Annual Report 2014 -15

TIFR Centre for Interdisciplinary Sciences

Professor K.V.R.Chary

Highlights

A putative UV inducible protein (UVI31+) from *Chlamydomonas reinhardtii* that exhibits RNA and DNA endonuclease activity was structurally characterized. S114A and S55A mutants of UVI31+ were shown to reduce and enhance the DNA endonuclease activity, respectively, as compared with its wild type.

In studying the liaison between myristoylation and cryptic EF-Hand motif that confers Ca^{2+} sensitivity to neuronal calcium sensor-1 (NCS-1), the disability of EF-1 was shown to be a prerequisite to append myristoylation signaling while preserving structural robustness and Ca^{2+} sensitivity and specificity in NCS-1.

In an *in-cell* NMR study, metabolic changes of live C. reinhardtii were followed during mixotrophic and heterotrophic conditions by monitoring $[1,2-^{13}C]$-labelled acetate assimilation and studied differential accumulation and mobilization of starch or/and lipids in *Chlamydomonas reinhardtii*.

A fast NMR methodology namely Ile, Thr and Val (ITV) specific (3, 2)D-CB(CACO)NNH was proposed to show the spectral signatures of the C-terminal sequential neighbors of Ile, Thr and Val in a highly resolved manner. This accelerates resonance assignment process significantly.

Text

Identification of C-terminal neighbours of residues that have only one $^{1}H^{\beta}$ attached to $^{13}C^{\beta}$: (Ile, Thr and Val) - specific (3,2)D-CB(CACO)NNH experiment: Sequence specific resonance assignment is the first and foremost step in determining the 3D structure of $^{13}C/^{15}N$-enriched proteins. Several double- and triple-resonance NMR experiments have been proposed in this direction for achieving unambiguous assignments. A fast NMR methodology namely Ile, Thr and Val (ITV) specific (3, 2)D-CB(CACO)NNH, which shows the spectral signatures of the C-terminal sequential neighbors of Ile, Thr and Val in a highly resolved manner, proposed. This helps in the generation of additional starting points along a given polypeptide chain, apart from the known conventional Ala, Gly, Ser

and Thr residues, and thus accelerate resonance assignment process significantly *(Chandra K, Patel S, Atreya H.S (IISc Bangalore) and Kandala V. R. Chary)*

Structure and Dynamics of a putative UV inducible protein (UVI31+) from *Chlamydomonas reinhardtii* that exhibits RNA and DNA endonuclease activity: *Chlamydomonas 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. The structure, dynamics and the putative function of UVI31+ has been studied. The calculated 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. The 3D structure of UVI31+ has three α-helices on one side of the protein, while the other side is formed by three β-strands and are glued by a strong hydrophobic core, providing a compact 3D protein structure. Twenty-three residue long polypeptide stretch connecting $\|_1$ and $\|_2$ strands was found to be highly flexible. Further, UVI31+ is found to recognize DNA primarily by its β-sheet domain with a dissociation constant of 52 nM. Point mutation at S114 of UVI31+ to Ala (S114A) reduced the endonuclease activity drastically, whereas shortening of the flexible loop did not affect the endonuclease activity. The S114A mutation showed DNA binding 10 fold weaker than wild-type-UVI31+. The proteins specific motif along with the long flexible loop holds the key to its multiple functions. *(Himanshu Singh, Sunita Patel, B. J. Rao, Kandala V R. Chary)*

Post-Translational Modification In Proteins: *In-Vivo* And *In-Vitro* Studies: Chlamydomonas reinhardtii is a unicellular algae, which undergoes apoptosis under UV-C irradiation. In order to understand UV induced apoptosis, an *in-silico* genome analysis was carried out that revealed the presence of UVI31+, a UV inducible gene. In an endeavour to understand the changes in UVI31+ upon UV exposure, we studied the possibility of various post-translational modifications of UVI31+ in general and phosphorylation in particular. With the help of NMR and mass spectrometry, UVI31+ was found to undergo reversible phosphorylation at position S67 in the presence of kinases. Phosphorylation brings about subtle conformational changes in UVI31+, as studied by CD and TNS binding studies, which in turn was found to affect the interaction of UVI31+ with pyrenoid, yet the endonuclease activity remained unaffected. Based on these observations, we attribute that phosphorylation might be an important event in controlling the localisation of the protein and hence its role in UV damage response. *(Deepshika Verma, Manish Shukla (DBS), B J Rao (DBS), K V R Chary).*

Site-specific fluorescence dynamics in a RNA thermometer reveals the role of ribosome binding in its temperature-sensitive switch function: Certain short mRNA sequences in the 5'-untranslated region have emerged as regulatory switches controlling translation. RNA thermometers control translation of several heat shock and virulence genes by using temperature-sensitive transitions in their structure. Changes in the structure and dynamics of MiniROSE RNA, which regulates translation in a certain range of temperature (20 to 45 °C) were studied by site-specifically replacing seven Ade residues with the fluorescent analog, 2-aminopurine (2-AP), one at a time. Fluorescence lifetime, fluorescence depolarization time and dynamic quenching constant of 2-AP labeled MiniROSE RNA were compared in free versus ribosome-bound states. Based on all the results, we proposed a four-state model where, for the first time, we invoked that ribosome binding of the RNA thermometer critically regulates the temperature sensing switches in MiniROSE RNA functions. (In collaboration with *Satya Narayan, M.H. Kombrabail, Sudipta Das (IIT, Kanpur), Himanshu Singh, K.V.R. Chary, B. J. Rao (DBS) and G. Krishnamoorthy).*

Liaison between Myristoylation and Cryptic EF-Hand Motif Confers Ca^{2+} Sensitivity to Neuronal Calcium Sensor-1: Many members of the neuronal calcium sensor (NCS) protein family have a striking coexistence of two characteristics, that is, N-myristoylation and the cryptic EF-1 motif. We investigated the rationale behind this correlation in neuronal calcium sensor-1 (NCS-1) by restoring Ca^{2+} binding ability of the disabled EF-1 loop by appropriate mutations. This study established the presence of the strong liaison between myristoylation and cryptic EF-1 in NCS-1. Breaking this liaison resulted in the failure of Ca^{2+} specific signal transduction to downstream effecter molecules despite Ca^{2+} binding. Thus, the EF-1 disability is a prerequisite in order to append myristoylation signaling while preserving structural robustness and Ca^{2+} sensitivity and specificity in NCS-1. *(K. Chandra, Y.Sharma (CCMB, Hyderabad), K.V.R. Chary).*

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 described 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 (DBS) , B J Rao (DBS), KVR Chary).*

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

- Elected Fellow of The World Academy of Sciences (FTWAS; 2014).
- J.C. Bose National Fellow, Department of Science and Technology, GoI, New Delhi, (2012-Present).
- Elected as Member, International Advisory Board, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2014-2016).
- Elected Chairperson, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2012-2014).
- Member, Expert Committee for review of the Department of Biotechnology, IIT Roorkee (2014-).
- Ex-officio, Executive Council, Indian Biophysical Society (2013-2015).
- Member, IUPAB National Committee of INSA (2012-16).
- Advisor, Royal Society of Chemistry, West India Section (2012-present).
- Council Member, International Council on Magnetic Resonance in Biological Systems (ICMRBS), 2005-2014.
- General Secretary, Executive Committee, ICMRBS, (2010-2012).
- Member, Project Management Committee of the 600 MHz NMR Facility, Indian Institute of Chemical Biology, Kolkata (2006-present). Member and Secretary of the International Union for Pure and Applied Biophysics (IUPAB), Task Force on NMR of Biological Systems (1998-present).
- Executive Council Member, Elected Hon. Chairman, Royal Society of Chemistry, West India Section, (2010-2012).
- 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-Present).
- 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 (CRSI), India and Indian Chemical Society, India.

Visits

- The Chemistry and Strcutural Biology Division, Institute for Molecular Bioscience, The University of Queensland, Australia, in August 2014.
- School of Chemistry, University of New South Wales, Sydney, on August 29, 2014.
- Prof. Martin Greens Laboratory, University of New South Wales, Sydney, on August 29, 2014

Awards and Distinctions

- Elected Fellow of The World Academy of Sciences (FTWAS; 2014).
- Elected as Member, International Advisory Board, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2014-2016).
- Elected as Chairperson, International Council on Magnetic Resonance in Biological Systems (ICMRBS), (2012-2014).
- Elected as an Ex-officio, Executive Council, Indian Biophysical Society (2013-2015).
- Elected as Treasurer and Steering Committee Member, Asian Biophysics Association (2013-present).
- Invited Speaker at International Union for Pure and Applied Biophysics (IUPAB) held at at the Brisbane Convention & Exhibition Centre, Brisbane, Australia, August 3-7, 2014.

Invited Talks in Conferences and Meetings

- Invited talk on Macromolecular Interactions by NMR: Functional manipulation of a calcium binding protein from E. *histolytica* guided by paramagnetic NMR, at the National Conference on Frontiers in Biotechnology and Bioinformatics 2014 D.Y. Patil College, New Mumbai, January 31, 2014.

- Invited talk on, Conformational Heterogeneity and Dynamics of a $\beta\gamma$-crystallin, an Intrinsically Disordered Protein, at the International Union for Pure and Applied Biophysics (IUPAB) held at the Brisbane Convention & Exhibition Centre, Brisbane, Australia, August 3-7, 2014.

- Plenary talk on Structure and Dynamics of Intrinsically Ordered and Disordered Proteins, at the Indo-US conference on Recent advances in Structural Biology and Drug Discovery (RASBDD-IIT-2014) from 9-11 October 2014 at IIT Roorkee.

Non DAE Research Projects

- Marie-Curie International Research Staff Exchange Scheme: Call identifier: FP7-PEOPLE-2009-IRSES (WW-NMR) under the Seventh Framework Programme of European Union.

Publications

1. 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.* 2015 Jan 21.

2. Narayan S, Kombrabail MH, Das S, Singh H, Chary KV, 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.* 2015 Jan 9;43(1):493-503.

3. Singh H, Shukla MR, Chary KV, Rao BJ. Acetate and bicarbonate assimilation and metabolite formation in *Chlamydomonas reinhardtii*: a 13C-NMR study. *PLoS One.* 2014 Sep 10;9(9):e106457.

4. Singh H, Rao BJ, Chary KV. ^{1}H, ^{13}C and ^{15}N NMR assignments of a mutant of UV inducible transcript (S55A-UVI31+) from *Chlamydomonas reinhardtii. Biomol NMR Assign.* 2014 Oct; 8(2):371-4. doi: 10.1007/s12104-013-9520-4. Epub 2013 Aug 27.

5. Lallan Mishra, Ruchi Gaur, A L Susmitha and K V R Chary, Water soluble Calcium-Sodium based coordination polymer: SelectiveRelease of Calcium at Specific Binding Sites on Protein, RSC Adv., 2014 (in press).

6. Sunita Patel, Atul Srivastava, Venkatraman Ramanujam and Kandala V R Chary, Conformational Propensities and Dynamics of a $\beta\gamma$-crystallin, an Intrinsically Disordered Protein, PCCP, 2014, 1-36.

7. Singh,H., Varma, D., Basuthkar J Rao, Kandala V R Chary, ^{1}H, ^{13}C and ^{15}N NMR assignments of Mg^{2+} bound form of UV inducible transcript protein (UVI31+) from *Chlamydomonas reinhardtii*. Biomol NMR Assignments, 2014, 8(1), 71-4.

Graduate Courses

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

Ph.D. Theses / M.Sc. Theses

- Ms. Susmitha (2008-2014) JRF/SRF of ICMR received her Ph.D from BHU, Varanasi.

Professor N.D. Hari Dass

Highlights

Solved the problem of repeated weak measurements in quantum theory.
Repeated weak measurements in quantum theory: an outstanding problem in quantum measurements has been whether repeated weak measurements can determine an unknown state. I have solved this problem and the answer is NO.
Ontology and Quantum Mechanics: The issue of ontology in quantum mechanics, is critically examined within standard quantum theory. It is argued that though no strict ontology is possible within quantum theory, ingenious measurement schemes may still make the notion of a FAPP Ontology i.e ontology for all practical purposes meaningful and useful.

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

- Editorial Boards of the international journals QUANTA, Journal of Quantum Information Science, Applied Mathematics and Information Science Letters.

Visits

i. Visited the Institute of Mathematical Sciences, Chennai, during April 2014.

ii. Visited the Institute of Mathematical Sciences, Chennai, during 16-26 Jan 2015.

iii. Visited the Chennai Mathematical Institute, Chennai, during 2-6 Mar 2015.

Publications

a) In Journals

- Ontology and Quantum Mechanics, published in QUANTA Vol 3 No 1 (2014) p.47-66.

b) In Proceedings

- The superposition principle in quantum mechanics - did the rock enter the foundation surreptitiously?, being published in the proceedings of the conference '100 years of the Bohr Atom 1913-2013 by the Royal Danish Academy of Sciences.

c) Web Publications

- Repeated weak measurements on a single copy are invasive, submitted to Physical Review Letters, recommended by one referee for publication in Physical Review E; arXiv 1406.0270[quant-ph].

Lectures / Lecture Courses Given Elsewhere

i. A massive saga, colloquium at the Institute of Mathematical Sciences, 23 April 2014.

ii. Non-GR approaches to Gravitational Radiation, at the Institute of Mathematical Sciences, Chennai, on 20 Jan 2015.

Graduate Courses

1. Classical Electrodynamics-II (Jan-Apr 2014 semester at TCIS).

2. Field Theory (Jan-Apr 2015 at TCIS).

Dr. Kanchan Garai

Highlights

My paper titled The binding of apolipoprotein E to oligomers and fibrils of amyloid-β alters the kinetics of amyloid aggregation published in Biochemistry. 2014 was chosen to be highlighted in the journal website. This paper examines the biophysical characteristics of the apoE-Aβ interactions which is an extremely important event in the pathology of Alzheimer's disease. The key progress made in the last one year is the following:

a) Established the biochemistry lab at TCIS for protein expression, purification and characterization using fluorescence based assays. We have successfully purified two recombinant proteins apoE and α-synuclein.

b) We have built a fluorescence correlation spectroscopy (FCS) set up in house for characterization of protein dynamics and protein-protein interactions.

c) We are developing assays for measurement of solubility of amyloid proteins. We discovered that these proteins have at least two solubilities, one for the native random coil state and the other for the (mis-)folded amyloid state.

d) We have made significant progress in development of a quantitative framework to measure amyloid fibril stability. Our results suggest that under denaturing conditions amyloid fibrils denature rapidly but dissociate slowly.

Invited Talks in Conferences and Meetings

a) Invited speaker at annual conference Frontiers in Physics-2014 from October 17 to 18, 2014

b) Invited speaker at International conference: STATPHYS - KOLKATA VIII (2014) at Kolkata during Dec 1-4, 2014.

Other conferences attended:

a) Attended International Conference on Soft Materials (ICSM) in Jaipur during Oct 6-10, 2014.

b) Session chair and poster presentation at The Second International Symposium on Protein Folding and Dynamics at NCBS, Bangalore during Nov 5-7, 2014.

Publications

1. Holehouse AS, **Garai K**, Lyle N, Vitalis A, Pappu RV. Quantitative assessments of the distinct contributions of polypeptide backbone amides versus side chain groups to chain expansion via chemical denaturation. J Am Chem Soc. 2015 Mar 4;137(8):2984-95. doi: 10.1021/ja512062h.

2. **Garai K**, Verghese PB, Baban B, Holtzman DM, Frieden C. The binding of apolipoprotein E to oligomers and fibrils of amyloid-β alters the kinetics of amyloid aggregation. Biochemistry. 2014 Oct 14;53(40):6323-31. doi: 10.1021/bi5008172.

3. Sundaram GS, **Garai K**, Rath NP, Yan P, Cirrito JR, Cairns NJ, Lee JM, Sharma V. Characterization of a brain permeant fluorescent molecule and visualization of Aβ parenchymal plaques, using real-time multiphoton imaging in transgenic mice. Org Lett. 2014 Jul 18;16(14):3640-3. doi: 10.1021/ol501264q.

Lectures / Lecture Courses Given Elsewhere

a) Taught and coordinated the course of lab techniques in the chemical sciences in the first semester 2014 at TCIS.

b) Teaching Biophysics in the 2nd semester 2015 at TCIS jointly with Dr. Pramodh Vallurupally.

Professor Rama Govindarajan

Highlights

Particulate flows

- It is commonly believed that particles in a vortical flow leave regions of high vorticity and cluster in regions of high strain. We showed (Ravichandran, Perlekar and Govindarajan, Phys. Fluids 2014) that particles in a moving frame can cluster within closed streamlines. This could have implications a range of particulate flow, including for how cloud droplets aggregate in a cloud.

Droplets and bubbles

- We showed that a rising drop and a falling bubble are fundamentally different because of the tendency for vorticity to concentrate in the lighter fluid. We obtained a phase diagram for different regimes of bubbles rise though a quiescent liquid. This appeared in Nature Communications (Tripathi, Sahu and Govindarajan 2015).

- Regimes demarcated on the basis of bubble behaviour shape and behaviour, namely, axisymmetric (circle), asymmetric (solid triangle) and breakup (square). The axisymmetric regime is called region I. The two colors within the asymmetric regime represent the non-oscillatory region II (shown in green), and the oscillatory region III (blue) dynamics. The two colors within the breakup regime represent the peripheral breakup, region IV (light yellow), and the central breakup region V (darker yellow). The red dash-dotted line is the Mo = 0.001, above which oscillatory motion is not observed in experiments. Typical bubble shapes in each region are shown.

Figure / Photograph Captions

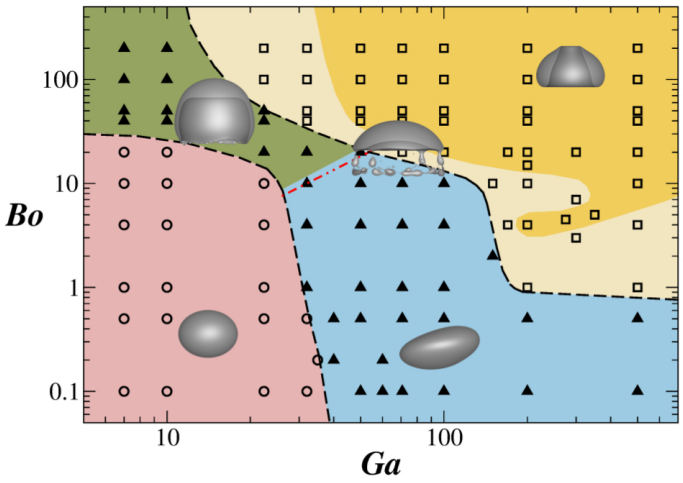


Figure 1: Phase Plot

Staff List

Project assistants

- Ritabrata Thakur
- Bharath Narayanan

Post-Doc

- Manoj Tripathi

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

- On the Editorial Board of Pramana
- On the Editorial Advisory Board of Physics of Fluids.

Visits

- Invited speaker at "Mathematical Modelling of Particles in Turbulent Flow", Banff International Research Station, Canada. 22-26 August 2014.

Awards and Distinctions

- Member, IUTAM Symposia Panel for Fluid Mechanics, 2014 onwards.
- Member, Frenkiel Award Committee, APS Division of Fluid Dynamics.
- Fellow of the American Physical Society in November 2013

Invited Talks in Conferences and Meetings

- "Mathematical Modelling of Particles in Turbulent Flow", Banff International Research Station, Canada. 22-26 August 2014.
- UOP India Technical Community Symposium, Gurgaon September 2014.
- (Royal Society) Commonwealth Science Conference, Bengaluru, November 2014.
- IIT Bombay Climate Workshop, 2014.
- Indian Statistical Physics Community Meeting Feb 2015.
- UoH, Workshop on writing for journals, feb 2015.
- IIT-TCIS Intergroup Annual meeting, Jan 2015.

Conference Organised by the School / Deptt. / Group

- IUTAM Symposium on Laminar-Turbulent Transition, December 2014. Co-organiser and scientific committee member.
- IITB-IITH-TCIS Annual Intergroup meeting, Jan 2015.

Non DAE Research Projects

- CEFIPRA
- OMM

Publications

a) In Journals **2015**

- Dynamics of an initially spherical gas bubble rising in quiescent liquid. Manoj Tripathi, Kirti Sahu & Rama Govindarajan. Nature Communications, 6, 6268.

- Morphological evolution of domains in spinodal decomposition. Charu Datt, Sumesh P. Thampi & Rama Govindarajan. Physical Review E Rapid Comm., 91, 010101(R).
- The effect of initial momentum flux on the circular hydraulic jump. Vishwanath Sastry, Ratul Dasgupta, Rama Govindarajan & KR Sreenivas. ASME Journal of Fluids Engineering, 137(6), 061301.
- Rolling motion in moving droplets. Sumesh Thampi & Rama Govindarajan, Pramana, 84, 409-421.

2014 (after March)

- Instability of a free shear layer in the vicinity of a viscosity-stratified layer, Kirti Chandra Sahu & Rama Govindarajan, Journal of Fluid Mechanics, 752 (2014): 626-648.
- Attracting fixed points for heavy particles in the vicinity of a vortex pair. Ravichandran Sivaramakrishnan, Prasad Perlekar and Rama Govindarajan. Physics of Fluids, 26, 013303.
- A minimal model for flow control on an airfoil using a poro-elastic coating. Divya Venkataraman, Alessandro Bottaro and Rama Govindarajan. Journal of Fluids and Structures, 47, 150164.
- Why a falling drop does not in general behave like a rising bubble, Manoj Kumar Tripathi, Kirti Chandra Sahu & Rama Govindarajan. Scientific Reports, 4, No. 4771.
- Nonlinear dynamical systems, their stability and chaos. (Lecture notes from the FLOW-NORDITA Summer School on Advanced Instability Methods for Complex Flows, Stockholm, Sweden, 2013) Amol Marathe and Rama Govindarajan, Applied Mechanics Reviews, 66(2), 024802.

b) In Proceedings

- Vortex Filament and Global Instability Analysis of the Crow Mode. Juan ngel Tendero, Pedro Paredes, Miquel Roura, Rama Govindarajan, Vassilios Theofilis. Instability and Control of Massively Separated Flows. Fluid Mechanics and Its Applications, 107, 229-234.
- Laminar Separation Bubbles in Two-Dimensional Straight-Diverging-Straight Channel Flows, Mamta Jotkar, Jos Miguel Prez, Vassilis Theofilis, Rama Govindarajan, Instability and Control of Massively Separated Flows, Fluid Mechanics and Its Applications Volume 107, 177-182.

Lectures / Lecture Courses Given Elsewhere

- SS Bhatnagar Anniversary Celebrations, Punjab University Chandigarh, Feb 2015.
- NITK Surathkal, Mar 2015.
- IIT Bombay, Sep 2014.
- ICTS
- TIFR-CAM: Jan 2015, set of three lectures & Several others.

Lectures by Visitors

- Several

Graduate Courses

- Mathematical Methods Aug semester
- Nonlinear dynamics: this semester (co-teaching with Surajit Sengupta)

Ph.D. Theses / M.Sc. Theses (Please indicate the University awarding the degree)

- Manoj Tripathi, IIT Hyderabad, Co-advisor.

Dr. Anukul Jana

Staff List

- Mr. Amit Malakar; Project Student (May 2014 to Dec 2014)
- Mr. Sourav Sarkar; Summer Project Student (May 2014 to June 2014)
- Mr. Debabrata Dhara; Project B and PhD Student (August 2014 to)
- Mr. Debdeep Mandal; Project B and PhD Student (August 2014 to)

Invited Talks in Conferences and Meetings

- **24-26th September, 2014:** Presented a poster in Whler Conference, Saarland University, Germany with a title of "Unsaturated Ge2 Moieties with Directly Attached and Remote Functional Groups"
- **10-11 December, 2014:** Attend a meeting of New Directions in Chemical Synthesis-II (Inorganic Synthesis) at IIT Bombay, India

Non DAE Research Projects

- Investigators: Anukul Jana
- Title: Design and utility of appropriate anionic ligands for the syntheses and mutual conversion of multiple bond of heavier Group 14.
- Funding Agency: Alexander von Humboldt Foundation
- Duration: one-time Equipment Grant
- Amount: EUR 20,000-

Publications

a) In Journals

1. ***Anukul Jana***, *Volker Huch, Henry S. Rzepa and David Scheschkewitz* "A Molecular Complex with a Formally Neutral Iron Germanide Motif (Fe_2Ge_2)"
   Organometallics ***2015***, *34, DOI: 10.1021/om501286g*
2. ***Anukul Jana***, *Volker Huch, Henry S. Rzepa and David Scheschkewitz* "A Multiply Functionalized Base-Coordinated GeII Compound and Its Reversible Dimerization to the Digermene"
   Angew. Chem. Int. Ed. **2015**, *54*, 289292.

3. ***Anukul Jana***, *Isabell Omlor, Volker Huch, Henry S. Rzepa and David Scheschkewitz* N-Heterocyclic Carbene Coordinated Neutral and Cationic Heavier Cyclopropylidenes
Angew. Chem. Int. Ed. **2014**, *53*, 99539956.

Lectures / Lecture Courses Given Elsewhere

- **5 November 2014:** "Multiple Bonded Compounds in Heavier Elements" at In-House Symposium 2014 of TCIS, Hyderabad, India.
- **19 February 2015:** "Recent Advances in Main Group Chemistry" at NISER Bhubaneswar, India.
- **26 February 2015:** "Low-Valent Main Group Chemistry: Beyond Academic Curiosity" at Jadavpur University, India.
- **2-7 March 2015:** Special lectures on "Chemistry of Low-Valent Low-Coordination" in TIFR Mumbai for Chemistry Graduate students as part of "Advanced Inorganic and Bioinorganic Chemistry" course.

Graduate Courses

- August - November 2014: "Advanced Inorganic and Organic Chemistry" course for first year Chemistry PhD students.

Any other information

- Member of the Chemistry Subject Board of TIFR Mumbai

Dr. Smarajit Karmakar

Highlights

I. DISTRIBUTION OF DIFFUSION CONSTANTS AND STOKES-EINSTEIN VIOLATION IN SUPERCOOLED LIQUIDS

It is widely believed that the breakdown of the Stokes-Einstein relation between the translational diffusivity and the shear viscosity in supercooled liquids is due to the development of dynamic heterogeneity *i.e.* the presence of both slow and fast moving particles in the system. In this study we *directly* calculate the distribution of the diffusivity for a model system for differenet temperatures in the supercooled regime. We find that with decreasing temperature, the distribution evolves from Gaussian to bimodal indicating that on the time scale of the α relaxation time, mobile (liquid like) and less mobile (solid like) particles in the system can be *unambiguously* identified. We also show that less mobile particles obey the Stokes-Einstein relation even in the supercooled regime and it is the mobile particles which show strong violation of the Stokes-Einstein relation. Finally, we show that the degree of violation of the Stokes-Einstein relation can be tuned by introducing randomly pinned particles in the system.

Authors : Shiladitya Sengupta (JNCASR, Bangalore and TIFR-H, Hyderabad) and **Smarajit Karmakar**

Publication : Distribution of Diffusion Constants and Stokes-Einstein Violation in supercooled liquids - Shiladitya Sengupta and Smarajit Karmakar J. Chem. Phys. **140**, 224505 (2014).

II. PHASE DIAGRAM OF GLASS FORMING LIQUIDS WITH RANDOMLY PINNED PARTICLES

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 pin concentration is a probable reason for this difference.

Authors : Saurish Chakrabarty (IISc, Bangalore), **Smarajit Karmakar**, Chandan Dasgupta (IISc, Bangalore).

Publication : Phase Diagram of Glass Forming Liquids with Randomly Pinned Particles - Saurish Chakrabarty, Smarajit Karmakar, Chandan Dasgupta arXiv:1404.2701 (Under review for publications).

III. THE STATIC LENGTHSCALE CHARACTERIZING THE GLASS TRANSITION AT LOWER TEMPERATURES

The existence of a static lengthscale that grows in accordance with the dramatic slowing down observed at the glass transition is a subject of intense interest. A recent publication compared two proposals for this length scale, one based on the point-to-set correlation technique and the other on the scale where the lowest eigenvalue of the Hessian matrix becomes sensitive to disorder. The conclusion was that both approaches lead to the same lengthscale, but the former is easier to measure at higher temperatures and the latter at lower temperatures. But even after using both methods together, the range of increase in the observed lengthscales was limited by the relaxation times reachable by standard molecular dynamics techniques (i.e. about 4-5 orders of magnitude). In this paper we therefore attempt to explore the typical scale at even lower temperatures, testing for this purpose two approaches, one based on the idea of vapor deposition and the other on a swap Monte Carlo technique. We conclude that the first approach does not help in getting to lower temperatures, but the second one does so quite effectively. We can reach a typical lengthscale that grows in accordance with at least 15 orders of magnitude increase in the relaxation time, competing with the best experimental conditions. We conclude by discussing the relationship between the observed lengthscale and various models of the relaxation time.

Authors : Ricardo Gutierrez (Israel), **Smarajit Karmakar**, Yoav G. Pollack (Israel), Itamar Procaccia (Israel).

Publication : The Static Lengthscale Characterizing the Glass Transition at Lower Temperatures - Ricardo Gutierrez, Smarajit Karmakar, Yoav G. Pollack, Itamar Procaccia, arXiv:1409.5067, (Euro. Phy. Lett 2014).

IV. 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 densitytemperature 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 con

rmed by suitable experiments on patchy colloids.

Authors : Chandana Mondal, **Smarajit Karmakar**, and Surajit Sengupta.

Publication : Glass-Like Slow Dynamics in a Colloidal Solid with Multiple Ground States - Chandana Mondal, Smarajit Karmakar, and Surajit Sengupta, The Journal of Physical Chemistry B 2015

Staff List (Students and Post Doctoral Fellows):

1. Jeetu S Babu (Mar 2014 - Mar 2015), Post Doctoral Fellow
2. Indrajit Tah, PhD Student
3. Rajshekher Das, PhD Student
4. Bhanu Prasad Bhowmik, PhD Student
5. Kallol Paul, PhD Student

Invited Talks in Conferences and Meetings

1. Discussion Meeting on Glass Formers and Glasses, JNCASR, Bangalore August 8-9 (2014).
2. Frontiers in Physics-2014, School of Physics, University of Hyderabad, October 17 - 18 (2014).

3. STATPHYS - KOLKATA VIII, S. N. Bose National Centre for Basic Science, Kolkata, December 1 - 5 (2014).

4. Fracture: from micro-scale processes to macro-scale response, IMSc, Chennai, January 06 - 10 (2015).

5. Current Trends in Condensed Matter Physics - 2015, NISER, Bhubaneswar, 19th-22nd February (2015).

6. Discussion Meeting on Glass Formers and Glasses, JNCASR, Bangalore, March 27 -28 (2015).

Publications

1. Distribution of Diffusion Constants and Stokes-Einstein Violation in supercooled liquids - Shiladitya Sengupta and Smarajit Karmakar J. Chem. Phys. **140**, 224505 (2014)].

2. Glass-Like Slow Dynamics in a Colloidal Solid with Multiple Ground States - Chandana Mondal, Smarajit Karmakar, and Surajit Sengupta, The Journal of Physical Chemistry B 2015 (DOI: 10.1021/jp512952u).

3. Phase Diagram of Glass Forming Liquids with Randomly Pinned Particles - Saurish Chakrabarty, Smarajit Karmakar, Chandan Dasgupta arXiv:1404.2701 (Under review for publications).

4. The Static Lengthscale Characterizing the Glass Transition at Lower Temperatures - Ricardo Gutierrez, Smarajit Karmakar, Yoav G. Pollack, Itamar Procaccia, arXiv:1409.5067 (Euro. Phy. Lett 2014).

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

V. MANUSCRIPTS UNDER PREPARATION :

1. Dynamics dependence of four-point susceptibility for glass forming liquids in two and three dimensions - Saurish Chakrabarty, Smarajit Karmakar, and Chandan Dasgupta (2015)

2. New Growing Length-scale, Fragility and Random First Order Transition Theory in glass forming liquids with Random Pinning - Saurish Chakrabarty, Smarajit Karmakar, and Chandan Dasgupta (2015)

3. β-relaxation in glass forming liquids - Smarajit Karmakar, Chandan Dasgupta and Srikanth Sastry (2015)

4. Excess Density of States and Brittle-Ductile Transition in Crystalline and Amorphous solids - Jeetu S Babu, Chandana Mondal, Surajit Sengupta, Smarajit Karmakar (2015)

5. Understanding Cavitation in Amorphous solids - Jeetu S Babu, Ratul Dasgupta, Smarajit Karmakar (2015)

6. Dynamics and Thermodynamics in two dimensional glass forming liquids with medium range crystalline order - Smarajit Karmakar, Shiladitya Sengupta, Chandan Dasgupta and Srikanth Sastry (2015)

Lectures / Lecture Courses Given Elsewhere

1. Colloquium: TIFR-Mumbai NSF Colloquium, 26th Nov. 2014.

2. Aug - Nov 2014 : Advanced Statistical Mechanics

3. Jan - April 2015 : Numerical Methods (together with P. Perlekar)

Dr. Aprotim Mazumder

Highlights

DNA damage is ubiquitous in nature, and cellular response to it as diverse. A vast body of literature has established an intimate link between DNA damage responses (DDR) and the emergence of cancer, neurodegeneration and premature aging. Perturbations of specific DNA repair pathways are often associated with cancers in specific tissues. The broad aims of my research are to elucidate the tissue-specific emergence of cancer with mutations in specific DNA repair pathways, and investigate the roles of DDR in tissue-specific differentiation. I have been at TIFR for just two months (as of April 2015) and before this was a postdoctoral researcher at the Massachusetts Institute of Technology (MIT). Going beyond cells in culture, in the past year I developed methods to assay single-cell DDR in primary mammalian tissue, as a part of a broader work reporting differential DDR in mice of different genotypes of interest. See the work by Ebrahimkhani et al in *PNAS* last year. This work was carried out at the Samson laboratory at MIT, Cambridge, MA, USA.

Staff List

- My lab is new and I am in the process of recruiting staff.

Visits

- **IFOM, Milan, Italy** - Visited to interact deliver a seminar in May 2014 upon invitation.
- **inStem, Bangalore, India** - Visited to interact deliver a seminar in August 2014 upon invitation.

Awards and Distinctions

- The Koch Institute Image Award (2014) (featured on www.cell.com)

Invited Talks in Conferences and Meetings

- Aprotim Mazumder, Young Investigators Meeting, March 2015.

Publications

Ebrahimkhani, M.R., Daneshmand, A., Mazumder, A., Allocca, M., Calvo, J.A., Abolhassani, N., Jhun, I., Muthupalani, S., Ayata, C., Samson, L.D. Aag-initiated base excision repair promotes ischemia reperfusion injury in liver, brain, and kidney. (2014) *PNAS of USA*, 11;111(45):E4878

Dr. T.N. Narayanan

Highlights

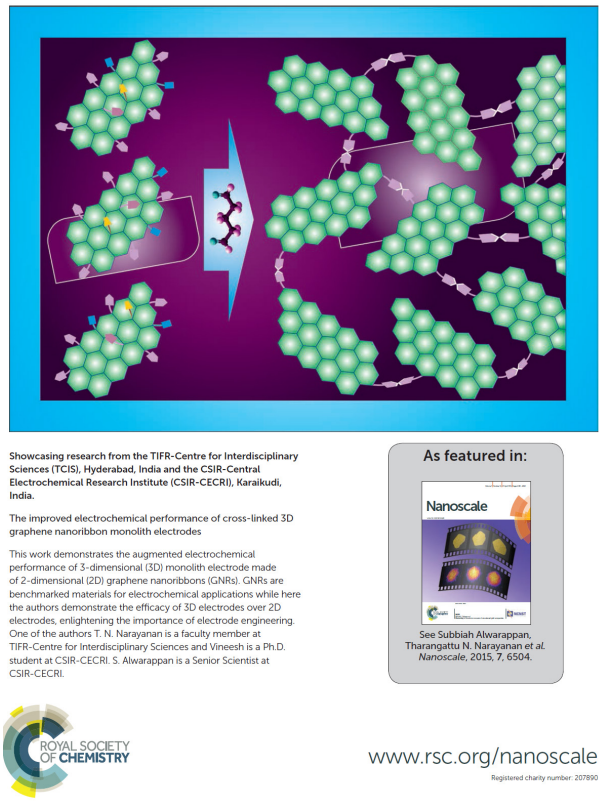
Our research group studies the interface induced properties of nanomaterials, and tuning the properties for finding applications in energy and environment related technologies. The key findings of the last one year include the following;

a) Developed new 3-dimensioanl architecture for electrodes using atomically thin graphene nanoribbons, and established that the new geometry has an enormous advantage over conventional electrode designs in energy technologies and catalysis.

b) Engineering the wettability of the surfaces is highly intriguing in many fields. But, engineering the wettability of a surface while keeping the optical transparency is fascinating. Our group developed a transparent polymer paint containing fluorinated graphene oxide nanosheet fillers, and using a simple spray painting technique, we established that the coatings have a water contact angle $\sim$174 °C, the highest ever reported contact angle. A detailed study has been conducted for understanding the effect of fluorine in graphene matrix in minimizing its surface energy.

c) Graphene has been identified as a potential electrode material, where it can act as a metal free light weight electrode with high optical transparency, conductivity and carrier mobility. Graphene synthesis technology is also reaching the technology readiness level 9 (TRL9), which implies immediate availability for commercialization. But pristine graphene is not interesting in many applications, particularly in electronic as well as electrochemical applications. Doped graphene is an attractive candidate for these applications but development of bulk amount of doped graphene is still infancy. Recently our group developed a 2-step simple process for the development boron doped graphene (an Indian patent application is field: A process for development of heteroatoms doped layered graphene from boron carbide, T N Narayanan, Deepak P, and Praveen Kumar, Indian Patent Application Number: 2354Del2014). Moreover, this graphene shows excellent properties compared to the existing reports when it is tested towards various electrochemical reactions and it acts like a bi-functional catalyst (water oxidation and oxygen reduction).

Figure / Photograph Captions:



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

- Affiliated Member of Royal Society of Chemistry (Membership Number#564616).

Invited Talks in Conferences and Meetings

1. 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. **(Invited Talk)**.

2. 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. **(Invited Talk)**

3. Fascinating Carbon Science, **T. N. Narayanan**, Sri Vyasa NSS College, Wadakkanchery, Kerala February 4, 2015 **(Invited Talk)**.

4. Engineered 2D Materials for Efficient Bio-Sensors, **T N Narayanan, MRS Fall Meeting**, Boston, USA, November 30 and December 5, 2014. **(Invited Talk)**

Publications

a) In Journals

1. The Improved Electrochemical Performance of 3D Graphene Nanoribbon Monolith Electrodes, T. V. Vineesh,S Alwarappan, and T N Narayanan,* Nanoscale 7, 6504, 6509 (2015). (*Corresponding Author) [Cover Page] [Paper]
2. Atomic Layers in Electrochemical Biosensing Applications Graphene and Beyond, O. V. Manila, A. Alwarappan, T. N. Narayanan,* Current Organic Chemistry. (Accepted). Corresponding author. *(Invited Review Article)*
3. Graphene-Protein Field Effect Biosensors: Glucose Sensing, Sowmya Viswanathan, T. N. Narayanan, Kathryn D. Fink, Jacobo Paredes,P. M. Ajayan, Slawomir Filipek, Przemyslaw Miszta, M. Gurusaran, H. Cumhur Tekin, Fatih Inci, Utkan Demirci, Pingzuo Li, Kirill I. Bolotin, Dorian Liepmann, and V. Renugopalakrishanan, Materials Today.
4. Above 170° Water Contact Angle and Oleophobicity of Fluorinated Graphene Oxide Based Transparent Polymeric Films, T. Bharathidasan, T. N. Narayanan,* S. Sathyanaryanan, and S. S. Sreejakumari, Carbon 84, 207-213 (*Corresponding Author) (Paper)
5. Probing the engineered sandwich network of vertically aligned carbon nanotube-reduced graphene oxide composites for high performance electromagnetic interference shielding applications, Avanish Pratap Singh, Monika Mishra, Daniel P. Hashim, T. N. Narayanan, Myung Gwan Hahm, Pawan Kumar, Jaya Dwivedi, Garima Kedawat, Ankit Gupta, Bhanu Pratap Singh, Amita Chandra, Robert Vajtai, S. K. Dhawan, Pulickel M. Ajayan and Bipin Kumar Gupta, Carbon 85, 79-88. (Paper)

b) In Proceedings

1. Engineered 2D Materials for Efficient Biosensors, T. N. Narayanan,* P. M. Ajayan, Sowmya Viswanathan, M. Gurusaran, and V. Renugopalakrishanan, Mater. Res. Soc. Symp. Proc. Vol. 1725 DOI: 10.1557/opl.2015.202 (2015). (*Corresponding author)

2. Small Angle Neutron Scattering Studies of Glucose Oxidase Immobilized on Single Layer Graphene: Relevant to Protein Microfluidic Chip, Manickam Gurusaran, Durgesh Rai, Shuo Qian, Kevin Weiss, Volker Urban, Pingzuo Li, Lulu Ma, T. N. Narayanan, Pulickel M Ajayan, Kanagaraj Sekar, Sowmya Viswanathan, Venkatesan Renugopalakrishanan, Biophysical journal, 108 (2), 327a-328b (2015).

Dr. Prasad Perlekar

Highlights

a) Two-dimensional homogeneous isotropic fluid turbulence with polymer additives

We carry out an extensive and high-resolution direct numerical simulation of homogeneous, isotropic turbulence in two-dimensional fluid films with air-drag-induced friction and with polymer additives. Our study reveals that the polymers (a) reduce the total fluid energy, enstrophy, and palinstrophy; (b) modify the fluid energy spectrum in both inverse- and forward-cascade rgimes; (c) reduce small-scale intermittency; (d) suppress regions of high vorticity and strain rate; and (e) stretch in strain-dominated regions. We compare our results with earlier experimental studies and propose new experiments.

b) Direct evidence of plastic events and dynamic heterogeneities in soft-glasses

By using fluid-kinetic simulations of confined and concentrated emulsion droplets, we investigate the nature of space non-homogeneity in soft-glassy dynamics and provide quantitative measurements of the statistical features of plastic events in the proximity of the yield-stress threshold. Above the yield stress, our results show the existence of a finite stress correlation scale, which can be mapped directly onto the cooperativity scale, recently introduced in the literature to capture non-local effects in the soft-glassy dynamics. In this regime, the emergence of a separate boundary (wall) rheology with higher fluidity than the bulk is highlighted in terms of near-wall spontaneous segregation of plastic events. Near the yield stress, where the cooperativity scale cannot be estimated with sufficient accuracy, the system shows a clear increase of the stress correlation scale, whereas plastic events exhibit intermittent clustering in time, with no preferential spatial location. A quantitative measurement of the space-time correlation associated with the motion of the interface of the droplets is key to spot the elastic rigidity of the system.

Invited Talks in Conferences and Meetings

- Prasad Perlekar, Two dimensional turbulence with polymer additives, Current Trends in Condensed Matter Physics, Bhubaneshwar, India, 19-20 Feb. 2015
- Prasad Perlekar, Two dimensional turbulence in symmetric binary mixtures, Compflu 2014, JNCASR, Bangalore, 22-24 December 2014

- Prasad Perlekar, Inertial particle clustering in rotating Rayliegh-Benard convection, Conference on Dynamics of Particles in Flows, NORDITA, Stockholm, June 2014.
- Prasad Perlekar, Active fluids: new challenges from experiments to HPC, Mariehamn, Finland.

Publications

a) In Journals

1. A. Gupta, P. Perlekar, and R. Pandit, Two-dimensional homogeneous isotropic fluid turbulence with polymer additives, Physical Review E, 91, 033013 (2015).
2. R. Benzi, M. Sbragaglia, A. Scagliarini, P. Perlekar, M. Bernaschi, S. Succi, and F. Toschi, Internal Dynamics and activated processes in soft-glassy materials, Soft Matter, 11, 1271 (2015).

Graduate Courses

1. Classical Mechanics
2. Numerical Methods

Professor Sriram Ramaswamy (Centre Director)

Highlights

Press coverage of our work:

Flocking at a distance in active granular matter, Nitin Kumar, Harsh Soni, Sriram Ramaswamy and A.K. Sood, Nature Communications **5**: 4688 doi:10.1038/ncomms5688 (2014); arXiv:1402.4262v2; highlighted in Science, Nature Materials, Nature India, The Telegraph

Staff List:

a) **TCIS Students:** Harsh Soni, Suropriya Saha, Ananyo Maitra (the first two were supported as JRFs at TCIS, TIFR; all three have submitted their PhD theses to IISc, two have defended and the third will shortly; all three have accepted postdoctoral positions, Maitra at Université Paris Sud, Saha at MPIPKS Dresden, Soni at Brown University)

b) **External Students:** Sabiha Sachdeva and Ranjan Krishna Modak (based at IISc where their primary supervisors are working)

c) **Student interns:** Surbhi Hablani, BS from Skidmore College, New York, working on a research project on colloidal microswimmers; Rahul Chajwa, IISER Mohali, working on instabilities in collective sedimentation (jointly with Narayanan Menon)

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

- Fellow of Indian Academy of Sciences since 1996, and Fellow of INSA since 2003.
- Member, Editorial Boards of: *Annual Review of Condensed Matter Physics* since 2011, *Advances in Physics* since 2007, *European Physical Journal E* since 2009, *Journal of Statistical Mechanics: Theory and Experiment* since 2003; member, Advisory Board of *Soft Matter* since 2008. Associate of the Higgs Centre, University of Edinburgh, since March 2013

Invited Talks in Conferences and Meetings

1) Invited lecture, German Physical Society (special session in honour of Siegfried Hess), Berlin, March 2015

2) Invited public lecture, S S Bhatnagar Institute for Chemical Engineering and Technology, Panjab University, Chandigarh, 21 Feb 2015

3) Invited lecture, Current Topics in Condensed Matter Physics, NISER, Bhubaneswar, 19-21 Feb 2015

4) Invited lecture, Mini Statmech Meeting, Berkeley, Jan 2015

5) Invited lecture, Focused Program on Physics Approach to Simplifying Complexity in Biology, Hong Kong University of Science and Technology, Dec 2014

6) Invited public lecture, Soft Matter Program, Syracuse University, October 2014

7) Invited lecturer, Beg Rohu summer school on statistical physics and condensed matter, Quiberon, Brittany, France, Sep 2014.

8) Invited speaker, conference in honour of Aneesur Rahman, Univ of Hyderabad, Aug 2014

9) Coordinator (with M C Marchetti and C Schmidt) of the Program on Active Matter: Cytoskeleton, Cells, Tissues and Flocks, KITP, UC Santa Barbara, Jan-May 2014.

Publications:

1) Anisotropic Isometric Fluctuation Relations in experiment and theory on a self-propelled rod, Nitin Kumar, Harsh Soni, Sriram Ramaswamy, and A.K. Sood, Phys Rev E (Rapid) **91**, 030102 (Rapid) (2015); `arXiv:1502.04466`

2) Active Viscoelastic Matter: from Bacterial Drag Reduction to Turbulent Solids, E. J. Hemingway, A. Maitra, S. Banerjee, M. C. Marchetti, S. Ramaswamy, S. M. Fielding, M. E. Cates, Phys. Rev. Lett. **114**, 098302 (2015) `arXiv:1410.6077`

3) Flocking at a distance in active granular matter, Nitin Kumar, Harsh Soni, Sriram Ramaswamy and A.K. Sood, Nature Communications **5**: 4688 `doi:10.1038/ncomms5688` (2014); `arXiv:1402.4262v2`;

4) Universal power law in crossover from integrability to quantum chaos, R Modak, S Mukerjee, S Ramaswamy, Phys. Rev. B **90** (2014) 075152; `arXiv:1309.1865`.

5) Aspects of the density field in an active nematic, S Mishra, S Puri and S Ramaswamy, Phil. Trans. R. Soc. A **372**: 20130364 (2014); `http://dx.doi.org/10.1098/rsta.2013.0364`

6) Activating membranes, A Maitra, P Srivastava, M Rao and S Ramaswamy, Phys Rev Lett **112** (2014) 258101; arXiv:1311.5055.

7) Clusters, asters and collective oscillations in chemotactic colloids, S Saha, R Golestanian, S Ramaswamy, Phys Rev E **89** (2014) 062316; arXiv:1309.4947.

Professor Surajit Sengupta

Highlights

Our paper: N. Ganai, S. Sengupta and G. I. Menon, *Chromosome positioning from activity-based segregation.* Nucleic Acids Research, **42**, 4145 (2014) got selected by the Journal Club of Condensed Matter Physics to be commented upon in the January 2015 edition (Chromosome positioning from activity-based segregation). According to the commentator: The paper of Ganai et al. is a very original paper, which studies in details an interesting conjecture that goes well with the intuition that the structure of the nucleus must have biological relevance.

Text

Polymorphism and the glass transition in patchy colloids

- We have studied 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 have determined the phase diagram in the densitytemperature plane. We obtained 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 showed 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. Our claim that geometrical frustration arising from the presence of many competing crystalline ground states is the cause for glassy ordering and dynamics in this solid is therefore substantiated. Our results may be easily confirmed by suitable experiments on patchy colloids.

  with Chandana Mondal, (Weizmann, Israel) and Smarajit Karmakar (TCIS, Hyderabad)

Tailoring defect densities in crystals using light fields

- Coarse-graining atomic displacements in a solid produces both local affine strains and non-affine fluctuations. We have studied the equilibrium dynamics of these coarse grained quantities to obtain space-time dependent correlation functions. We have shown how a subset of these thermally excited, non-affine fluctuations act as precursors for the nucleation of lattice defects and suggested how defect probabilities may

be altered by an experimentally realisable external field conjugate to the global non-affinity parameter. Our results are amenable to verification in experiments on colloidal crystals using commonly available holographic laser tweezer and video microscopy techniques, and may lead to simple ways of controlling the defect density of a colloidal solid.

with Saswati Ganguly (IACS, Kolkata) and Peter Sollich (Kings College, London)

Defect precursors in Graphene like crystals

- We have shown how certain localised displacement fluctuations in the planar honeycomb lattice may be identified as precursors to topological defects. These fluctuations are among the most pronounced non-affine distortions of an elemental coarse graining volume of the honeycomb structure at non zero temperatures. We have obtained the statistics of these precursor modes in the canonical ensemble, evaluating exactly their single point and two-point spatio-temporal distributions, for a lattice with harmonic nearest neighbour and next near neighbour bonds. As the solid is destabilised by tuning interactions, these precursor fluctuations diverge and correlations become long-lived and long-ranged.

with Amartya Mitra (TCIS, Hyderabad) , Saswati Ganguly (IACS, Kolkata) and Peter Sollich (Kings College, London)

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

- Partner/collaborator: FP7-PEOPLE-2013- IRSES grant no: 612707, DIONICOS.

Visits

1. University of Dusseldorf, groups of Profs J. Horbach, H. Lowen and S. Egelhaaf for scientific collaborative work. March 13 - April 13 (2014)
2. The Weizmann Institute for the TIFR-Weizmann meet TWIM 2014 June 8 - 10, (2014)

Invited Talks in Conferences and Meetings

1. Surajit Sengupta, Non-affine droplet fluctuations in crystalline solids, hidden critical points and a crystal to glass transition, TWIM-2014, June

2. Surajit Sengupta, Chromosome Positioning from Activity Based Segregation, IABS-2015, Kolkata, February 2, 2015

3. Surajit Sengupta, Chromosome Positioning from Activity Based Segregation, CTCNS-2015, Hyderabad, April 5, 2015

Lectures / Lecture Courses Given Elsewhere

- Introduction to Physics and Chemistry: Tata Institute of Social Sciences, Hyderabad, August 2014

Graduate Courses

- Electrodynamics I

Ph.D. Theses / M.Sc. Theses

- Ph. D. thesis, Equilibrium and rheological properties of model network formers, by Chandana Mondal, University of Calcutta, November 2014.

Any other information

- Attended Soft Matter Young Investigator Meet 2014 Pondicherry, December 18-20, 2014 as a Mentor.

Dr. Pramodh Vallurupalli

Highlights

Using a Combination of NMR spectroscopy and Molecular Dynamics simulations we have shown that the free energy barrier for T4 lysozyme to interconvert between its major and minor states is only 5RT. To the best of our knowledge this is the first report of a near barrierless transition between two compact conformations of a protein molecule.

Text

As the experimental facilities are yet to arrive, I have been performing computational studies of protein conformational dynamics.

Mechanism of the interconversion between the major and minor states of T4 Lysozyme L99A: At room temperature T4L L99A populates two conformations a major (∼99%) and a minor state with a population of ∼1% and a lifetime of ∼1ms. We have developed new NMR methods [1] and determined the structure of this minor conformer [2] (Figure 1). However the mechanism of interconversion is still not known. Using a Combination of NMR spectroscopy and Molecular Dynamics simulations we have determined the mechanism of interconversion. The simulations are in qualitative agreement with the experimental results suggesting that the forcefield models the underlying free energy surface reasonably well. We find that the free energy barrier for the interconvertion between the two states is only 5RT. To the best of our knowledge this is the first report of a near barrierless transition between two compact conformations of a protein molecule.

1. Proc Natl Acad Sci U S A. 2008 Aug 19;105(33):11766-71.
2. Nature. 2011 Aug 21;477(7362):111-4.

Figure / Photograph Captions

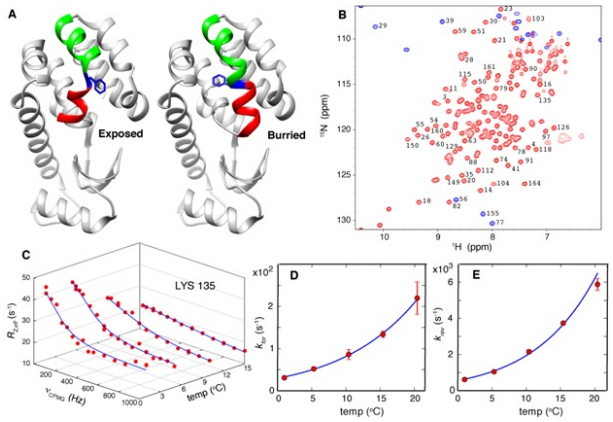


Figure 2: Exchange between the Phe114 exposed (E) and buried (B) conformers can be studied using CPMG relaxation dispersion (RD) NMR spectroscopy. A) The Phe 114 exposed and buried structures of T4L L99A. Helix f (residues 107-113) is in red and helix g (residues 115-123) is in green. Phe 114 is in blue. In the buried form Phe114 moves into a helical conformation with its sidechain buried in the protein and helices f and g now form one large helix. The exposed structure was determined by crystallography while the structure of the buried form, which is populated to only ∼3% was determined by CPMG NMR. B) $^{15}N-^{1}$H Trosy spectrum of T4L L99A,G113A,R119P recoded at 35 °. This experiment correlates amide ^{15}N and ^{1}H resonances and peaks are labeled according to the residue from which they arise. In the case of this mutant studied here the exposed form is the minor structure while the buried form is the major structure and the peaks in the spectrum correspond to the buried form. Peaks that are aliased in the indirect ^{15}N dimension are shown in blue. C) Amide ^{15}N CPMG RD curves of Lys 135 recorded at 1, 5.3, 10.4 and 15.4 °C on a 500 MHz spectrometer. Red dots correspond to the measured relaxation rates and the blue line is best fit to the data. Analysis of these curves provides information regarding the kinetics, thermodynamics of the Buried to Exposed exchange processes and can be used to reconstruct the spectrum of the invisible exposed form. The dispersions decrease in size with increasing temperature as the processes is endothermic and the exchange regime is moving from intermediate to fast. D, E) Arrhenius plots of the forward and reverse rate constants obtained from the CPMG data recorded at five temperatures. The experimental rates are shown as red circles with errorbars and the bestfit Arrhenius curve is shown in blue.

Lectures by Visitors

1) Junctions of Dirac Materials by Prof. Krishnendu Sengupta, IACS Kolkata on Apr 1st 2015.

2) Regulation of kinesin and dynein mediated transport by tubulin post-translational modifications by Dr. Minhaj Sirajuddin, NCBS Bangalore on Feb 18th 2015.

Graduate Courses

- Topics in Biophysics (being taught with Dr. Kanchan Garai)

Dr. Karthik V Raman

Highlights

Joined TCIS, TIFR Hyderabad on 2nd February 2015. Significant effort is being made currently to setup up the experimental lab facility.

Text

Spin polarized tunneling

A Project assistant was hired to work on simulating an experimental setup for Spin polarized tunneling using scanning tunneling miscrope apparatus. This involves understanding the physics of electron tunneling in a metal-insulator-superconductor geometry, followed by the implementation of the model by writing codes in MATLAB.

Staff List

- Shubham Agrawal Project Assistant

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

- Member, International Advisory Board for Spin in organic semiconductors (SPIN-OS) - October 2014 - present

Visits

- Conference visits for invited talks in US and Japan

Awards and Distinctions

- MPI-DST mobility grant holder- annual visits to MPI to initiate collaboration - 2015 - 2019

Invited Talks in Conferences and Meetings

1. *Interface-assisted Molecular Spintronics,* AVS Conference, Baltimore, Maryland (Nov 2014).
2. *Tailoring Interfaces at Molecular scale,* SPIN OS conference, Himeji, Japan (Oct. 2014).

Non DAE Research Projects

- Ramanujan Faculty fellowship from SERB (2013-2018)

Publications

1. *Tailoring ferromagnet-molecule interfaces: towards molecular spintronics,* **Karthik V. Raman***, N. Atodiresei & J. S. Moodera, ***SPIN 04**, 1440014 (2014). Selected for Press release: http://www.worldscientific.com/page/pressroom/2014-10-20-02

2. *Interface-assisted spintronics: Tailoring at the molecular scale,* N. Atodiresei & **Karthik V. Raman**, ***MRS Bulletin 39***, 596 (2014).

3. *Interface-assisted molecular spintronics,* **Karthik V. Raman**, ***App. Phys. Rev.* 1**, 031101 (2014).

4. *Origin of steep I-V nonlinearity in Mixed-Ionic-Electronic-Conduction (MIEC)based Access Devices,* A. Padilla *et al.,* **IEEE TED** 99, 1 (2015)

5. *MIEC (Mixed-Ionic-Electronic-Conduction)-based access devices for non-volatile crossbar memory arrays,* R. S. Shenoy *et al., (Invited Review)* ***Semiconductor Science & Technology 29***, 104005 (2014).

6. *The origin of massive nonlinearity in Mixed Ionic Electronic Conduction (MIEC)based Access Devices, as revealed by numerical device simulation,* A. Padilla, G. W. Burr, R. S. Shenoy, K. V. Raman *et. al.,* ***DRC, 72nd Annual***, 163-164 (2014).