend Asian Biophysics Association Conference to deliver a talk and Chair a session.
- SGPGIMS, Lucknow, on June 23, 2015 to attend National Workshop on "NMR in Biological Systems".
- University of Wisconsin, on August 4, 2015 to deliver an invited talk.
- Structural Biology Initiative CUNY Advanced Science Research Center (ASRC) Monday, August 10, 2015 to deliver an invited talk.
- National Institutes of Health, National Heart, Lung, and Blood Institute, Bethesda, Maryland, USA, on August 17, 2015 to deliver an invited talk.
- Nano Cell, University of Linz, Austria, on November 23, 2015 to deliver an invited talk.

Govindarajan Rama:

- Kavli Institute of Theoretical Physics , Santa Barbara, University of Oregon, for discussions about the OMM project.

Jana Anukul:

- Saarland University, Germany, 28th September - 09th October, 2015

Madhu PK:

- University of Leipzig, Leipzig, June 22-July 12, 2015.
- ENS, Lyon, France, October 26-29, 2015.

Mondal Jagannath:

- Columbia University, USA (Collaboration with research group of Prof. Bruce J. Berne)
- University of California at Berkeley (Collaboration with research group of Prof. Niren Murthy)

Raman Karthik V:

- PACIFICHEM Conference, USA December 2015

Sengupta Surajit:

- University of Dusseldorf, July 1 - July 11, 2015.
- Okinawa Institute of Science and Technology, April 25 - May 9, 2015.
- Institute of Industrial Science, University of Tokyo, May 8, 2015.

8. Awards & Distinctions:

Chary KVR:

- Elected Council Member of National Academy of Sciences, India, Allahabad (2016-2018).
- Elected as Member, International Advisory Board, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2014-2016).
- Elected as Treasurer and Steering Committee Member, Asian Biophysics Association (2013-present).
- Invited Speaker and Chairman of a Session at Asian Biophysics Association Conference held at Hangzhou, China (May 2015).
- Invited Speaker and Chairman of a Session at the forthcoming 27th International Council on Magnetic Resonance in Biological Systems (ICMRBS).

Krishnamurthy M:

- DAE-SRC Outstanding Investigator award (2015).

Mondal Jagannath:

- Awarded Ramanujan Fellowship. Elected as a young associate of Indian Academy of Sciences.

Narayanan T.N:

- Associate of Indian Academy of Sciences – July 2015 –December 2018.
- ACS membership award in recognition of engagement with ACS's mission of service, July 2015-July 2018.
- Adjunct Faculty (2015 December- 2018 December) – Academy of Scientific and Innovative Research (AcSIR)

Raman Karthik V:

- 2015 PACIFICHEM Early Career Research Award

9. Invited Talks in Conferences and Meetings:

Agarwal Vipin:

- Solid-State NMR as a tool for structural characterization of biomolecules and materials. 14th September 2015, DCS,TIFR Mumbai, India.
- Observation of long-range H^N-H^N contacts in non-deuterated proteins at 90 kHz MAS. NMR Meets Biology, 14th-19th January, Vaylar, Kerala, India. (2016)

Chary K.V.R:

- Structure and Dynamics of Intrinsically Ordered and Disordered Proteins by NMR: The state-of the-art." at Indian Science Congress 2015, Kalina Campus, Mumbai University, on Monday, January 5, 2015
- Key-note address on, "Bioinformatics and NMR Spectroscopy", at Lecture-Cum-Workshop on "Application of Bioinformatics in Drug Designing", held at DY Patil University, on Thursday, January 22, 2015.
- "NMR At The Interface Of Physics, Chemistry And Biology/Biotechnology", at Bio-Integration 2015 "Integrating Chemistry and Physics in Rediscovering Biotechnology" A National Seminar under Faculty QIP programme of SPPU, Pune held on Thursday, February 26, 2015.
- Structure and Dynamics of UV inducible protein (UVI31+) from Chlamydomonas reinhardtii that exhibits RNA and DNA endonuclease activity", during the Asian Biophysics Association Conference, held at the Hongzhou, China, from May 9-12, 2015.
- Echoes in NMR", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 23, 2015.
- NMR of Nucleic Acids", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 25, 2015.
- Evolution through Structure", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 25, 2015
- An unusual calcium binding protein from Entamoeba histolytica", DCS Annual Talks, held at TIFR, on November 4, 2015.
- Invited talk on, "βγ-crystallins: Intrinsic Order & Disorder", at the International Conference of FAOBAB, on Sunday, November 29, 2015.

Garai Kanchan:

- Invited speaker at Owls 2016 international conference.

Govindarajan Rama:

- Keynote lecture, IUTAM Symposium on Helicity, Structures and Singularity in Fluid and Plasma Dynamics, Venice, April 2016.
- GEOFLO16: Two phase continuum models for geophysical particle-fluid flows, MPI-PKS Dresden, March 2016. (Two lectures)
- Complex Systems Approach to Self-Organization (CSAS 2016), IIT Madras, Chennai, February 2016.

Invited talks in Indian meetings:

- Science Popularisation Programme, Madras Music Academy, Chennai, February 2016. The audience was about a 1000 people.

- Subir Kar Plenary Lecture, 42nd National Fluid Mechanics and Fluid Power Conference, NITK Surathkal, December 2015.

Jana Anukul:

- Rational design for the syntheses of multiple bonded compounds involving heavier Group 14 elements and their reactivity" at Banaras Hindu University for DST-SERB, PAC meeting. May 2, 2015
- Hydrocarbon Soluble Low-Valent Low-Coordinate Silicon Enriched Core: Elegant Approach Towards Syntheses of Heavier Group 14 Molecular Cluster" at INSA for INSPIRE interview. May 25, 2015
- Functionalized Low-Valent Low-Coordinate Heavier Group-14 Chemistry" at Department of Chemical Sciences Annual Talks 2015, TIFR Mumbai.

Karmakar Smarajit:

- XXVII IUPAP Conference on Computational Physics CCP2015, Guwahati 2-4th Dec. 2015.
- Compu-2016: Conference on Complex Fluids, IISER-Pune, 2-4th, January 2016.
- Discussion Meeting on Glass Formers and Glasses, JNCASR, Bangalore, April 29 - 30 (2016), JNCASR.

Krishnamurthy M:

- Neutral atom acceleration, First Newton-Bhabha Workshop on High Field Science, March 1-3, 2016, Kerala, India.
- Acceleration of neutral atoms, positive and negative ions with novel targets" at the International Conference on Extreme Light (ICEL) Bucharest, Romania 2015.
- Ionisation and Recombination in NanoClusters for neutral atom acceleration, Invited talk at Gordon Research conference on Clusters and Nanostructures, Barcelona (2015).
- Intense laser matter interaction, talk given at BITS Hyderabad on Science day, Hyderabad (2015).

Madhu P.K:

- Heteronuclear spin decoupling in solid-state NMR: Towards higher efficiency and unification, Emerging NMR methods, IISc, Bangalore, July 16-17, 2015
- Structure, function, and dynamics of biomolecules with solid-state NMR, 1st western region structural biology meet, IIT Bombay, Mumbai, August 1, 2015
- Heteronuclear spin decoupling in solid-state NMR: Towards higher efficiency and unification, ISMAR (International Society of Magnetic Resonance), Shanghai, China, August 16-21, 2015
- Chemistry and biophysics of amyloid oligomers, Indo-German workshop on molecular amplification, Tutzing, Munich, Germany, October 20-23, 2015
- Spin decoupling in NMR, NMR meets Biology, Kerala, India, January 14-19, 2016
- Chair of a session, EUROMAR, Prague, Czech Republic, July 5-10, 2015
- Chair of a session, ISMAR, Shanghai, China, August 16-21, 2015

Mazumder Aprotim:

- "Scientific talk in the Optics Within Life Sciences (OWLS) meeting, TIFR, Mumbai (March, 2016)
- "Scientific seminar in Aurora College, Hyderabad, India (August, 2015)
- "Scientific seminar in CDFD, Hyderabad, India (April, 2015)

Mondal Jagannath:

- How does a kinase inhibitor withstands gatekeeper residue Mutation", DCS annual talks, Tata Institute of Fundamental Research, Mumbai, 4-6 November, 2015.
- "Role of osmolytes on conformational propensities of polymer", Soft Matter Young Investigators Meet, Pondicherry, 17-20 December, 2015.

Narayanan T.N:

- Recent Advances in Carbon Nanotechnology, T. N. Narayanan, St. Teresas College, Kochi, India, February 24th 2016
- Tuning the Electrochemical and photophenomena of Atomic Layers – A *Mix and Match* Approach, T. N. Narayanan, 4th International Conference on Frontiers in Nanoscience and technology [Cochin Nano -2016] February 20-23, 2016, Kochi, India.
- Engineering Atomic Layers for Efficient Sensors, NUCRET Boot Camp Hands-on Workshop Series Sensors: State-of-the-Art Science & Technology – Hands on Design of a Biosensor 2015, November 10-12, 2015, Northeastern University, Boston, USA
- Recent Trends in Carbon Nanotechnology, National Conference on "Recent Developments in Physics", NSS College, Ottapalam, Kerala, 19-20 October, 2015.
- Department of Science and Technology "INSPIRE SCIENCE CAMP" lectures for XIth class students having their SSC score above 93.2% in board examination, Dayanand Science College, Latur, Maharastra, India, September 18-22, 2015.

- Engineering the Atomic Layers Interfaces for Novel Solids, Institute of Physics, Bhubaneswar, India, September 14, 2015.
- New solids with novel interfaces with tunable properties, T. N. Narayanan, School of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, India, March 2, 2015.
- New solids with novel interfaces for energy technology ,T. N. Narayanan, International Conference on Energy Harvesting, Storage and Conversion (IC-EEE), Kochi, India February 5-7, 2015.
- New Trends in Energy and Water Technologies – A Nanotechnology Approach, T. N. Narayanan, National Seminar on Advanced Materials for Energy and Environment" (NSMEE-2015), Vimala College, Thrissur, February 9-10, 2015.
- Fascinating Carbon Science", T. N. Narayanan, Sri Vyasa NSS College, Wadakkanchery, Kerala February 4, 2015

Perlekar Prasad:

Three and Two dimensional binary mixture turbulence IUPAP Conference on Computational Physics, IIT Guwahati, 25 December 2015

Raman Karthik V:

- Interface-assisted molecular spintronics, PAIFICHEM 2015, December 2015 (USA)

Ramaswamy Sriram:

- Invited speaker, SFB on Collective Behavior of Soft and Biological Matter, Hohegeiss, Germany, Nov 2015.
- Invited speaker, Soft Matter Gordon Research Conference, 10-14 Aug 2015
- Invited speaker, Quantitative Biomedicine Symposium, Warwick Univ, May 2015
- Invited speaker, (i) Active Matter Conference, Suzhou, China and (ii) Spring School on Active Matter, Beijing Computational Science Research Centre, May 2015
- Invited lecture, Cell Mechanics Conference, Raman Research Institute, Bangalore, 24-26 April 2015

Sengupta Surajit:

- From crystal to glass: relating plastic deformation to amorphization of a crystalline solid, Growing Length Scale Phenomena (GLSP) in Condensed Matter Physics, JNCASR, Bangalore October 8-10, 2015.

Vallurupalli Pramodh:

Invited talk at the NMR meets Biology Conference Jan 14-16, Kerala, India - Using NMR to Study Conformational Exchange Involving Transiently Populated (Invisible) Minor Conformers of Proteins.

10. Conference Organised by the School / Deptt. / Group:

Chary K.V.R:

- National Poster Symposium on Advances in Chemical Sciences, jointly Organized by Royal Society of Chemistry – India Deccan Local Section, India & Tata Institute of Fundamental Research, Centre for Interdisciplinary Sciences, Hyderabad (December 12, 2015).

Karmakar Smarajit:

- XXVII IUPAP Conference on Computational Physics CCP2015, Guwahati 2 - 4th Dec. 2015
- Compu-2016: Conference on Complex Fluids, Hyderabad, 12-14th, December 2016, Session Organizer for Granular and Glassy systems
- Third Annual TCIS Summer Research Symposium, 1st July, 2016, TCIS, TIFR, Hyderabad.

Krishnamurthy M:

- First Newton-Bhabha Workshop On High Field Science, March 1-3, 2016, Kerala, India.

Madhu P.K:

- NMR Meets Biology, Alleppey, Kerala, January 14-19, 2016.

Perlekar Prasad:

- Spinodal decomposition in the inverse cascade of two dimensional, binary fluid turbulence" European Turbulence Conference, TU Delft, The Netherlands 25-28 August 2015
- Two dimensional turbulence in symmetric binary mixtures, ICTS Discussion Meeting, Bangalore. 6-8 April 2015

Ramaswamy Sriram:

- Co-organiser, Workshop on "Active Liquids", 21 – 25 September 2015, Lorentz Center, University of Leiden, Netherlands (on critical issues in the statistical mechanics and dynamics of collections of self-driven particles)

11. Non DAE Research Projects:

Chary K.V.R:

- The DST-DIISRTE joint research project (Australia-India Strategic Research Fund (AISRF)), DST, 2015-17.

Govindarajan Rama:

Indo-French grant

- Project Title : Rotating and Curved Boundary Layer Instabilities. Duration : 4 years (from 1.2.2013 to 31.1.2017).

OMM grant

- Project Title: Coupled Physical processes in the Bay of Bengal and Monsoon Air- Sea Interaction Duration : 3 years (from 4.4.2015 to 3.4.2018)

Jana Anukul :

Sl. No	Grant Agency	Title of the project	Total Amount
1	AvH Foundation	Design and utility of appropriate anionic ligands for the syntheses and mutual conversion of multiple bond of heavier Group 14.	Euro 20,000.00 (one time grant for capital equipment)
2	DST-SERB	Rational design for the syntheses of multiple bonded compounds involving heavier Group 14 elements and their reactivity File No: EMR/2014/001237	Rs. 25,90,000.00 (2015-2018)
3	CSIR	Syntheses and Reactivities of Compounds Involving Formal Zero Oxidation State of Mono- and Di-Nuclear Group 14 Elements File No: 01(2863)/16/EMR-II	Rs. 4,50,000.00 (2016-2019)

Madhu P.K:

- Danish-Indian collaboration programme entitled "Solid-state NMR methods and applications"
- Indo-French IFCPAR/CEFIPRA project entitled "Novel nanocatalysts synthesis guided by DNP NMR"

Mondal Jagannath:

- Jagannath Mondal, 'Mechanistic Investigation anti microbial peptides in action using large-scale computer simulations', Extreme Science and Engineering Discovery Environment (XSEDE), USA for Computational allocation (allocation provided in San diego Supercomputer), 1 year (July 2015-June 2016)
- Jagannath Mondal, Ramanujan research grant, DST/SERB, 5 years.

Mote Kaustubh R:

- Investigator: Kaustubh R. Mote Title: Structural and Mechanistic Characterization of the Mitochondrial Pyruvate Carrier Funding Agency: Department of Sciences and Technology, India (INSPIRE Faculty Award) Duration: 2015-2020

Narayanan T.N:

- DST-Fast Track Young Scientist Research Grant - (2014-2017) Topic: "2-dimensional nanosheets based ultra-low density sponges for energy and environmental applications".

Raman Karthik V:

- Ramanujan Fellowship SERB, DST 2013-18
- MPI-DST Mobility grant 2015-18

Ramaswamy Sriram:

- J C Bose Fellowship, DST, 2007-present (renewed 2012)

Surajit Sengupta:

- Surajit Sengupta and EU collaboration, DIONICOS: Dynamics of and in Complex Systems, European Commission, Feb 2014 to Feb 2017.

12. Publications

a) In Journals:

Agarwal Vipin:

- Susanne Penzel, Albert Smith, Vipin Agarwal, Andreas Hunkler, Ago Samoson, Anja Böckmann, Matthias Ernst, and Beat H. Meier, Protein resonance assignment at MAS frequencies approaching 100 kHz: A quantitative comparison of J-coupling and dipolar-coupling-based transfer methods J. Biomol. NMR, 63, 165-186 (2015)
- Kshama Sharma, P.K. Madhu and Vipin Agarwal, Systematic evaluation of heteronuclear decoupling at rotary resonance conditions in the regime of fast MAS, J. Magn. Reson. 270, 136-141, (2016)

- Kong Ooi Tan, Vipin Agarwal, Beat H. Meier and Matthias Ernst, A Generalized Theoretical Framework for the Description of Spin Decoupling in Solid-State MAS NMR: Properties of Low-Power decoupling, J. Chem. Phys., 145 (2016)

- Kaustubh Mote, Vipin Agarwal and P.K. Madhu, Five Decades of Homonuclear Dipolar Decoupling in Solid-State NMR: Status and Outlook Prog. Nucl. Magn. Reson. Spect. 97, 1-39, (2016)

Barma Mustansir:

- R. Kapri, M. Bandyopadhyay and M. Barma, Order-parameter scaling in fluctuation-dominated phase ordering , Phys. Rev. E 93, 012117 (2016)

Chary K.V.R:

- Manish R Shukla, Basuthkar J Rao, Kandala V R Chary, Differential accumulation and mobilization of starch and lipid in *Chlamydomonas reinhardtii,* Himanshu Singh, *Algal Research*, 18, 33-44 (2016).

- Verma D, Bhattacharya, A and Chary, K V R. ^{1}H, ^{13}C and ^{15}N NMR assignments of a calcium-binding protein from *Entamoeba histolytica*. *Biomol. NMR Assign,* 10, 67-70, (2016)

- Rajanikanth V, Sharma AK, Rajyalakshmi M, Chandra K, Chary KV, Sharma Y, Liaison between Myristoylation and Cryptic EF-Hand Motif Confers Ca^{2+} Sensitivity to Neuronal Calcium Sensor-1. *Biochemistry*, 54(4), 1111-22, (2015).

- Narayan S, Kombrabail MH, Das S, Singh H, Chary K.VR, Rao BJ, Krishnamoorthy G., Site-specific fluorescence dynamics in an RNA 'thermometer' reveals the role of ribosome binding in its temperature-sensitive switch function. Nucleic Acids Res, 43(1), 493-503, (2015).

Jana Anukul:

- David Nieder, Cem B. Yildiz, Anukul Jana, Michael Zimmer, Volker Huch and David Scheschkewitz, Dimerization of a marginally stable disilenyl germylene to tricyclic systems: evidence for reversible NHC-coordination. Chem. Commun. 52, 2799–2802, (2016).
- Anukul Jana, Volker Huch, Henry S. Rzepa and David Scheschkewitz, A Molecular Complex with a Formally Neutral Iron Germanide Motif (Fe_2Ge_2). Organometallics, 34, 2130–2133, (2015).

Karmakar Smarajit:

- Chandana Mondal, Smarajit Karmakar, and Surajit Sengupta, Glass-Like Slow Dynamics in a Colloidal Solid with Multiple Ground States. The Journal of Physical Chemistry B, 119 (34), 10902 - 10910 (2015).

- Saurish Chakrabarty, Smarajit Karmakar, Chandan Dasgupta, Phase Diagram of Glass Forming Liquids with Randomly Pinned Particles. Scientific reports 5 (2015).

- Saurish Chakrabarty, Smarajit Karmakar, Chandan Dasgupta, Vanishing of configurational entropy may not imply an ideal glass transition in randomly pinned liquids. Proc. Natl. Acad. Sci. (USA), 112, E4819 - E4820 (2015).

- Bhanu Prasad Bhowmik, Rajsekhar Das and Smarajit Karmakar, Understanding Stokes-Einstein in Supercooled Liquids using Random Pinning. J. Stat. Mech. : Theory and Experiments 074003 (2016).

- Saurish Chakrabarty, Rajsekhar Das, Smarajit Karmakar, Chandan Dasgupta, Understanding the Dynamics of supercooled liquids with Random Pinning within the Random First Order Transition Theory. J. Chem. Phys. 145, 034507 (2016).

- Ricardo Gutierrez, Smarajit Karmakar, Yoav G. Pollack, Itamar Procaccia, The Static Lengthscale Characterizing the Glass Transition at Lower Temperatures. Euro. Phy. Lett. 111 (5), 56009, (2015).

- Karmakar Smarajit, Dasgupta Chandan, Sastry Srikanth, Length scales in glass forming liquids and related systems by Report on Progress in Physics. 79, 016601 (2015).

- Karmakar Smarajit, Dasgupta Chandan, Sastry Srikanth, Length scales in glass forming liquids and related systems. Report on Progress in Physics 79, 016601 (2016).

- Smarajit Karmakar, Chandan Dasgupta and Srikanth Sastry , Short-Time Beta Relaxation in Glass-Forming Liquids Is Cooperative in Nature. Phys. Rev. Lett., 116, 085701 (2016).

- Jeetu S Babu, Chandana Mondal, Surajit Sengupta, Smarajit Karmakar, Excess vibrational density of states and the brittle to ductile transition in crystalline and amorphous solids, Soft Matter 12, 1210-1218 (2016).

manuscripts under preparation:

karmakar Smarajit:

- Supercooled Liquids with Medium Range Crystalline Order, Indrajit Tah, Shiladitya Sengupta, Srikanth Sastry, Chandan Dasgupta and Smarajit Karmakar (2016).

- Dynamics dependence of four-point susceptibility for glass forming liquids in two and three dimensions - Saurish Chakrabarty, Smarajit Karmakar, and Chandan Dasgupta (2016).

- Block Analysis: A new method to extract dynamic heterogeneity length scale in experimental colloidal glasses - Saurish Chakrabarty, Smarajit Karmakar, and Chandan Dasgupta (2016).

- Understanding Cavitation in Amorphous solids - Kallol Paul, Ratul Dasgupta, Smarajit Karmakar (2016).

Krishnamurthy M:

- M. Kundu, Kartik Bane, Amit D. Lad, Prashant Kumar Singh, Gourab Chatterjee, G. Ravindra Kumar and Krishanu Ray, Anharmonic resonance driven hot electrons from femtosecond laser produced biological target plasma. M. Krishnamurthy, Opt. Exp. 23, 17909 (2015)

- R. Rajeev, Malay Dalui, T. Madhu Trivikram, K.P.M. Rishad, and M.Krishnamurthy, Anisotropic energetic negative ion emission from cluster nano-plasmas. Phys. Rev. A 91, 063403 (2015)

- Malay Dalui, W.-M. Wang, T. Madhu Trivikram, Subhrangshu Sarkar, Sheroy Tata, J. Jha, P. Ayyub, Z. M. Sheng and M. Krishnamurthy, Preferential enhancement of laser-driven carbon ion acceleration from optimized nanostructured surfaces, Sci. Rep. (2015)

- R. Rajeev, Madhu Trivikram, K.P.M. Rishad, V. Narayanan and M. Krishnamurthy, Anisotropic emission of high energy neutral atoms in a nano-plasma accelerator. New. J. Phys. 17 230033 (2015).

- Y. Mishima, H. Habara, P.K. Singh, A. Adak, G. Chatterjee, Amit D. Lad, P. Brijesh, Malay Dalui, M. Inoue, J.Jha, Sheroy Tata, T. Madhu Trivikram, M. Krishnamurthy, G. Ravindra Kumar and K. A. Tanaka, Efficient Production of Fast Electron Via Surface Plasmon Resonance Induced by Intense Laser Light.Rev. Laser Engg. 43 1 (2015).

Madhu P.K:

- A. Equbal, M. Leskes, N. C. Nielsen, P. K. Madhu, S. Vega, Relative merits of rCW^{A} and XiX heteronuclear spin decoupling in solid-state magic-angle-spinning NMR spectroscopy: A bimodal Floquet analysis. J. Magn. Reson. 263, 55-64, (2016).

- A. Equbal, M. Bjerring, K. Sharma, P. K. Madhu, N. C. Nielsen, Heteronuclear decoupling in MAS NMR in the intermediate to fast sample spinning regime. Chem. Phys. Lett. 633, 243-249, (2016).

- K. R. Mote, P. K. Madhu, High resolution proton-detected solid-state NMR spectroscopy of fully protonated proteins at slow to moderate magic-angle spinning frequencies. J. Magn. Reson. 262, 149-157, (2015).

- M. Chandrakeshan, D. Bhowmik, B. Sarkar, R. Abhyankar, H. Singh, P. K. Madhu, S. Maiti, V. S. Mithu, Steric crowding of the turn region alters the tertiary fold of amyloid-beta 18-35 and makes it solube, J. Biol. Chem. 290, 30099-30107, (2015).

- D. Bhowmik, K. R. Mote, C. M. MacLaughlin, N. Biswas, B. Chandra, J. K. Basu, G. C. Walker, P. K. Madhu, S. Maiti, Lipid-coated nanoparticles confer Raman enhancement to membrane proteins and reveal membrane-attached amyloid-beta conformation. ACS Nano, 9, 9070-9077, (2015).

- A. Equbal, M.Bjerring, P. K. Madhu, N. C. Nielsen, Improving spectral resolution in biological solid-state NMR using phase-alternated rCW heteronuclear decoupling. Chem. Phys. Lett. 635, 339-344, (2015).

- H. I. Dabora, E. Nimerovsky, P. K. Madhu, A. Goldbourt, Site-resolved backbone and side-chain intermediate dynamics in a carbohydrate-bidning module protein studied by magic-angle spinning. NMR, Chem. Eur. J. 21, 10778-10785, (2015) .

- A. Equbal, M. Bjerring, P. K. Madhu, N. C. Nielsen, A unified heteronuclear decoupling strategy for magic-angle spinning solid-state NMR spectroscopy, J. Chem. Phys. 142, 1842011-1842018, (2015).

- S. Stahlberg, B. Skolova, P. K. Madhu, A. Vogel, K. Vavrova, D. Huster, Probing the role of ceramide acyl chain length and sphingosine unsaturation in model skin barrier lipid mixtures by 2H solid-state NMR spectroscopy. Langmuir, 31, 4906-4915, (2015).

Mondal Jagannath:

- J. Mondal, P. Tiwary and B. J. Berne, How does kinase inhibitor withstand gatekeeper residue mutation, J. Am. Chem. Soc. 138, 4608 (2016) (As Corresponding author)

- S. Roy, D. Skoff, D. Perroni, J. Mondal, A. Yethiraj, M. K. Mahanthappa, M. T. Zanni and J. L. Skinner, Water Dynamics in Gyroid phases of self-assembled gemini surfactants J. Am. Chem. Soc.138, 2472 (2016)

- P. Tiwary, J. Mondal, J. A. Morrone and B. J. Berne, Role of water and steric constraints in the kinetics of cavity-ligand unbinding, Proc. Natl. Acad. Sci. USA 112,12015 (2015)

- J. Mondal, D. Halverson, I.T.S. Li, G. Stirnemann, G. C. Walker and B. J. Berne , How osmolytes inuence hydrophobic polymer conformations: A unified view from experiment and theory. Proc. Natl. Acad. Sci. USA 112, 9270 (2015)

Mote Kaustubh R:

- B. Singh, K.R. Mote, C.S. Gopinath, P.K. Madhu, V. Polshettiwar, SBA-15-oxynitrides as a solid-base catalyst: Effect of nitridation temperature on catalytic activity, Angew. Chem. Int. Ed. 54 5985–5989 (2015).

- K.R. Mote, P.K. Madhu, Proton-detected solid-state NMR spectroscopy of fully protonated proteins at slow to moderate magic-angle spinning frequencies, J. Magn. Reson. 261, 149–156 (2015).

- D. Bhowmik, K.R. Mote, C.M. MacLaughlin, N. Biswas, B. Chandra, J.K. Basu, et al., Cell-membrane-mimicking lipid-coated nanoparticles confer Raman enhancement to membrane proteins and reveal membrane-attached amyloid-β conformation, ACS Nano. 9, 9070–9077 (2015).

Narayanan T.N:

- P. M. Sudeep, S. Vinayasree, P. Mohanan, P. M. Ajayan, T. N. Narayanan, and M. R. Anantharaman, Fluorinated Graphene Oxide for Enhanced S and X-band Microwave Absorption, Applied Physics Letters106, 221603 (2015).

- S. Kundu, R. M. Yadav, T. N. Narayanan, M. V. Shelke, R. Vajtai, P. M. Ajayan and V. K. Pillai, Synthesis of N, F and S Co-doped graphene quantum dots, Nanoscale, 7, 11515-11519 (2015).

- Pratik Shah, T. N. Narayanan, Chen-Zhong Li, Subbiah Alwarappan, Probing the biocompatibility of MoS_2nanosheets by cytotoxicity assay and electrical impedance spectroscopy, Nanotechnology, 26, 315102 (2015).

- M.J. Jaison, T. N. Narayanan, T. Prem Kumar, and Vijaymohanan K. Pillai, A Single step room temperature electrochemical synthesis of nitrogen doped graphene nanoribbons from carbon nanotubes, J. Materials Chemistry A, 3, 18222-18228 (2015).

- Sumana Kundu, Sujoy Ghosh, Michael Fralaide, T. N. Narayanan, Vijayamohanan K. Pillaiand Saikat Talapatra, Fractional Photo-current Dependence of Graphene Quantum Dots Chemically Unzipped from Carbon Nanotubes, Physical Chemistry Chemical Physics 17, 24566-24569 (2015).

- T. N. Narayanan, Kathryn D. Fink, Jacobo Paredes,P. M. Ajayan, Slawomir Filipek, Przemyslaw Miszta, M. Gurusaran, H. CumhurTekin, FatihInci, Utkan Demirci, Pingzuo Li, Kirill I. Bolotin, Dorian Liepmann, and V. Renugopalakrishanan, Graphene-

Protein Field Effect Biosensors: Glucose Sensing, Sowmya Viswanathan, Materials Today, 18 (9), 513-522 (2015).

- P. M.Sudeep, S. Vinod, S. Ozden, R. Sruthi, ÁkosKukovecz, ZoltánKónya, Robert Vajtai, M. R.Anantharaman, P. M. Ajayan, and T. N. Narayanan*, Functionalized boron nitride porous solids, RSC Advances 5, 93964-93968 (2015).

- B M Krishna Mariserla , M K L Man , S Vinod , C Chin , T Harada , Jaime Taha-Tijerina , C Tiwary , P Nguyen , P Chang , T N Narayanan , A Rubio , P M Ajayan , S Talapatra, and K Dani, Engineering photophenomena in large, 3D structures composed of self-assembled van der Waals heterostructure flakes, Advanced Optical Materials 3, 1551-1556 (2015).

- T.V. Vineesh, M. Azeezulla, S. Krishnamoorthy, T. N. Narayanan* and S. Alwarappan, Synergistic Effects of Dopants on the Spin Density of Catalytic Active Centers of N-doped Fluorinated Graphene for Oxygen Reduction Reaction, Applied Materials Today 1(2), 74-79 (2015).

- Beena Mol, Lija Joy, Hysen Thomas, Vinoy Thomas, Cyriac Joseph, T. N. Narayanan, Salim Al-Harthi, N. Unnikrishnan, M. R. Anantharaman, Evidence for enhanced optical properties through plasmon resonance energy transfer in silver silica nanocomposites, Nanotechnology 27, 085701 (10pp) (2016).

- Kiran Kumar Tadi, T. N. Narayanan*, Sivaram Arepalli, Kaustav Banerjee, Sowmya Viswanathan, P. M. Ajayan, and V. Renugopalakrishnan, Engineered 2D Nanomaterials-Protein Interfaces for Efficient Sensors, Journal of Materials Research, 30 (23) 3565-3574 (2015).

- T. V. Vineesh, M. Praveen Kumar, C. Takahashi, G. Kalita, S. Alwarappan, Deepak K. Pattanayak, T. N. Narayanan*, Bifunctionalelectrocatalytic activities of boron doped graphene derived from boron carbide, Advanced Energy Materials, 5(17), 1500658 (1-8) (2015).

- Kiran K. Tadi, Shubhadeep Pal, T. N. Narayanan,* Fluorographene based Ultrasensitive Ammonia Sensor, Scientific Reports6, 25221 DOI: 10.1038/srep25221 (2016).

Perlekar Prasad:

- M. De Pietro, M.A.T. van Hinsberg, L. Biferale, H.J.H. Clercx, P. Perlekar, and F. Toschi, Clustering of vertically constrained passive particles in homogeneous, isotropic turbulence, Phys. Rev. E, 91, 053002 (2015).

- D. Vincenzi, P. Perlekar, L. Biferale, and F. Toschi, Impact of the Peterlin approximation on polymer dynamics in turbulent flows. Phys. Rev. E, 92, 053004 (2015).

- C.M. Lee, A. Glyfason, P. Perlekar, and F. Toschi, Inertial particle acceleration in strained turbulence, J. Fluid Mech., 785, 31 (2015).

Raman Karthik V:

- "Materials chemistry: A magnetic facelift for non-magnetic metals," Karthik V. Raman*, Jagadeesh S. Moodera. Nature, 524, 42, 2015

Ramaswamy Sriram:

- A Cavagna, I Giardina, T S Grigera, A Jelic, D Levine, S Ramaswamy, and M Viale Silent Flocks: Constraints on Signal Propagation Across Biological Groups Phys Rev Lett *114*, 218101 (2015)

Sengupta Surajit:

- Tamoghna Das, Saswati Ganguly, Surajit Sengupta and Madan Rao, Pre-Yield Non-Affine Fluctuations and A Hidden Critical Point in Strained Crystals, Scientific Reports (Nature Publishing Group), 5, 10644, (2015).

- Saswati Ganguly, Surajit Sengupta, Peter Sollich, Statistics of non-affine defect precursors: tailoring defect densities in colloidal crystals using external fields, Soft Matter, 11, 4517 (2015).

- Amartya Mitra, Saswati Ganguly, Surajit Sengupta, Peter Sollich, Non-affine fluctuations and the statistics of defect precursors in the planar honeycomb lattice, J. Stat. Mech. P06025 (2015)

- Anirban Pal, Smita Gohil, Surajit Sengupta, H. K. Poswal, Surinder M Sharma, Shankar Ghosh and Pushan Ayyub, Structural phase transitions in trigonal Selenium induce the formation of a

disordered phase, J. Phys.: Condens. Matter, 27, 415404 (2015)

- Jeetu S Babu, Chandana Mondal, Surajit Sengupta and Smarajit Karmakar, Excess Vibrational Density of States and the Brittle to Ductile Transition in Crystalline and Amorphous Solids, Soft Matter, 12, 1210 (2016).

Vallurupalli Pramodh:

- Vallurupalli, P*; Chakrabarti, N; Pomes, R and Kay, Atomistic picture of conformational exchange in a T4 lysozyme cavity mutant: an experimentguided molecular dynamics study. *CHEMICAL SCIENCE*, 7(6), 3602-3613, (2016). Published online Jan 7 2016 *Corresponding Author

b) In Proceedings [Authors, Title, Title of Proceedings, Volume, Page, Year]

c) Web Publications

d) In Books

***Anukul Jana**, and Herbert W. Roesky*, Chapter 14: "Silicon(II) as a Synthon for the access of different Silicon(IV) and Silicon(II) Compounds" in "Efficient Methods for Preparing Silicon Compounds" *Elsevier*, 2016, ISBN: 9780128035306, 183–204.

e) Books/Book Reviews

f) Technical Reports/Internal Reports

13. Lectures / Lecture Courses Given Elsewhere

Agarwal Vipin:

- Nuclear Magnetic resonance: Introduction and perspective, Visiting Students of Birla Institute of Technology, March 2016.

Barma Mustansir: "Fluctuations and Order", Fourth S. S. Bhatnagar Anniversary Lecture, Panjab University, Chandigarh (2016).

Chary K.V.R:

- Invited talk on, "Structure and Dynamics of Intrinsically Ordered and Disordered Proteins by NMR", at State Key Laboratory of Bio-organic and Natural Product Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Science on Friday, May 8, 2015
- Invited talk on, "Echoes in NMR", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 23, 2015.
- Invited talk on, "NMR of Nucleic Acids", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 25, 2015.
- Invited talk on, "Evolution through Structure", at National Workshop on "NMR in Biological Systems", held at SGPGIMS, Lucknow, on June 25, 2015.
- Invited talk on, "NMR of Biological Systems: From Molecules to Human", at the Workshop on "Application of Bioinformatics in Drug Designing", Saturday, held in Kottayam, August 1, 2015.
- Invited talk on, "Structure and Dynamics of Intrinsically Ordered and Disordered Proteins by NMR", at University of Wisconsin, on August 4, 2015.
- Invited talk on, "Conformational Propensities and Dynamics of a βγ-crystallin, an Intrinsically Disordered Protein", at Structural Biology Initiative CUNY Advanced Science Research Center (ASRC) Monday, August 10, 2015.
- Invited talk on, "Flagella "A Biological product" as a Novel Alignment Medium for the Measurement of Residual Dipolar Couplings in Proteins", National Institutes of Health, National Heart, Lung, and Blood Institute, Bethesda, Maryland, USA, on August 17, 2015.
- Invited talk on, "Novel Methods in NMR and βγ-crystallins: Intrinsic Order & Disorder", at Nano Cell, University of Linz, Austria, Monday, November 23, 2015.

Garai Kanchan:

- Teaching Biophysics in the 2nd semester 2016 at TCIS jointly with Dr. Pramodh Vallurupalli

Krishnamurthy M:

- Two lectures given at the 7th Asian Summer School and Symposium on Laser-Plasma Acceleration and Radiation, Shanghai 2016.
- Lectures in SERB school on Lasers and Nonlinear optics, Pondicherry, April 2016.
- Three lectures in: "Special lectures series in Physics; focus: Laser atom interaction", University of Mysore, Mysore 2016

Madhu P.K:

- Structural insights into Aβ oligomers, University of Leipzig, Germany, July 2, 2015.
- Heteronuclear spin decoupling in solid-state NMR, ENS, Lyon, France, October 27, 2015.

Mondal Jagannath:

- Lecture on "Introduction to Chemistry" as a part of the science course conducted at Tata Institute of Social Sciences.

Sengupta Surajit:

- Okinawa Institute of Science and Technology, April 27, 2015 Tailoring defect densities in crystals using light fields: Amorphization and plastic flow of a solid in a non-affine field

- Institute of Industrial Science, University of Tokyo, May 8th, 2015 Tailoring defect densities in crystals using light fields: Amorphization and plastic flow of a solid in a non-affine field

14. Lectures by Visitors

Agarwal Vipin:

- Sylvia Britoo, University of Cambridge, U.K. (De)lithiation Mechanism of Vanadium Sulfide, a Promising Conversion Electrode Material for Rechargeable Lithium Ion Batteries, 22nd December , 2015.

- Yusuke Nishiyama, RIKEN CLST-JEOL Collaboration center, Japan. Proton detection at fast magic angle spinning (60-120 kHz MAS), 13th July, 2015

Chary K.V.R:

- Invited talk by Professor J B Joshi (Adjunct Professor; Emeritus Professor, HBNI, Mumbai.

Madhu P.K:

- Chandrasekhar Ramanathan, Univ. of Dartmouth, USA, Many body systems in solid-state NMR, May 29, 2015.

Mazumder Aprotim:

- Jyotsna Dhawan, CCMB Hyderabad
- Satyajit Mayor, NCBS - TIFR, Bangalore
- Maithreyi Narasimha, TIFR, Mumbai

Narayanan T N:

- Nikhil Koratkar (RPI, Troy, NY, USA) Colloquium
- Pulickel M. Ajayan (Rice University, Houston, USA) - Sawaal-Jawaab and Colloquium.

Vallurupalli Pramodh:

- Organized (with Roopa Prasad) the seminar program at TCIS/TIFRH.

15. Graduate Courses

Agarwal Vipin:

- Solid-State Nuclear Magnetic Resonance, January-May, 2016, TCIS, TIFR, Hyderabad.

Barma Mustansir:

- Phase Transitions, Ordering and Dynamics (taught by M. Barma and S. Ramaswamy)

Chary K.V.R:

- Course on “NMR in Biological Systems” (Jan – May, 2015)

Jana Anukul:

Advanced Inorganic and Organic Chemistry, for the Chemistry PhD and IPhD students, August-December 2015

Karmakar Smarajit:

- Aug - Nov 2015 : Advanced Statistical Mechanics
- Jan - April 2016 : Numerical Methods (together with Dr. P. Perlekar)

Madhu P.K:

- Nuclear Magnetic Resonance, January-May, 2016, TIFR, Mumbai.
- Solid-State Nuclear Magnetic Resonance, January-May, 2016, TCIS, TIFR, Hyderabad.

Mazumder Aprotim:

- Basic Cell Biology (August - December, 2015)

Mondal Jagannath:

- Statistical Mechanics I (August 2015 to November 2015)

T. N. Narayanan:

- Physics & Chemistry of Materials: Bulk to Nano (Jan. 2016- May 2016)
- Experiments Methods and Advanced Experimental Methods (Aug.2015-Nov.2015 & Jan. 2016-May 2016)

Perlekar Prasad:

- Classical Mechanics and Advanced Computational Physics.

Raman Karthik V:

- Taught a graduate level course on Physics & Chemistry of Materials: Bulk to Nano

Sengupta Surajit:

- Electromagnetic Theory - I

Vallurupalli Pramodh:

- Topics in biophysics (Taught with Kanchan Garai)

16. Ph.D. Theses / M.Sc. Theses

Agarwal Vipin:

- Arpita Sundaria (M. Tech): completed her final year M. Tech. thesis in the lab. She was a final year M. Tech. (Biotechnology) student from the University of Rajasthan, Jaipur and was awarded the M. Tech degree in May 2016. The title of her thesis was " Over expression and purification of protein for solid-state NMR studies. "

Sengupta Surajit:

- Chandana Mondal. topic: "Equilibrium and Rheological Properties of Model Network Formers". (degree obtained from the University of Calcutta)

- Nirmalendu Ganai, topic: "Studies of Ordering in Equilibrium and Non-equilibrium Systems" (degree obtained from the University of Calcutta)

17. Popular Science Articles / Lectures

18. Radio & TV Programmes

NONE

19. Any other information:

Agarwal Vipin:

- NMR Meets Biology, Kerala, India, January 14-19, 2016

Jana Anukul:

- Member of the Chemistry Subject Board of TIFR Mumbai**.**

- Member of infrastructure and services (space, electricity, AC, furniture, telecom, lab safety, security, maintenance) committee of the Narsingi campus of TCIS Hyderabad.

- Member of seminars and colloquia committee of TCIS Hyderabad.

Madhu P.K:

- EUROMAR, Prague, Czech Republic, July 5-10, 2015
- Emerging NMR Methods, IISc, Bangalore, July 16-17, 2015

- 1st Western Region Structural Biology Meet, IIT Bombay, Mumbai, India, August 1, 2015

- ISMAR, Shanghai, China, August 16-21, 2015

- Indo-German Workshop on Molecular Amplification, Tutzing, Munich, Germany, October 20-23, 2015

- NMR Meets Biology, Kerala, India, January 14-19, 2016

Mondal Jagannath:

- Reviewed manuscripts for Journal of Physical Chemistry, Journal of Chemical Physics, Journal of Molecular Liquids.