

TIFR Centre for Interdisciplinary Sciences

NMR Spectroscopy

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 investigated the unification of a large number of schemes under high magic-angle spinning (MAS) and radiofrequency amplitude conditions. This has enabled us to place all the schemes in vogue under a general framework. Currently the focus is to investigate design of schemes in this regime under the unified perspective to take into account offset effect, a major impediment in low radiofrequency amplitude regime. [P. K. Madhu, Kshama Sharma, Asif Equbal]

Theoretical analysis of offset effects in solid-state NMR pulse schemes

Multi-mode Floquet theory has been used to obtain a comprehensive understanding of the effects of offset in radiofrequency irradiation for a generic recoupling scheme. The offset influence could be ascribed to a change in the spin-interaction resonance conditions which may have a bearing on the recoupling efficiency. This may be used in a constructive way to improve the efficiency by avoiding or manipulating such resonance conditions. Such effects are expected to show up in decoupling experiments as well. [P. K. Madhu, Anders Nielsen, Ravi Shankar (Univ. of Aarhus, Denmark)]

Recoupling pulse schemes and strategies

The standard rotational-echo double resonance (REDOR) experiment used in solid-state NMR has proven to be one of the most useful and robust schemes in distance measurements. We have proposed a variant to this employing non-linearly placed pulses, based on Uhrig's dynamic decoupling, denoted as UDD pulse scheme. UDD pulses give a quantitative scaling factor and performs as good as conventional REDOR. Both of these were compared with another existing variant, namely, shifted-REDOR scheme. Our analysis clearly points out the experimental problems with shifted-REDOR none of which are present with the conventional REDOR and UDD scheme. [P. K. Madhu, Mukul Jain, G.Rajalakshmi, Kaustubh Mote, Asif Equbal, Vipin Agarwal]

Recoupling pulse schemes in an asynchronous nature of implementation

We have in detail explored another subtle feature of recoupling schemes designed on the basis of the symmetry of internal spin interactions. These schemes rely on a proper synchronization of the MAS frequency and radiofrequency irradiation. However, our experiments and theoretical analysis (based on multimode Floquet theory) points to a substantial efficiency enhancement upon a small mis-adjustment in the synchronous condition. This is primarily due to the effect of offset terms and higher-order terms in the Hamiltonian analysis that are normally difficult to analyse with the average Hamiltonian theory, a prime theoretical tool in the design of symmetry schemes. We have demonstrated applications of this approach on a couple of recoupling schemes and the results agree with theory and simulations. [P. K. Madhu, Matthias Ernst (ETH, Zurich), Kshama Sharma]

Towards spin exchange optical pumping of Xe

Production and characterisation of hyperpolarized ^{129}Xe gases by optical method is a multi-step process electron spin polarisation in Rb using optical pumping method, transfer of electron polarisation from Rb to Xe nucleus through spin exchange interactions and subsequent NMR detection of the nuclear spin of the hyperpolarised Xe gas. We have tested the spin exchange optical pumping (SEOP) in a sealed Rb-Xe cell and are in the process of setting up a Xe gas flow SEOP system. The development of electronics for detection of low-field NMR signal from Xe is also underway. A Rb vapour magnetometer based on nonlinear magneto-optical rotation was developed to measure external magnetic fields in the range of 0.1-1 microTesla. This method can be used to detect NMR signals optically at low to zero field. [P. K. Madhu, G. Rajalakshmi, Naresh Kumar, Vineeth Francis, Shashank Yadav]

Heteronuclear spin decoupling in solid-state NMR

In solid-state NMR, the quality of the heteronuclear decoupling critically determines the achievable resolution and sensitivity of a NMR spectrum. This is also critical for distance measurements in experiments, such as REDOR, where coherence lifetime technically decides the range of distances that can be experimentally measured. Last year, two particular

aspects of heteronuclear decoupling were shown. One, development of a theoretical model to analyze the performance and offset behaviour of any decoupling sequence. Two, the number of literature reports discussing decoupling at rotary resonance recoupling conditions could be avoided by carefully choosing decoupling conditions. [Vipin Agarwal Kshama Sharma, P.K. Madhu]

Parameter independent low-power decoupling for fast magic-angle spinning in solid-state

We tailored the rCW_{ApA} decoupling sequence in the regime of low-power radio-frequency irradiation and fast magic-angle spinning. The robustness of the refocused continuous-wave (rCW) schemes to experimental parameters such as pulse lengths and offset irradiation were demonstrated. Numerical simulations and analytical theory were used to understand the effects of various nuclear spin interactions on the decoupling performance of the low-power rCW decoupling scheme relative to other state of the art decoupling methods. This has led to the design of an 'optimum low-power decoupling sequence' that can be used without parameter optimization. This result is particularly important in the context of samples with low signal to noise. [P.K. Madhu, Vipin Agarwal, Asif Equbal, Beat H. Meier (ETH, Zurich), Matthias Ernst (ETH, Zurich), N. C. Nielsen (Univ. of Aarhus, Denmark)]

Different strategies to improve heteronuclear decoupling

The strategy of using π pulses to refocus CW fields has led to robust and efficient rCW family of heteronuclear decoupling sequences. We used π pulses to refocus residual interactions in the XiX decoupling scheme. The refocused XiX or rXiX has refocusing π pulses along 135° axes in a super-cycledXiX scheme. The π pulses create a half-wave symmetry in the interaction frame Hamiltonian and thereby eliminate the influence of J-coupling and minimize the effect of strong homonuclear induced second-order residual couplings. The r-XiX scheme has been tested in the fast magic-angle spinning and low-amplitude radio-frequency (RF) irradiation regime. The rXiX scheme shows improved decoupling efficiency, better-offset tolerance, and easier decoupling setup compared to XiX. [Vipin Agarwal, Mukul Jain, Asif Equbal, K. Sreedevi, P. K. Madhu]

Qualitative 1H - 1H distance in fully protonated proteins

In the fast MAS regime, the second-order recoupling sequences typically used to determine structures of protein in solids do not work. In this project we are developing methods to measure quantitative and qualitative 1H - 1H distances. Such distance restraints would form the basis of calculating protein structure in

fully protonated samples at fast MAS frequencies. We have developed a new experimental method to obtain long-range selective (e.g H^N - H^N) contacts on the order of 5-6 Å despite the presence of other protons at shorter distances in fully protonated proteins. The novel method is dubbed as "Band-Selective Spectral Spin Diffusion" (BASS-SD). These long-range distance restraints are critical to access tertiary structures of protein but are difficult to observe in a dense proton matrix. The selective 1H-1H contacts obtained with BASS-SD alleviate the need for perdeuterated protein with protonation at selective sites. Numerical simulations and experiments show BASS-SD to outperform the currently used experiments in terms of sensitivity and the number of observed long-range contacts. The method has been demonstrated on GB1 and the β -barrel membrane protein AlkL. We are currently probing way to use them to calculate protein structures using this method. [Vipin Agarwal, Mukul Jain, Chandrakala Gowda, Guido Pintacuda (CNRS, Lyon, France)]

Accelerating proton spin diffusion in perdeuterated proteins at 100 kHz MAS

Fast magic-angle spinning (>60 kHz) has many advantages but makes spin-diffusion-type proton-proton long-range polarization transfer inefficient and highly dependent on chemical-shift offset. Using 100%- H^N - $[^2H, ^{13}C, ^{15}N]$ -ubiquitin as a model substance, we quantified the influence of the chemical-shift difference on the spin diffusion between proton spins and compared two experiments which lead to an improved chemical-shift compensation of the transfer: rotating-frame spin diffusion and a new experiment, reverse amplitude-modulated MIRROR. Both approaches enable broadband spin diffusion, but the application of the first variant is limited due to fast spin relaxation in the rotating frame. The reverse MIRROR experiment, in contrast, is a promising candidate for the determination of structurally relevant distance restraints. The applied tailored rf-irradiation schemes allow full control over the range of recoupled chemical shifts and efficiently drive spin diffusion. The longer longitudinal relaxation time leads to a higher signal-to-noise ratio in the spectra acquired with reverse MIRROR. [Vipin Agarwal]

Folding of multidomain proteins

Newly developed NMR relaxation dispersion experiments have been used to study the folding of FF and SH3 domains. Folding intermediates were identified and their structures were obtained by these methods. We have now established conditions to study the folding of T4L using CEST type NMR experiments. Folding proceeds via an intermediate where the structure of the N terminus is affected but is not disordered. The structure of this intermediate

populated to 2% will be determined to understand the folding of this protein. [Pramodh Vallurupalli]

Single, double and triple quantum experiments to study faster process

New double and triple quantum ^1H experiment have been developed to study fast dynamics at methyl sites in proteins. Peak positions of residues undergoing exchange shift between the Single, Double and Triple quantum experiments providing information regarding fast (50 microsecond) process. [Pramodh Vallurupalli]

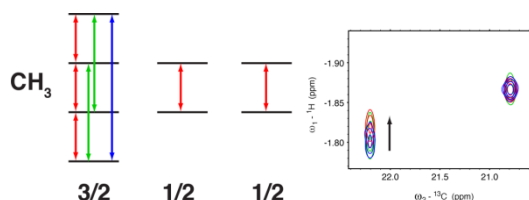


Figure 1: The angular momentum of three equivalent protons in methyl groups can be added to give a spin $3/2$ manifold and two spin $1/2$ manifolds. In the spin $3/2$ manifold we can excite double (green) and triple (blue) transitions in addition to the conventional single quantum transitions. In sites of the molecule undergoing chemical exchange the peaks arising from the three different transitions will not overlap with SQ peak shifted towards the minor state.

Towards tailoring plant protease inhibitors for control of the crop pest *Helicoverpa armigera*

We continued our efforts in the development of 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. Plasmids

Laser Spectroscopy

A group working on high intense laser spectroscopy has designed and developed a delivery mechanism for microparticles into an effusive jet in vacuum for laser plasma studies, and developed a device for generating ultrashort femtosecond electron pulses from nanotips. [M. Krishnamurthy]

Soft Matter

Glass susceptibility: Growth kinetics and saturation under shear

The mode-coupling theory, despite its limitations, offers analytical predictions about the growth of relaxation times in a liquid approaching structural arrest. The glass transition within this approximation is a self-consistently generated nonzero infinite-time limit of the temporal density autocorrelator. When control parameters are such that the "equilibrium" state of the system is a glass, and the system is allowed to evolve towards such a state from a fluid-state initial condition, the peak value of the three-point correlator that plays the role of glass susceptibility undergoes a steady

growth towards its final value. Earlier we had calculated this coarsening of glassiness. Here we show how the growth is cut off and the relaxation time rendered finite when a background shear flow is imposed. We obtain reliable analytical predictions for the growth, the cutoff time, and the steady-state time of the sheared liquid. We find the relaxation time of the sheared fluid scales as $(\text{shear-rate})^{-0.8}$. [Sriram Ramaswamy]

containing IRD7 and IRD12 genes were transformed into independent *E. coli* strains BL21 (λ DE3) for recombinant production of the PIs used in our NMR studies. Sequence-specific resonance assignments of IRD7 and IRD12 are achieved using a suite of 3D experiments. Chemical shift values of CA and CB of Cys residues indicated that all the eight Cys residues are in oxidized state forming stable disulphide bridges. 2D TOCSY and NOESY spectra were used to identify all the disulphide bond connectivities in IRD7 and IRD12. Heteronuclear spin relaxation data was used to study the overall and internal dynamics of IRD7 and IRD12. The calculated structure of IRD12 using CYANA clearly indicates the presence of three β strands in the region 14-18, 23-27 and 46-49, which are anti-parallel to one another. Further structure refinement is in progress. Structure calculation of IRD7 is also in progress. (This project is being undertaken under DST-DIISRTE joint research project (Australia-India Strategic Research Fund (AISRF))). [K.V.R. Chary, Janeka Gartia, Glenn King, (The Queen'sland University, Brisbane, Australia), Ashok Giri (NCL Pune)]

Fluid Dynamics

It is known that multiphase flows are ubiquitous in nature. The fluid dynamics group at TCIS is currently investigating a variety of multiphase flow phenomena varying from flow in bacterial suspensions to turbulent emulsions. [Prasad Perlekar]

growth towards its final value. Earlier we had calculated this coarsening of glassiness. Here we show how the growth is cut off and the relaxation time rendered finite when a background shear flow is imposed. We obtain reliable analytical predictions for the growth, the cutoff time, and the steady-state time of the sheared liquid. We find the relaxation time of the sheared fluid scales as $(\text{shear-rate})^{-0.8}$. [Sriram Ramaswamy]

Understanding the dynamics of glass-forming liquids with random pinning within the random first order transition theory

Extensive computer simulations were performed for a few model glass-forming liquids in both two and three dimensions to study their dynamics when a randomly chosen fraction of particles are frozen in their equilibrium positions. For all the studied systems, we find that the temperature-dependence of the α relaxation time extracted from an overlap function related to the self-part of the density autocorrelation function can be explained within the framework of the Random First

Order Transition (RFOT) theory of the glass transition. We propose a scaling description to rationalize the simulation results and show that our data for the α relaxation time for all temperatures and pin concentrations are consistent with this description. We find that the fragility parameter obtained from fits of the temperature dependence of the α relaxation time to the Vogel-Fulcher-Tammann form decreases by almost an order of magnitude as the pin concentration is increased from zero. Our scaling description relates the fragility parameter to the static length scale of RFOT and thus provides a physical understanding of fragility within the framework of the RFOT theory. Implications of these findings for the values of the exponents appearing in the RFOT theory are discussed. [Saurish Chakrabarty, Rajsekhar Das, Smarajit Karmakar, Chandan Dasgupta (IISc Bangalore)]

Pinning susceptibility: A novel method to study growth of amorphous order in glass-forming liquids

Existence and growth of amorphous order in supercooled liquids approaching glass transition is a subject of intense research. Even after decades of research, there is still no clear consensus on the molecular mechanisms that lead to a rapid slowing down of liquid dynamics approaching this putative transition. The existence of a correlation length associated with amorphous order has recently been postulated and this has been estimated using multi-point correlation functions, which cannot be calculated easily in experiments. Thus the study of growing amorphous order remains mostly restricted to systems like colloidal glasses and simulations of model glass-forming liquids. In this study, we propose an experimentally realizable yet simple correlation function to study the growth of amorphous order. We then demonstrate the validity of this approach for a few well-studied model supercooled liquids and obtain results, which are consistent with other conventional methods. [Rajsekhar Das, Saurish Chakrabarty, Smarajit Karmakar]

Equilibrium and dynamic pleating of a crystalline bonded network

We describe a phase transition that gives rise to structurally non-trivial states in a two-dimensional ordered network of particles connected by harmonic bonds. Monte Carlo simulations reveal that the network supports, apart from the homogeneous phase, a number of heterogeneous “pleated” phases, which can be stabilized by an external field. This field is conjugate to a global collective variable quantifying “non-affineness,” i.e., the deviation of local particle displacements from local affine deformation. In the pleated phase, stress is localized in ordered rows of pleats and eliminated from the rest of the lattice.

The kinetics of the phase transition is unobservably slow in molecular dynamics simulation near coexistence, due to very large free energy barriers. When the external field is increased further to lower these barriers, the network exhibits rich dynamic behaviour: it transforms into a metastable phase with the stress now localized in a disordered arrangement of pleats. The pattern of pleats shows ageing dynamics and slow relaxation to equilibrium. Our predictions may be checked by experiments on tethered colloidal solids in dynamic laser traps. [Saswati Ganguly, Parswa Nath, Jurgen Horbach (Universität Düsseldorf, Germany), Peter Sollich (King’s College, London, United Kingdom), Smarajit Karmakar, and Surajit Sengupta]

Glass transition in supercooled liquids with medium range crystalline order

The origins of rapid dynamical slowdown in glass forming liquids in the growth of static length scales, possibly associated with identifiable structural ordering, is a much-debated issue. Growth of medium range crystalline order (MRCO) has been observed in various model systems to be associated with glassy behaviour. Such observations raise the question about the eventual state reached by a glass former, if allowed to relax for sufficiently long times. Is a slowly growing crystalline order responsible for slow dynamics? Are the molecular mechanisms for glass transition in liquids with and without medium range crystalline order the same? If yes, glass formers with MRCO provide a paradigm for understanding glassy behaviour generically. If not, systems with MRCO form a new class of glass forming materials whose molecular mechanism for slow dynamics may be easier to understand in terms of growing crystalline order, and should be approached in that manner, even while they will not provide generic insights. In this study we perform extensive molecular dynamics simulations of a number of glass forming liquids in two dimensions and show that the static and dynamics of glasses with MRCO are different from other glass forming liquids with no predominant local order. We also resolve an important issue regarding the so-called Point-to-set method for determining static length scales, and demonstrate it to be a robust, order agnostic, method for determining static correlation lengths in glass formers. [Smarajit Karmakar]

This research group has also studied the ways in which a flat membrane can be made to pleat into a compact form by inducing a first order phase transition: the sort of transition that we see when water freezes. There are many possible applications of this work, including folding soft membranes for use as catalyst etc. This work was also highlighted in the media. [Surajit Sengupta, Smarajit Karmakar]

Material Sciences

The interest of Material Sciences research group lies in the development of functional mesoscopic interfaces, and probing the novel and unprecedented phenomena emanating from these junctions. The mesoscopic structures and their membranes developed are studied for their applications in various energy technologies. [T. N. Narayanan]

Electro-catalysis - Development of new catalysts for full cells

Cost effective methods for carbon neutral/negative renewable fuels are receiving tremendous attention in recent research. Hydrogen is identified as one of the best carbon-negative renewable futuristic energy sources, and water electrolysis (electrochemical water splitting) is identified as the best method to produce H_2 without the emission of greenhouse gases. Electrocatalysis is of having paramount interest in many modern energy technologies, particularly hydrogen production via water splitting. The success of graphene research surged the development of metals free graphene based catalysts, and recently graphene based multifunctional catalysts have been developed in our laboratory at TCIS. During the last one year, various catalysts based on atomic layers of graphene and metal dichalcogenides are developed for both hydrogen production and oxygen evolution. Development of water electrolysis full cells having their operation potential close to thermodynamic potential (1.23 V) is also demonstrated, without the aid of any benchmarked catalysts.

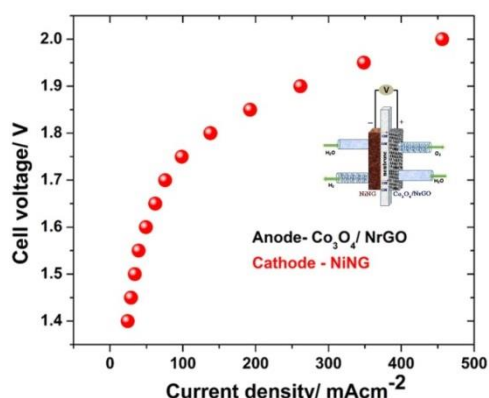


Figure 2. Performance of an alkaline water electrolysis cell developed at the laboratory without benchmarked catalysts.

Solid state ion transport membranes

Recent security threats in conventional liquid electrolytes based Li-ion batteries invoke the search for high ionic conductivity solid electrolytes (SEs) for solid

state batteries. We recently started to look in to the development of multifunctional polymer SEs (ionic conductivity $\sim 0.03 \text{ mS cm}^{-1}$) having exotic properties such as high Li-ion transport number (~ 0.69) with large electrochemical window (2-5 V), high mechanical robustness and flexibility (Young's modulus $\sim 1 \text{ MPa}$), visible light transparency ($\sim 85\%$), and hydrophobicity (contact angle $>100^\circ$).

In one such example, poly(ethylene oxide) (PEO) and poly(dimethyl siloxane) (PDMS) based polymer complex is studied as a Li-ion transport membrane, and lithium perchlorate (LiClO_4) as the Li source. It is found that a 'salting in' phenomenon induced by the ClO_4^- -PEO interactions modifies the crystalline melting temperature of PEO leading

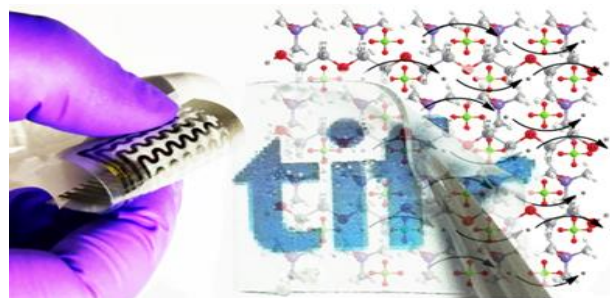


Figure 3: Showing a high Li ion conductivity transparent flexible solid electrolyte developed at TCIS for solid state devices. A symmetric parallel plate capacitor developed using this membrane is also shown.

to the amorphization of the PEO-PDMS matrix and hence in to a high Li-ion conductivity by microstructure modifications. This transparent flexible SE is shown for its applicability in flexible symmetric capacitors and Li-ion cells without the use of liquid electrolyte interfaces. Now, this study is extending to other important ions' transport studies too and correlation of structural, mechanical and transport properties of membranes is also intensely pursuing.

Atomic layers synthesis and transport properties

Development of defect free crystals is important to study the physico-chemical properties of ultra-thin atomic layers such as graphene and metal dichalcogenides. Chemical vapor deposition and shear assisted exfoliation of atomic layers from bulk crystals are identified as methods to get defect free large area/amount of atomic layers. In this aspect, we focus on both the methods to develop graphene, fluorographene, and metal dischalcogenides such as MoS_2 . Recently we have developed novel transfer techniques too to develop devices out of these grown

individual atomic layers. In one such study, we have developed MoS₂/graphene van der Waals solids having different stacking sequences and studied the role of stacking sequence in photo-electrocatalytic (PEC) hydrogen production. Molecular origin of number of layers and stacking sequence-dependent PEC hydrogen evolution reaction (HER) performance of MoS₂/graphene van der Waals vertical heterostructures is studied. Density functional theory based calculations show that the presence of MoS₂ induces p-type doping in graphene, which facilitates hydrogen adsorption in the graphene side compared to the MoS₂ side with ΔG_H closer to 0 eV in the MoS₂/graphene bilayer vertical stacks. Further, it is found that the activity maximizes in graphene with monolayer MoS₂ and reduces further for bilayer and multilayers of MoS₂.

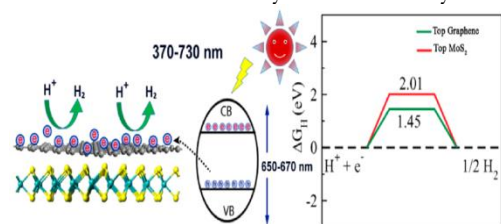


Figure 4: Stacking dependent PEC HER performance of van der Waals solids.

Another group is engaged in building an ultra high vacuum cluster tool system with the capability to make devices in-situ and characterize the samples using RHEED and STM. The group has initiated efforts in exploring the formation of Majorana Fermions at proximity induced interfaces between a high spin-orbit, high Zeeman material and s-wave superconductors. The results highlighted the contributions played by the spin-orbit and spin-scattering centers in the observation of zero bias conductance peak. [Karthik V. Raman]

Cell and Molecular Biology

Efforts have been made for devising a novel image-analysis based assay for detection of cell cycle stage, in order to gain insight into DNA damage responses at the single cell level. Additionally, we are trying to develop novel two color single molecule detection of transcripts in cells. A fruit fly facility also has been set up, and a confocal microscope system is under procurement. [Aprotim Mazumder]

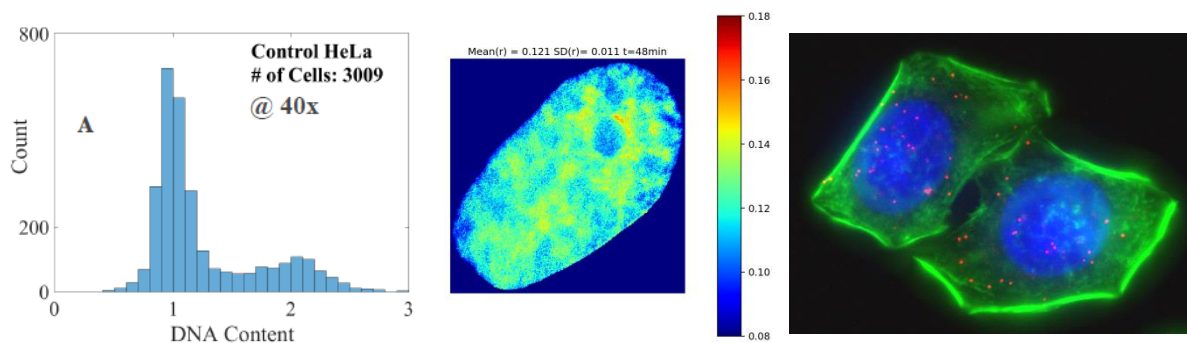


Figure 5: **Left:** DNA content histogram of HeLa cells obtained from microscopy. G1 and G2 peaks can be seen. Usually flow cytometry is used to generate such histograms. **Middle:** Fluorescence anisotropy map of histone H2B-GFP labeled chromatin in a HeLa cell nucleus. Warmer colors indicate higher anisotropy, and hence greater compaction. Assays like this are being used to study chromatin compaction changes under DNA damage. **Right:** Single ATR mRNA molecules (red) in HeLa cells. The nuclei (stained with DAPI, blue) and actin (stained with phalloidin-Atto488, green) are also shown. Assays like this are being used to study transcriptional changes in response to DNA damage.

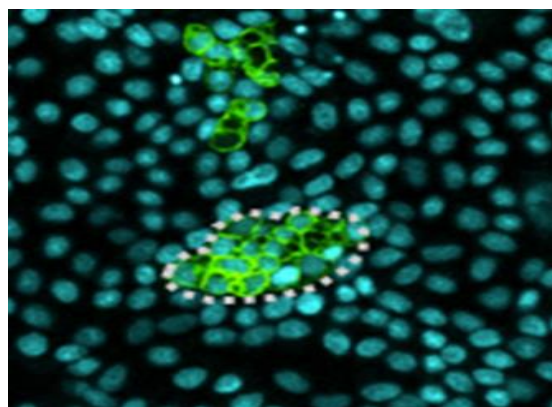


Figure 6: Competition between wild-type and Ras oncogene-expressing (green) clones leads to extrusion and eventual demise of the latter.

Molecular Genetics

The Molecular genetics group is setting up a research program in genetics and genomics to study underlying causes of neuro-metabolic diseases. The goal of this program is to accelerate discovery of disease-linked mutations and associated mechanisms using “Integrated-Human-Drosophila-Pipeline” in collaboration with clinical geneticists in India. [Manish Jaiswal]

Biophysical Chemistry

The Biophysical Chemistry group at TCIS has recently built a novel and highly sensitive multi-channel fluorescence correlation spectrometer (FCS) which is capable of measurements in standard cuvettes.

Efforts are being made to study the dissolution mechanism of amyloid fibrils. [Kanchan Garai]

Transport through Golgi: Instabilities in coupled driven systems

Over the past few years, strongly coupled multi-species driven diffusive systems have been studied intensely, with a focus on the speed and decay of coupled-species fluctuations, propagating through a uniform background.

A striking effect was demonstrated in such systems: macroscopic instabilities which destroy the homogeneous state altogether. This was shown for a generic two-way coupled field system, which may be visualized as particles sliding down a fluctuating landscape: particle motion is governed by local slopes, while landscape evolution is influenced by the presence of particles. The homogeneous state was shown unstable against phase separation; moreover, there are several different phases, in both one and two dimensions. A complete characterization of static and dynamic properties of all phases has been completed as well. This constitutes a first step towards the important goal of classifying ordered phases in coupled driven systems. [Mustansir Barma, S. Chakraborty, S. Pal, S. Chatterjee (S. N. Bose Centre for Basic Sciences, Kolkata)]

Coarsening and persistence in a dense collection of arrowheads

Left and right pointing arrowheads provide a simple representation of bent-core molecules which collectively exhibit interesting orientationally ordered phases. The large scale effects of entropy-driven ordering were studied, arising from the interplay between shape and hard core interactions in a system of arrowheads on a line, evolving under reorientation dynamics. Interestingly, in the high density limit, there are two non-equivalent types of domain wall, diffusive (A) and static (B). The approach to the ordered state is governed by the kinetics of AB annihilation, quite different from the customary Glauber-Ising kinetics AA annihilation. Persistence properties reveal a new power law exponent, close to $1/4$. In a generalization where the B walls diffuse slowly, the exponent varies continuously, indicating a breakdown of universality. [[Mustansir Barma, M. D. Khandkar (Pillai College of Engineering, New Panvel), R. B. Stinchcombe (University of Oxford)]]

Nonequilibrium biogenesis and transport through Golgi-like cisternae

A central issue in cell biology is the physico-chemical basis of the formation of organelles such as Golgi in intracellular tracking pathways. At a basic level, morphologically and chemically distinct compartments

should arise from an interplay between the molecular transport and chemical maturation.

Minimalist models that incorporate this interplay in physical space, and include both single-particle and collective aspects in the motion of proteins, were formulated. Our analysis showed that in limiting cases, the model exhibits a phase transition to a state with striking mass fluctuations and intermittency in time. Further, beyond elucidating the conditions for de novo biogenesis of distinct cisternae, new measures were proposed that can discriminate between various models - this includes measures of the dynamics in steady state, and the response to perturbations of a kind amenable to live-cell imaging. [[Mustansir Barma, H. Sachdeva; Institute of Science and Technology, Austria and Madan Rao, NCBS, Bengaluru]

Synthetic Organometallic Chemistry

At the synthetic organometallic chemistry front, following have been achieved:

- N-Heterocyclic Carbene (NHC) stabilized 2-hydrophosphasilenes using silicon(IV) precursors were achieved and demonstrated the proof of donor acceptor bonding between NHC and the silicon centre of the "Si=P" moiety.
- 2-hydroiminosilane was synthesized and its reactivity towards small molecules activation; such as addition of O-H bond of H₂O across Si=N bond was explored.
- Importance of electron rich olefins is known and it can act as one electron donor or two electron donor under the formation of radical cation and dication. We have considered N-alkyl substituted N-Heterocyclic Carbene (NHC) and Cyclic Alkyl Amino Carbene (CAAC) moieties for the electron rich olefins; and were able to isolate corresponding radical cation and dication.

Chemical Synthesis

The Chemical Synthesis group is engaged in developing novel synthetic methods for total chemical synthesis of natural and non-natural proteins that would have implications in developing inhibitors of specific disease related protein-protein interactions. The very first step to achieve this would be to develop an efficient method for the synthesis of peptide having a thioester moiety at the C-terminus. Making a peptide thioester by traditional Fmoc solid phase peptide synthesis is nontrivial due the usage of nucleophilic base piperidine during the synthesis. Inspired by intein splicing, the nature's way of making protein thioester, we have designed and synthesized three synthetic precursors. All those three precursors would, quite easily, rearrange to peptide thioester upon treatment with mild reagents. We made significant progress last

year along this line. We hope that we will be able to apply these methods for the chemical protein synthesis by the end of this year. [Kalyaneswar Mandal].

Computational Chemistry

The theoretical chemistry and physics group has deciphered the molecular mechanisms of an anti-cancer drug in circumventing bacterial resistance using computational techniques. The work has been highlighted in India bioscience. [Jagannath Mondal]

Deductive and Inductive Modeling of Matter:

This group working on the big-data-driven inference of molecular/materials properties and chemical physics phenomena has one vital contribution. A machine-learning model has been developed, to infer electron correlation of arbitrary molecular potentials. [Raghunathan Ramakrishnan]

Science Education:

This team has initiated contacts with several schools in the neighbourhood of TCIS, interacted with students of TSWREIS (Telangana Social Welfare Residential Educational Institutions Society) and visited their science laboratories. [Jayashree Ramadas].

Members

Surajit Sengupta, Rama Govindarajan (till July 01, 2016), Sriram Ramaswamy (till October 26, 2016), Smarajit Karmakar, Prasad Perlekar, Anukul Jana, Kanchan Garai, Pramodh Vallurupalli, T.N. Narayanan, Aprotim Mazumder, Karthik V. Raman, M. Krishnamurthy, K.V.R Chary, P.K. Madhu, Vipin Agarwal, Jagannath Mondal, Raghunathan Ramakrishnan (from April 29, 2016), Kalyaneswar Mandal from May 25, 2016), Tamal Das (from November 01, 2016), Manish Jaiswal (from December 02, 2016), Jayashree Ramadas (from January 19, 2017)

Subodh R Shenoy(till December 31, 2016), N. D Haridass, Mustansir Barma, Kaustubh R. Mote, Anand Yethiraj (till June 23, 2016), Pushpita Ghosh (from August 22, 2016), Subodh R Shenoy (from January 01, 2017)

Research Scholars

Anshul Deep Singh Parmar, Vinutha H A, Sharath K Jose (till July 31, 2016), Ravichandran S (till December 31, 2016), Habeeba Tamkeen K S, Shivnarayan T Dhuppar, Pankaj Popli, Pardeep Kumar (till July 31, 2016), Sumit Kumar Birwa(till October 31, 2016), S Ganga Prasath (till September 30, 2016), Rashmi Ramadugu, Shubhadeep Pal, Rayan Chatterjee, Debabrata Dhara, Debdeep Mandal, Timir Baran Sil, Rahul K Gupta, Rajsekhar Das, Saurabh Chaudhary, Sudeshna Patra, Mrinmoy Mucherjee, Bhanu Prasad Bhowmik, Pappu Acharya, Subhrajyoti Dolai, M P Kumar (till March 28, 2017), Mukul G Jain, Indrajit Tah, Subhendu Pandit, Khandekar Jishan Bari, Naresh Kumar(till April 29, 2016), Dheeraj P Dube, Sripati V Rahul, Lokrshi Prawar Dadhichi, Navdeep Rana, Keerthan Subramanian, Archit Bhardwaj, Vikash Pandey, Shashank Yadav, K. Jaya Krishna, Kallol Paul, Ritabrata Thakur(till September 30, 2016, Janeka, Kshama Sharma, Debankur Das, Anusha Bargavi Gopalan, P. S Kesavan, Shamasree Ghosh, Rahul Chajwa(till October 31, 2016), Rahul Sharma, Nikhita Pasnuri, Subhajit De(till July 28, 2016), Avijit Maiti, Sumit Bawari, Aslam Uddin(till July 29, 2016), Subhajit Ghosal(till June 07, 2016), Vishnu V Krishnan, Bhupendra R Dandekar, Mithun Maddheshiya (from August 01, 2016), Subinoy Adhikari (from August 01, 2016), Abhisek Kar (from August 01, 2016), Suman (from August 05, 2016), Soham Mukhopadhyay (from August 01, 2016), Satyabrata Bandyopadhyay (from August 01, 2016), Anamika Biswas (from August 01, 2016), Tanya Singal(from August 01 to September 13, 2016), Pravin Pralhad Taware (from August 01, 2016), Mithilesh Kumar Nayak (from August 01, 2016), Sabyasachi Chakraborty (from August 01, 2016), Anku Guha (from August 01, 2016), Phani Shilpa Pothapragada (from August 01, 2016), Paswa Nath (from August 04, 2016), Geetika (from August 01, 2016), Satyaki Sasmal (from August 01, 2016), Anoop Mutneja (from August 01, 2016), Krishna Rani Sahoo (from August 01, 2016), Pallavi (from August 03, 2016)

Post-Doctoral Fellows

M. Anand (till August 17, 2016), C. Neeraja, Kiran Kumar Tadi (till July 20, 2016), Deepa Jaiswal, Sitara Roy , Abhijeet A Joshi (till June 20, 2016), Deepu P (till June 29, 2016), Y Balaji (till July 15, 2016), Satya Prakash (till March 06, 2017), Biswajit Santra, K. Praveen Kumar Naik (till November 22, 2016), S. Mathimalar, Guntupalli Gopi Krishna, Sarada Seetharaman (till October 19, 2016), Sunita Patel (till July 29, 2016), Ravi Kumar Biroju, Laxman Mahadev Alakonda, Angana Ray (till February 28, 2017), Chandrakala M Gowda, Venkata Subbarao R (from June 01, 2016), Bankanidhi Sahoo (from June 03, 2016), Anand Puthirath Balan (from July 03, 2016), Naddi Shankaraiah (from August 08, 2016), Tapas Singha (from September 14, 2016), Navjeet Ahalawat (from October 03, 2016), Milan KR Barman (from October 04 to March 28, 2017), Jamad Mannuthodikayil (from October 19, 2016), Shrikanth Sharma (from October 21, 2016), Bal Krishnan Mishra (from November 03 to December 09, 2016), Ronald Benjamin (from January 03, 2017), Atul Singh Bharadwaj (from January 19, 2016), Rajasekhar Pothala (from February 15, 2017), Angana Roy (from March 01, 2017), Vivek Gupta (from March 06, 2017), Rahul Kumar (from March 23, 2017).

Junior / Senior Research Fellows

Sarika Kumari, Akshi Gupta, Swapneel Amit Pathak (till December 30, 2016), Paswa Nath (till August 03, 2016), Subrata Kuilya (till July 12, 2016), Sambit Mohapatra, Sreedevi K.N. (till December 21, 2016), Ramapada Dolai, Naresh Kumar (from May 18, 2016), Subhajit De (from August 11 to September 09, 2016), Manisha Yadav (from July 19 to January 17, 2017), Saayak Halder (from July 29, 2016), Vineeth Francis (from September 01, 2016), Syed Muhammed Muazzam Kamil (from September 06, 2016), Rakesh Kumar Y (from November 10, 2016), Arka Provo Das (from March 10, 2017).

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

Aditya Kandaswamy (till May 23, 2016), Kapil Bhorkar (till May 17, 2016), Arpita Sundaria (till July 12, 2016), Nirdosh Dadwal (till July 13, 2016), Arthi Appathurai (till July 22, 2016), Karthik Menon (till May 31, 2016), Sakuntala (till May 05, 2016), Mamta Jotkar (till April 27, 2016), Jennifer Joseph (from June 01 to August 31, 2016), Aslam Uddin (from August 01 to November 30, 2016), Asif Equbal (from September 19, December 28, 2016), Rajath Krishna R (from November 01 to November 30, 2016), Nikhil Jaisinghani (from January 09, 2017)

Scientific/Technical staff

Ram Gopal, Rajalakshmi G, N. Kalyan Kumar, Krishnaro Doddapuneni, Suman Saurav, Deepa S, Velmurugan G.V., Sreejith Raran-Kurussi (from November 07, 2016) Rajasekhar Rajapurmath, N. Srenaiiah (from August 12, 2016), Krishna A Elipilli (from October 03, 2016)

Administrative Staff

D. Hariprasad, J. Ratna, Mruduta R. Barde, Vivek Baban Hadawale, D. Raghuram Dathu, M. Varalakshmi (from April 18, 2016), Roopashri R Prasad (from August 11, 2016), Hemalatha P (from September 08, 2016), Hanumanth Rao (from March 30, 2017)

Project Staff

Ramachandraiah (till June 30, 2016), N Srenaiiah (till August 09, 2016), Pittala Kumar, P. Kasiviswanath, Rajdip Das (from December 05, 2016), M Varalakshmi (till April 12, 2016), Roopashri R Prasad (till August 09, 2016), Hemalatha P (till September 07, 2016), T. Srinu Babu (till June 09, 2016), Narsimulu (till September 09, 2016), V Gopinath (till January 05, 2016), Lalitha Minocha, Nakkireddy Swapna, Pemberla Rajitha, Mallikarjun S., K. Archana, Vikas Kumar Arandker (from March 27, 2016), T. Srinu Babu (from June 20, 2016), Narsimulu (from September 18, 2016)

National and International Involvement

Mondal J.: 1.Member of "Biophysical Society".2. Member of "American Chemical Society"3.Elected young associate of "Indian Academy of Sciences" **Mandal K.:** Member, "American Peptide Society ". **Chary K.V.R.:** 1.Invited to be a member of Peer Team to Visit "Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, Karnataka" on 6th and 7th December 2016 for Assessment and Accreditation of the institution.2.Elected Council Member of "The National Academy of Sciences", India (2016-2018).3.Member of Fellowship Scrutinizing Group of "The National Academy of Sciences", India (2016-)4..Elected EC Member, "National Magnetic Resonance Society", India (2017-) Elected as Treasurer and Steering Committee Member, "Asian Biophysics Association" (2013-present). 5.Elected as a Member, "International Advisory Board", International Conference on Magnetic Resonance in Biological Systems (ICMRBS), which was held in Kyoto, Japan (2014-2016). 6.Elected as a Member, "International Advisory Board", International Conference on Magnetic Resonance in Biological Systems (ICMRBS), to be held in Dublin, UK (2016-2018). 7.Member, IUPAB "National Committee of INSA "(2012-16).8. Executive Council Member (2008-present), Elected Hon. Vice-Chairman (2008-2010), Elected Hon. Chairman (2010-2012), Advisor (2012-present), "Royal Society of Chemistry", West India Section, (2010-2012).9.Member, Editorial Advisory Board, of the Journal "Current Bioinformatics", launched by Bentham Science Publishers, The Netherlands and U.S.A. (2005-present); 10.Member, Editorial Board, of "The Open Magnetic Resonance Journal", launched by Bentham Science Publishers, The Netherlands and U.S.A., (2007- Present).11.Fellow of "Royal Society in Chemistry (FRSC)" (2004-present).12.Member, J.N. "Tata Endowment Selection Committee", Mumbai (2005-Present)13. Member, Management Advisory Committee for the "National Facility for High Field NMR", TIFR.14.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".15.Invited to deliver a talk and to chair a plenary session during the International Conference on "Magnetic Resonance in Biological Systems" (ICMRBS) held at Kyoto, Japan in August 2016. 16.Invited to deliver a talk during the annual symposium of "National Magnetic Resonance Society", India held at IIT Kharagpur in February 2016.17.Served on the Selection Committee as the Visitors Nominee to interview candidates for the post of Professor in the Department of Bio-technology, IIT Madras (2015-).**Raman K.V.:** Member, International Advisory Board, "SpinOS" (2015-present). **Madhu P.K.:**1.Head: Research, finance, and administration, TCIS, TIFR, Hyderabad. 2.Convener, "MagRes academic advisory body (MRAAB)", TIFR, Hyderabad.3.Editorial board member of "Journal of Magnetic Resonance".4.Editorial board member of "Solid State

Nuclear Magnetic Resonance".5.Editorial board member of "Journal of Biomolecular NMR" International advisor, "European School on Solid-State NMR".6. Member, MAC, "National Facility for High-Field NMR", TIFR Scientific programme committee member, EUROMAR, Quebec, Canada, July 23-28, 2017.Member, National Magnetic Resonance Society, India: **Vallurupalli P.** Reviewer for: Science, "J Biomol NMR". **Ramakrishnan R:** 1.Expert member for "National Supercomputing Mission", supported by Ministry of Communications and Information Technology, Government of India. 2.Editorial board member: "Scientific Reports", a journal published by Springer Nature3. Member of Selection Panel: University of Hyderabad - Freie Universität Berlin Student Exchange Program **Narayanan T.N.**:Peer reviewed articles from the following journals: Science Advances, Advanced Materials, Scientific Reports, Journal of Materials Research, AIP conference proceedings. **Agarwal V.:** Member, "National MagneticResonanceSociety", India.

Visits

Madhu P.K.:1.University of Leipzig, Leipzig, June 12- July 12, 2016 2.University of Leipzig, Leipzig, Feb. 26-March 4, 2017.**Mazumder A, Raman K.V.:** 104th Indian Science Congress, Tirupati, India (January, 2017) (represented the whole TIFR system along with two student colleagues from TCIS). **Das T.** Cell Biology and Physics of Morphogenesis (BioPhyMorph 2017) Mahabaleshwar Seminars, Alibaug, 28th February to 4th March 2017.**Agarwal V:** Visiting researcher at Prof Pintacuda's Lab at the Centre de RMN à Tres Hauts Champs, Institut des Sciences Analytiques, Villeurbanne, Lyon, France15 October- 15 November 2016. 2.Prof Bernd Reif's group, Technical University Munich, Germany. 27 -29 October 2016 .3.Prof Arno Kentgen's Group, Radboud University, Nijmegen, The Netherlands 19 -22 March 2017 **Chary K.V.R.** International Congress on Recent Advances in Chemistry And Chemical Engineering (ICRACACE-2016), held at JNTU, Hyderabad. 2. Department of Chemistry, IIT Indore, August 16, 2016.3.Kyoto, Japan, to deliver a talk and to chair a plenary session during the International Conference on Magnetic Resonance in Biological Systems (ICMRBS) held at Kyoto, Japan in August 2016. 4. BITS, Pilani, Goa, Royal Society of Chemistry – West India Local Section, India Symposium, November 13, 2016. **Narayanan T.N.:** 1. Visited Indian Space Research Organization (ISRO), Bangalore, India, August 19th, 2016 and delivered a talk. 2. Visited the following universities at Israel and given lectures, Bar-Ilan University, Weizmann Institute of Science, and Ariel University during July 24-27, 2016. 3. Visited Rice University, USA during April 23-30, 2017.

Invited talks

Jana A.

- 1.N-Heterocyclic Carbene Stabilized 2-Hydrophosphasilene: A Heavier Analogue of Alkene at Department of Chemical Sciences Annual Talks 2016, TIFR Mumbai. 21 Dec 2016
- 2.Functionalization of CO₂ using Compounds Involving Main Group Elements at Brain Storming Session on Environmental Geotechnics, 24-25 January 2017, Goa sponsored by SERB-DST. 24 January 2017

Chary K.V.R.:

- 1.“Intrinsic Order and Disorder”, an invited talk at International Congress on Recent Advances in Chemistry And Chemical Engineering (ICRACACE-2016), held at JNTU, Hyderabad.
- 2.“Sequence to Structure”, an invited talk at the Department of Chemistry, IIT Indore, August 16, 2016.
- 3.“Structural characterization of a putative UV inducible protein (UVI31+) from *Chlamydomonas reinhardtii* that exhibits DNA endonuclease activity”, an invited talk at the International Conference on Magnetic Resonance in Biological Systems (ICMRBS) held at Kyoto, Japan on August 22 ,2016.
- 4.“Order and Disorder in Protein Structures as Studied by NMR”, and invited talk at the Royal Society of Chemistry – West India Local Section, India Symposium, held at BITS, Pilani, Goa, November 13, 2016.

Das T.:

- 1.“Motion and Force Measuring Techniques at Multicellular Scale: Mechanotransduction During Collective Migration of Epithelial Cells”, Cell Biology and Physics of Morphogenesis (BioPhyMorph 2017) Mahabaleshwar Seminars, Alibaug, 2nd March 2017
- 2.“Mechanobiology of Collective Cell Migration”, Cell Biology and Physics of Morphogenesis (BioPhyMorph 2017) Mahabaleshwar Seminars, Alibaug, 3rd March 2017

Mondal J.:

1. “Atomistic Simulation of Protein-Ligand Binding”, ARCAM, University of Hyderabad, on the occasion of Anisur Rahman Day (2016)
2. “Molecular Recognition: Insights from computer Simulation”, School of Chemistry, University of Hyderabad (2016)
3. “Multiscale simulation in the interface of chemistry and biophysics”, Kaleidoscope, Goa, India (2016)
4. “How does a small molecule find a solvent inaccessible cavity?”, Theoretical Chemistry Symposium, Hyderabad (2016)
5. “Self-organization inside a bacterial cell”, Complex Fluid , IIIT Hyderabad, India (2016)
6. “Self-organization in E coli cell”, Soft Matter Young Investigators' conference, Goa, India (2016)
7. “Is Protein single molecule dynamics under force described by two or more states?”, IIIT Hyderabad (2017)

Madhu P.K.:

- 1.Paramagnetic relaxation, pNMR meeting, University of Aarhus, Denmark, July 9-10, 2016
2. Summer school on NMR relaxation, Schloss Windishleuba, Germany, September 4-10, 2016:

- a. Phenomenology of relaxation
 - b. Bloembergen-Pound-Purcell theory
 - c. Redfield relaxation theory
 - d. Superoperators and explicit calculation of spectral densities
 - e. Relaxation in experiments: NOE to TROSY
3. Summer school on Solid-state NMR, Schloss Windishleuba, Germany, February 19-25, 2017:
 - a. Recoupling in solid-state NMR
 - b. Recoupling applications and cross-polarisation dynamics
 - c. Quadrupolar nuclei-I
 - d. Quadrupolar nuclei-II
 - e. Future of solid-state NMR
 4. Solid-state NMR in materials science applications, Catalysis by design using NMR, Lille, France, March 15-17, 2017

Ramakrishnan R.:

1. Invited speaker at the "International Conference of Young Researchers on Advanced Materials" at IISc, Bangalore on 13 December 2016
2. Invited speaker at "Spectroscopy and Dynamics of Molecules and Clusters" at Pondicherry University, Pondicherry on 16-19 February 2017

Sengupta S.:

1. CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop on: "Emergent dynamics of out-of-equilibrium colloidal systems at nano- to microscales", Lausanne April 18-20, 2016.
2. CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop on: "Exploiting finite size effects in simulations", Paris, April 18-21, 2017.

Ramaswamy S.:

1. Invited speaker, CompFlu, Hyderabad, Dec 2016
2. S Datta Majumdar Memorial Lecture, IIT Kharagpur, 16 Nov 2016
3. Mechanical Forces in Cell Biology: Information at the Cell and Tissue scale, NCBS, Bangalore, 4-6 Oct 2016
4. NISER Foundation Day lecture, 6 Sep 2016, NISER, Bhubaneswar
5. Plenary speaker, STATPHYS26, Lyon, France, July 2016
6. Invited speaker, IASBS-ICTP School on Active Matter and Chemotaxis, Zanjan, Iran, May 2016

Narayanan T.N.:

1. Engineered Atomic Layers & Their Hybrids for Electrocatalysis" International Conference of Young Researchers on Advanced Materials (IUMRS-ICYRAM 2016)" held at Indian Institute of Science, Bangalore, India during December 11-15, 2016.
2. Engineered Graphene Layers & Their Hybrids for Electrocatalysis, "1st International Conference on Nanoscience and Nanotechnology (ICNAN'16" held at Vellore Institute of Technology (VIT), Vellore, Tamilnadu, India October 19-21, 2016.
3. Engineering Atomic Layers for Energy and Sensing Applications, Laboratory for Electro Optic System (LEOS), Indian Space Research Organization (ISRO), Bangalore, India, August 19th, 2016.
4. Engineering Electrodes for Energy Technologies – Fundamentals to Applications, Department of Physics, Bar-Ilan University, Israel, July 27th, 2016.
5. Engineering Atomic Layers for Functional Solids, Department of Materials Science and Interfaces, Weizmann Institute of Science, Israel, July 26th, 2016.
6. Tunability in the Wetting Phenomena of Graphene, International Conference on Materials Technology and Modeling (MMT-2016), Ariel University, Israel, July 25th, 2016.
7. Recent Advances in Carbon Nanotechnology, T. N. Narayanan, St. Teresas College, Kochi, India, February 24th 2016.

Agarwal V.:

1. Low-power recoupling and decoupling in fast rotating MAS solids. 19th October, CRMN, Lyon, France. (2016)
2. Selective polarization exchange amongst protons in fully protonated proteins at 100 kHz MAS frequencies. 28th October, Technical University, Munich, Germany. (2016)
3. Selective ¹H-¹H distance restraints in fully protonated proteins at 111 kHz and above MAS frequencies, 7th Asia-Pacific NMR Symposium 16-19th February 2017, Bangalore, India. (2016)
4. Rotor-Synchronized Heteronuclear Recoupling for Fast MAS Solid-State NMR Spectroscopy, NMR-CAT: Catalysis by design using NMR (Indo-French symposium of NMR and catalysis), 14th -17th March 2017, University of Lille, Lille, France
5. Low-power recoupling and decoupling at 60-111 kHz MAS in solids. 21st March, Solid-state NMR department, Radboud University, Nijmegen. The Netherlands (2017)

Conferences Organized by the Department

1. Complex Fluids – Compflu-2016, IIT-Hyderabad, 12-14 Dec, 2016.
2. Third Annual TCIS Summer Research Symposium, 1st July, 2016, TCIS, TIFR, Hyderabad.

Non DAE Research Projects

Mandal K.: Investigator: Kalyaneswar Mandal, Title: "Systematic development of novel therapeutics against malaria", Funding Agency: Wellcome Trust/ DBT India Alliance, Duration: 60 months

Jana A.: 1.CSIR India , Synthesis and Reactivities of Compounds Involving Formal Zero Oxidation State of Mono- and Di-Nuclear Group 14 Elements (2016-19), 2.AvH Foundation, Germany , Molecular Manifestations of Transition Metal Tetrelides MxEy (M = Cr, Mn, and Fe; E = Si and Ge) for Thin Film Deposition (2017-19)

Mazumder A.:"Developing novel methods for single cell detection of transcripts and proteins in primary cells and tissue to explain variable sensitivities of body cells to DNA-damaging chemotherapeutic agents", SERB Early Career Research Grant, 3 years starting from March, 2017.

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".

Madhu P.K.:1..Danish-Indian collaboration programme entitled "Solid-state NMR methods and applications". 2 .Indo-French IFCPAR/CEFIPRA project entitled "Novel nanocatalysts synthesis guided by DNP NMR"

Vallurupalli P.:Understanding Protein Conformational Dynamics using T4 Lysozyme as a model system, Agency: SERB ECR/2016/001088. Investigator: PramodhVallurupalli, Duration: 3 Years, starting from March 2017, Total: 37 Lakhs

Mondal J.: Elucidation of kinetic pathways of protein-ligand recognition and improvement of virtual drug discovery using Computer simulation", Investigator: Jagannath Mondal, Funding agency: DST under "early career research proposal" (2016). *Das T.*:Tamal Das, Max Planck Partner Group with Max Planck Institute for Medical Research, Max Planck Society, 1st March 2017 – 29th February 2020. *Chary K.V.R.*:The DST-DIISRT joint research project (Australia-India Strategic Research Fund (AISRF)), DST, 2015-17.

Lectures given elsewhere

Agarwal V

1. Theory and applications of Solids-State NMR Spectroscopy, at the school on Role of NMR Spectroscopy in Structural Biology, Metabonomics and Drug Discovery , 22 November, ICGEB, Delhi, India. (2016)
2. Solids-State NMR Spectroscopy of Biomolecules, at the school on Role of NMR Spectroscopy in Structural Biology, Metabonomics and Drug Discovery , 23 November, ICGEB, Delhi, India. (2016)

Chary K.V.R.

1. Intrinsic Order and Disorder an invited talk at International Congress on Recent Advances in Chemistry And Chemical Engineering (ICRACACE- July11-13, 2016), held at JNTU, Hyderabad.
2. Sequence to Structure, an invited talk at the Department of Chemistry, IIT Indore, August 16, 2016.
3. Structural characterization of a putative UV inducible protein (UVI31+) from *Chlamydomonas reinhardtii* that exhibits DNA endonuclease activity , an invited talk at the International Conference on Magnetic Resonance in Biological Systems (ICMRBS) held at Kyoto, Japan on August 22, 2016.
- 4.Order and Disorder in Protein Structures as Studied by NMR and invited talk at the Royal Society of Chemistry – West India Local Section, India Symposium, held at BITS, Pilani, Goa, November 13, 2016.

Madhu P.K.

1. Structural reorganisation accompanying A β aggregation, IISER Mohali, Mohali, October 21, 2016
2. Asynchronous MAS recoupling and static decoupling in solid-state NMR, Univ. of Leipzig, March 1, 2017

Narayanan T.N.

1. Engineering Electrodes for Energy Technologies – Fundamentals to Applications, T N Narayanan, Global Initiative of Academic Networks (GIAN) workshop – Nanotechnology – From Fundamentals to Practice, Indian Institute of Science Education and Research (IISER), Thiruvananthapuram, Kerala, India, June 13-17, 2016.

Sengupta S.

1. Invited talk at the CECAM workshop on "Emergent dynamics of out-of-equilibrium colloidal systems at nano- to microscopes", April 18, 2016 to April 20, 2016, Lausanne, Switzerland.
2. Invited talk at the StatPhys Kolkata conference, 13th to 16th December, 2016, Saha Institute for Nuclear Physics, Kolkata.
3. Invited talk at the conference on "Plasticity and failure in disordered materials", January 04 - 07, 2017 at The Institute of Mathematical Sciences, Chennai.

Lectures at TIFR

Mazumder A.

1. Dr. Aditi Bhattacharya, InStem, 27th July, 2016
 2. Dr. Ashesh Dhawale, Harvard University, 17th March, 2016
- Madhu P.K.

1. M. H. Levitt (Univ. of Southampton, UK), Nuclear spins far from equilibrium, January 9, 2017, TCIS, TIFR, Hyderabad
2. Matthias Ernst (ETH, Zurich), Hyperpolarisation in NMR and MRI: Dissolution dynamic nuclear polarization, February 14, 2017, TCIS, TIFR, Hyderabad

Publications

1. Assembly of NHC-Stabilized 2-Hydrophosphasilenes from Si(IV) Precursors: A Lewis Acid-Base Complex" Debabrata Dhara, Debdeep Mandal, Avijit Maiti, Cem B. Yildiz, Pankaj Kalita, Nicolas Chrysochos, Carola Schulzke, Vadapalli Chandrasekhar and Anukul Jana Dalton Trans. 45, 19290–19298, 2016
2. Structure of Ca²⁺-binding protein-6 from Entamoeba histolytica and its involvement in trophozoite proliferation regulation, Verma D, Aruna Murmu, Gourinath S, Bhattacharya, A and Chary, K V R, PLOS Pathogens, 2017 (in press)
3. ¹H, ¹³C and ¹⁵N NMR assignments of an unusual Ca²⁺-binding protein from Entamoeba histolytica in its apo form. Verma D, Mutyala S, Aruna Murmu, Bhattacharya, A and Chary, K V R Biomol. NMR Assign., 1-5. 2016
4. Differential accumulation and mobilization of starch and lipid in Chlamydomonas reinhardtii, Himanshu Singh, Manish R Shukla, Basuthkar J Rao, Kandala V R Chary, Algal Research, , 18, 33-44. 2016
5. The significance of symmetry in the nuclear spin Hamiltonian for efficient heteronuclear dipolar decoupling in solid-state NMR: A Floquet description of spycycled rCW schemes, A. Equbal, R. Shankar, M. Leskes, S. Vega, N. C. Nielsen, P. K. Madhu, J. Chem. Phys. 2017.
6. Five decades of homonuclear dipolar decoupling in solid-state NMR: Status and outlook, K. R. Mote, V. Agarwal, P. K. Madhu, Prog. Nucl. Magn. Reson. Specy. 97, 1-39, 2016.
7. A suite of pulse sequences based on multiple sequential acquisitions at one and two radiofrequency channels for solid-state magic-angle spinning NMR studies of proteins, K. Sharma, P. K. Madhu, K. R. Mote, J. Biomol. NMR, 65, 127-141, 2016.
8. Systematic evaluation of heteronuclear spin decoupling in solid-state NMR at the rotary-resonance conditions in the regime of fast magic-angle spinning, K. Sharma, P. K. Madhu, V. Agarwal, J. Magn. Reson. 270, 136-141, 2016.
9. A detailed analysis of the morphology of fibrils of selectively mutated amyloid \square (1-40), J. Adler, M. Baumann, B. Voigt, H. A. Scheidt, D. Bhowmik, T. Hüpl, B. Abel, P. K. Madhu, J. Balback, S. Maiti, D. Huster, Chem. Phys. Chem. 17, 1-11, 2016.
10. Positron annihilation and nuclear magnetic resonance study of the phase behavior of water confined in mesopores at different levels of hydration, P. Maheswari, D. Dutta, S. Mukherjee, P. K. Madhu, K. R. Mote, P. K. Pujari, Phys. Chem. Chem. Phys. 18, 12886-12895, 2016.
11. Relative merits of rCW^A and XiX heteronuclear spin decoupling in solid-state magic-angle-spinning NMR spectroscopy: A bimodal Floquet analysis, Equbal, M. Leskes, N. C. Nielsen, P. K. Madhu, S. Vega, J. Magn. Reson. 263, 55-64, 2016.
12. Heteronuclear decoupling in MAS NMR in the intermediate to fast sample spinning regime, Equbal, M. Bjerring, K. Sharma, P. K. Madhu, N. C. Nielsen, Chem. Phys. Lett. 633, 243-249, 2016.
13. Two-dimensional turbulence in symmetric binary-fluid mixtures: Coarsening arrest by the inverse cascade, Nairita Pal, and Rahul Pandit, Scientific Reports, 7, 44789, 2017
14. Deviation-angle and trajectory statistics for inertial particles in turbulence, Akshay Bhatnagar, Anupam Gupta, Dhrubaditya Mitra, Michael Wilkinson, and Rahul Pandit. Phys. Rev. E, 94, 063112, 2016
15. Coherent structures and extreme events in rotating multiphase flows, Luca Biferale, Fabio Bonaccorso, Irene M. Mazzitelli, Michel A.T. van Hinsberg, Alessandra S. Lanotte, Stefano Mussachio, Prasad Perlekar, and Federico Toschi, Phys. Rev. X, 6, 041036, 2016
16. How long do particles spend in vortical regions in turbulent flows?, Akshay Bhatnagar, Anupam Gupta, Dhrubaditya Mitra, Rahul Pandit, and Prasad Perlekar, Phys. Rev. E, 94, 053119, 2016
17. Front structure and dynamics in dense colonies of motile bacteria: Role of active turbulence, Rayan Chatterjee, Abhijeet A. Joshi, and Prasad Perlekar, Phys. Rev. E, 94, (2016), 022406, 2016
18. Dynamics of circular arrangement of vorticity in two dynamics, Rohith V. Swaminathan, S. Ravichandran, Prasad Perlekar, Rama Govindarajan. Phys. Rev. E, 94, (2016), 013105, 2016
19. Binary-fluid turbulence: Signatures of multifractal droplet dynamics and dissipation reduction, Nairita Pal, Prasad Perlekar, Anupam Gupta, and Rahul Pandit. Phys. Rev. E, 93, 063115, 2016
20. Probing conformational dynamics in biomolecules via chemical exchange saturation transfer: A primer. Pramodh Vallurupalli, Ashok Sekhar, Tairan Yuwen, Lewis E. Kay, J Biomol NMR. 2017
21. Simultaneous NMR characterisation of multiple minima in the free energy landscape of an RNA UUCG tetraloop, Aditi N. Borkar, Pramodh Vallurupalli, Carlo Camilloni, Lewis E. Kay and Michele Vendruscolo, Chem Chem Phys 19, 2797-2804. 2017
22. Enhancing the Sensitivity of CPMG Relaxation Dispersion to Conformational Exchange Processes by Multiple-Quantum Spectroscopy. Tairan Yuwen, Pramodh Vallurupalli, Lewis E. Kay, Angew Chem Int Ed Engl. 55, 11490-4., 2016
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Science Popularization and Public Outreach

Summer Symposium, July 1st, 2016, Sawaal Jawaab, Jul 16th, 2016, “Shapes and geometry of Surfaces”, Prof. Mahan Mj., TIFR, Mumbai Hosting visits from Multiple Schools at TCIS: Multiple Schools Visit at TCIS – “Fun with Magnets” and “Scientific Origami” 12th

January, 2017, Pune University, Pune March 6, 2017, BITS Pilani 26 March, 2016 Talk: Sriram Ramaswamy, TEDx lecture on Active Matter, National Institute of Technology Karnataka,, Surathkal, 18 Oct 2016



