מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Interaction Meeting on Materials, Chemistry, and Biology

January 15-17th 2019
Tata Institute of Fundamental Research Mumbai
Venue: Homi Bhabha Auditorium

Program Schedule
Talk Abstracts
Posters

Organizing Committee

TIFR
Ankona Datta (ankona@tifr.res.in)
Sandhya Koushika (spkoushika@tifr.res.in)
Ravi Venkatramani (ravi.venkatramani@tifr.res.in)

WIS
David Margulies (david.margulies@weizmann.ac.il)
Ulyana Shimanovich(ulyana.shimanovich@weizmann.ac.il)

Official TWIM-2019 email: twim2019@gmail.com

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January 15th Tuesday	January 16th Wednesday	January 17th Thursday
8:30 – 9:00 am Registration 9 – 9:10 am Director`s Address		
9:10 am - 9:40 Koby Levy	9:10 am – 9:40 am Shachi Gosavi	9:10 am – 9:40 am Akash Gulyani
9:40 – 10:10 am P. V. Shivaprasad	9:40 am – 10:10 am Talila Volk	9:40 am – 10:10 am Emmanuel Levy
10:10 – 10:40 am Malay Patra	10:10 – 10:40 am Ullas Kolthur	10:10 – 10:40 am A. S. R. Koti
10:40 – 11:00 am Tea	10:40 – 11:00 am Tea	10:40 – 11:00 am Tea
11:00 – 11:30 am Roop Mallik	11:00 – 11:30 am Ankona Datta	11:00 – 11:30 am Vidita Vaidya
11:30 – 12:00 noon Ron Naaman	11:30 – 12:00 noon Amnon Horovitz	11:30 – 12:00 noon Gilad Haran
12:00 – 12:30 Jeffery Gerst	12:00 – 12:30 pm Jyotishman Dasgupta	12:00 – 12:30 pm Vijaykumar Krishnamurthy
12:30 – 2:00 pm Lunch	12:30 – 12:45 pm Sponsor Slot 12:45 – 2:00 pm Lunch	12:30 – 2:00 pm Lunch
2:00 – 3:30 pm Poster Session (Odd Numbered)	2:10 - 2:40 pm Nidhi Agarwal	2:00 – 3:30 pm Poster Session (Even Numbered)
3:40 – 4:10 pm Sandhya Koushika	2:40 – 3:10 pm Purna Gadre/ Souvik Modi	3:40 - 4:10 pm Shyamalava Mazumdar
4:10 – 4:40 pm Ankita Das/Barun Maity	Activity: Excursion to South Mumbai	4:10 – 4:40 pm David Marguiles
4:40-5:00 pm Tea		4:40 – 5:00 pm Tea
5:00 – 5:30 pm Ulyana Shimanovich		5:00 – 5:30 pm Sudipta Maiti
5:30 – 6:00 pm Aprotim Mazumder		5:30 – 6:00 pm Koyel Banerjee-Ghosh
6:00 – 6:30 pm Shirshendu Ghosh	7:30 pm Conference Dinner	6:00 – 6:30 pm Ravi Venkatramani

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January 15th Tuesday
8:30 – 9:00 am Registration *9 – 9:10 am Director`s Address*
Session I (Chair: Jyotishman Dasgupta)
9:10 am - 9:40 am *Koby Levy - Molecular principles for optimizing protein-DNA interactions*
9:40 – 10:10 am *P. V. Shivaprasad - Insights into the mechanism of small RNA-mediated regulation of plant genomes*
10:10 – 10:40 am *Malay Patra - Potential of metal complexes in diagnosis and therapy of cancer*
10:40 – 11:00 am Tea (Almond Grove)
11:00 – 11:30 am *Roop Mallik - Who let the fat out ?*
11:30 – 12:00 noon *Ron Naaman - Chiral molecules and the electron's spin- From spintronics to enantio-separation*
12:00 – 12:30 pm *Jeffery Gerst - Intracellular and intercellular mRNA trafficking in eukaryotes*
12:30 – 2:00 pm Lunch (Almond Grove)
2:00 – 3:30 pm Poster Session (Odd Numbered)
Session II (Chair: A. S. R. Koti)
3:40 – 4:10 pm *Sandhya Koushika – Cargo crowding in neurons causes local traffic jams*
4:10 pm-4:40 pm Ankita Das - Hammering on a C-H Bond with Light inside a Nanocage *Barun Maity - Role of order and disordered regions of Abeta40 oligomers in multistep toxicity pathway*
4:40-5:00 pm Tea (Almond Grove)
5:00 – 5:30 pm *Ulyana Shimanovich - Silk-based materials*
5:30 – 6:00 pm *Aprotim Mazumder - Measuring EGFR-mediated gene expression at a single molecule resolution in drosophila tissues*
6:00 – 6:30 pm *Shirshendu Ghosh - T-cell Microvilli as Activation Hubs*

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January 16th Wednesday

Session I (Chair Vidita Vaidya)

9:10 am – 9:40 am
Shachi Gosavi - Understanding 3D-domain-swapping in proteins

9:40 am – 10:10 am
Talila Volk - Mechanotransduction in muscle nuclei: signals affecting epigenetic response and DNA replication

10:10 – 10:40 am
Ullas Kolthur - Metabolic inputs and protein domains in physiology and aging

10:40 – 11:00 am Tea (Auditorium Terrace Area)

11:00 – 11:30 am
Ankona Datta - Reversible chemical tools for timing and probing biology

11:30 – 12:00 noon
Amnon Horovitz - Unraveling the determinants that confer dependence on the chaperonin GroEL for folding

12:00 – 12:30 pm
Jyotishman Dasgupta - Probing charge Transfer States in Macromolecules using Ultrafast Raman Spectroscopy

12:30 – 12:45 pm Sponsor Slot
Edwards India Pvt Ltd

12:45 – 2:00 pm Lunch (Auditorium Terrace Area)

Sesssion II (Chair Ankona Datta)

2:10 - 2:40 pm
Nidhi Agarwal – Controlling the self-assembly – Reality and illusion?

2:40 – 3:10 pm
Purna Gadre - Somatic EGFR signaling defines the rate of germ cell divisions in Drosophila testis
Souvik Modi - Mitochondrial positions in C. elegans axons correlate with spontaenous calcium sparks and influence behavioural responses

Activity: Excursion to South Mumbai

7:30 pm
Conference Dinner (West Lawn)

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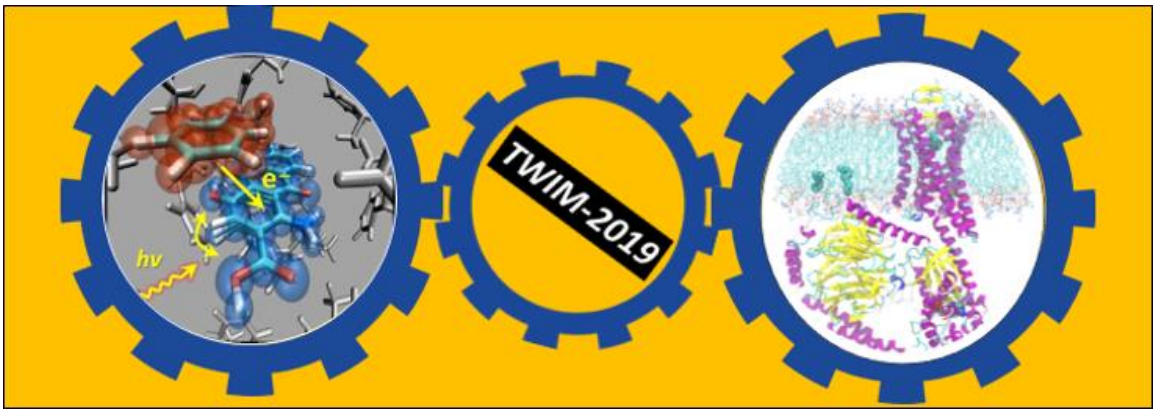
Venue: Homi Bhabha Auditorium

January 17th Thursday
Session I (Chair: Roop Mallik)
9:10 am – 9:40 am *Akash Gulyani - Sensing across scales: biosensors, fluorescent probes and natural light sensing*
9:40 am – 10:10 am *Emmanuel Levy - A synthetic protein system connects molecular structure to mesoscale phenotypes of phase separation in vivo*
10:10 – 10:40 am *A. S. R. Koti – Mechanistic Origins of Proteins Malleability*
10:40 – 11:00 am Tea (Auditorium Terrace Arrea)
11:00 – 11:30 am *Vidita Vaidya - Serotonin – a regulator of neuronal mitochondrial energetics and biogenesis*
11:30 – 12:00 noon *Gilad Haran - How fast are functional motions of proteins?*
12:00 – 12:30 pm *Vijaykumar Krishnamurthy – Guiding self-organized developmental patterns*
12:30 – 2:00 pm Lunch (Auditorium Terrace Arrea)
2:00 – 3:30 pm Poster Session (Even Numbered)
Session II (Chair: Ullas Kolthur)
3:40 - 4:10 pm *Shyamalava Mazumdar - Thermostable cytochrome P450- Stability and catalytic properties*
4:10 – 4:40 pm *David Marguiles - Molecules that Generate 'Fingerprints': A New Class of Fluorescent Probes for Medical Diagnosis and Chemical Biology*
4:40 – 5:00 pm Tea (Auditorium Terrace Arrea)
5:00 – 5:30 pm *Sudipta Maiti - Protein disorder and function*
5:30 – 6:00 pm *Koyel Banerjee-Ghosh - Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates*
6:00 – 6:30 pm *Ravi Venkatramani - Protein Dynamics as a marker to sense and regulate protein-protein interactions*
Closing Remarks

Weizmann Institute of Science

Interaction Meeting on Materials, Chemistry, and Biology

Talk Abstracts



Molecular principles for optimizing protein-DNA interactions

Yaakov (Koby) Levy

Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel

Yaakov (Koby) Levy discussed the complexity of protein-DNA interactions that may exhibit some conflicting thermodynamic and kinetic properties. The remarkable efficiency and specificity of protein-DNA recognition presents a major theoretical puzzle given the size of the genome, the large number of molecular species *in vivo* at a given time, and the crowded environment they inhabit. The fast association between proteins and DNA is governed by nonspecific interactions that allow protein sliding along DNA where the protein binds DNA nonspecifically and performs a helical motion when it is placed in the major groove. We have explored using various computational approaches the interplay between the molecular characteristics of the proteins (e.g., DNA recognition motifs, degree of flexibility, and oligomeric states) and the nature of sliding, intersegment transfer events and the overall efficiency of the DNA search. Another important aspect of the search is how the in-vivo conditions (for example, crowding in the cell or coverage of DNA by nucleosomes) affect the efficiency of DNA search. Protein sliding may occur on single-stranded DNA as well, yet via a different mechanism than that for double-stranded DNA. Furthermore, the interaction between proteins and DNA also has to result with high affinity complexes. In my presentation, I discussed the molecular features of proteins and of the nucleic acids that allow fast dynamics and high affinity binding on both single- and double-stranded DNA.

Insights into the mechanism of small RNA-mediated regulation of plant genomes

P. V. Shivaprasad

National Centre for Biological Sciences, Tata Institute of Fundamental Research, Bengaluru, India

Please add a brief abstract here. Abstracts can contain citations and/or images but should fit in a single page subject to the font and margin constraints provided here. A number of epigenetic regulatory layers are superimposed on the genome. In plants, small RNA regulators play a major role in the establishment and maintenance of gene silencing and epigenetic marks. We are interested in understanding the mechanism of small RNA biogenesis, their functions and their role in establishment of epigenetics using a number of model systems. Small RNAs associate with protein partners called Argonautes to target nucleic acids having high base-pair complementarity. Small RNAs regulate various aspects of plant development, typically acting as second-generation gene switches controlling expression of primary gene switches, the transcription factors and their co-factors. Intriguingly, they are also capable of arresting invading viruses and promote resistance to bacterial and fungal infections. Our lab focuses on various aspects of small RNA biogenesis and their functions, using genetic, molecular, bioinformatic and biochemical approaches. We have identified at least two novel mechanisms that regulate small RNA biogenesis in plants and identified a novel polymerase that can generate RNA substrates from transposon-rich regions.

Although functions of most conserved small RNAs are well-known, functions of less conserved small RNAs are relatively unknown. We work on a set of less-conserved small RNAs in non-traditional model systems such as grapes, brassicas, and rice. I will be discussing functions of few small RNAs that regulate phenotypes such as leaf area, domestication-associated phenotypes, male sterility and secondary metabolism.

Potential of metal complexes in diagnosis and therapy of cancer

Malay Patra,[1] J. P. Holland[2] and S. J. Lippard [3]

[1]*Department of Chemical Sciences, Tata Institute of Fundamental Research,Mumbai, India*

[2]*Department of Chemistry, University of Zurich, Switzerland*

[3]*Department of Chemistry, MIT, Boston, USA*

Early diagnosis and appropriate therapy are essential for successful treatment of cancer. Monoclonal antibodies (mAbs), immunoglobulin fragments and other proteins are important scaffolds in the development of radiopharmaceuticals for diagnostic immuno-positron emission tomography (immuno-PET) and targeted radioimmunotherapy (RIT). The problem is that conventional methods for radiolabelling proteins with metal ions like ^{68}Ga, ^{64}Cu, ^{89}Zr, and ^{90}Y etc require multi-step procedures involving pre-purification, functionalization with a chelate, and subsequent radiolabeling. Standard coupling chemistries are time consuming, difficult to automate, and involve isolation and storage of an intermediate, new molecular entity (the conjugated mAb) whose biochemical properties can differ from those of the parent protein. To circumvent these issues, we developed a photoradiochemical approach that uses fast, chemo- selective, light-induced protein modification under mild conditions with novel metal ion binding chelates derivatized with arylazide (ArN3) groups. Experiments show that one-pot photochemical conjugation and radiolabeling of fully formulated mAbs can be achieved in <15 min.

The three FDA approved platinum anticancer drugs, cisplatin, carboplatin and oxaliplatin, are widely used in the clinic to treat various forms cancer including testicular, ovarian, cervical, head and neck, non-small-cell lung, and colorectal cancer. Despite their phenomenal clinical success, however, the severe undesired side effects such as nephrotoxicity, myelosuppression, peripheral neuropathy, ototoxicity, and nausea are main drawbacks of platinum-based chemotherapy. The side effectes could be mitigated by introducing tumor-targeting properties into platinum anticancer compounds, thereby reducing the nonspecific platinum accumulation in the healthy tissues. Glucose transporter GLUT1 is known to widely overexpress in many human cancers and its expression levels in tumor biopsy samples correlate well with poor prognosis. We designed various D-glucose-platinum(II) conjugates (Glc-Pts) for targeted delivery of platinum anticancer drugs to cancer cells. The design, synthesis, biological evaluation of antibody-radiometal conjugates for diagnosis and glucose-platinum conjugates for therapy of cancer will be presented in the research seminar.

Who let the fat out?

Roop Mallik

Department of Biological Sciences, Tata Institute of Fundamental Research, Mumbai, India

The liver secretes lipids in a controlled manner despite vast changes in its internal lipid content. This buffering function of the liver is essential for lipid/energy homeostasis, but its molecular and cellular mechanism is unknown. We show that the motor protein kinesin transports triglyceride-rich lipid droplets (LDs) to the endoplasmic reticulum in liver cells. This supplies triglycerides for packaging into lipoprotein particles (VLDL) that are subsequently secreted from the liver. However, when fasting induces massive lipid accumulation in liver, kinesin is removed from LDs to inhibit triglyceride supply and homeostatically temper lipid secretion from liver. Most interestingly, this entire pathway is controlled by insulin, and can therefore respond to fed/fasted states of the animal.

Chiral molecules and the electron's spin- from spintronics to enantio-separation

Ron Naaman

Department of Chemical and Biological Physics Weizmann Institute, Rehovot 76100, Israel

Spin based properties, applications, and devices are commonly related to magnetic effects and to magnetic materials. However, we found that chiral organic molecules act as spin filters for photoelectrons transmission,[1] in electron transfer,[2] and in electron transport.[3]

The new effect, termed Chiral Induced Spin Selectivity (CISS),[4,5] was found, among others, in bio-molecules and in bio-systems. It has interesting implications for the production of new types of spintronics devices[6,7] and on electron transfer in biological systems.[8] Recently we found that charge polarization in chiral molecules is accompanied by spin polarization.[9] This finding shed new light on enantio-specific interactions and it opens the possibility to construct novel methods for enantio-separation.

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2. *Mishra, D.; Markus, T.Z.; Naaman, R.; Kettner, M.; Göhler, B.; Zacharias, H.; Friedman, N.; Sheves, M.;Fontanesi, C. PNAS,* ***2013,*** *110, 14872.*
3. *Xie, Z.; Markus, T. Z.; Cohen, S. R.; Vager, Z.; Gutierrez, R.; Naaman, R. Nano Letters,* ***2011,*** *11, 4652.*
4. *Naaman, R.; Waldeck, D.H. J. Phys. Chem. Lett. (feature)* ***2012,*** *3,* ***2178.***
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9, *A. Kumar, E. Capua, M. K. Kesharwani, J. M. L. Martin, E. Sitbon, D. H. Waldeck, R.Naaman, PNAS,* ***2017,*** *114, 2474.*

Intracellular and intercellular mRNA trafficking

Jeffrey E. Gerst, Rohini Nair, Rita Gelin-Licht, Camila Baez,
Gal Haimovich, Raman Singh, Sandipan Dasgupta

Department of Molecular Genetics, Weizmann Institute, Rehovot, Israel

In eukaryotes, mRNA trafficking and localized translation is proving to be a critical mechanism for controlling protein localization and, hence, cell physiology. In my lab we are examining both intracellular and intercellular RNA trafficking. By using yeast as a model organism for the study of intracellular trafficking, we have developed RNA tagging and single-species RNA pulldown procedures that have led us to identify both RNA-binding proteins (RBPs) and multiplexed mRNAs that associate with tagged RNAs. Mutations in genes that lead to the inhibition of RNA trafficking or multiplexing lead to phenotypes in respiration, secretion, chemotropism, and mating [1,2]. In addition, we use the yeast as a model system to study ribosome heterogeneity, in which specific ribosomal proteins assemble into ribosomes and are able to select subsets of mRNAs for translation [3,4]. Finally, we have identified a process in mammalian cells that leads to the transfer of full-length mRNAs from one cell to another by means of membrane nanotubes [5]. Ongoing work seeks to discover the extent of the mammalian transferome and its physiological role in healthy and diseased cells.

References:

1. *Gelin-Licht, R., Paliwal, S., Levchenko, A., and Gerst, J.E.* ***2012*** *Cell Rep. 1:483-494.*
2. *Zabezhinsky, D., Slobodin, B., Rapaport, D., and Gerst, J.E.* ***2016*** *Cell Rep. 15:540-549.*
3. *Segev, N. and Gerst, J.E.* ***2018*** *J. Cell Biol. 217:117-126.*
4. *Gerst, J.E.* ***2018*** *Trends Genet. 34:832-845.*
5. *Haimovich, G., Ecker, C.M., Dunagin, M.C., Eggan, E., Raj, A., Gerst, J.E. and Singer, R.H.* ***2017*** *Proc. Natl. Acad. Sci. USA 114:E9873-E9882*

Cargo crowding in neurons causes local traffic jams

Sandhya P. Koushika

Department of Biological Sciences, Tata Institute of Fundamental Research, Mumbai, India

Abstract

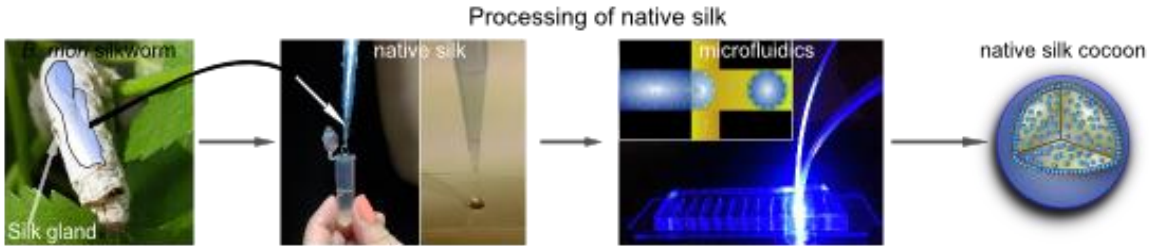
Axonal cargo flow is central to the functioning of healthy neurons. A substantial fraction of synaptic vesicles, a major cargo, remains stationary up to several minutes predominantly at actin-rich regions along the touch neuronalprocess. Stationary vesicles at actin-rich regions and stationary synaptic vesicles alone increase the likelihood of moving vesicles to stall at the same location, resulting in traffic jams arising from physical crowding. Repeated touch stimulation of C. elegans reduces the density of stationary pre-SVs, indicating that these traffic jams perhaps act as functional reservoirs.

Silk-based materials

Ulyana Shimanovich

Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, 76100, Israel

Natural proteins display critical structural and bioactive properties that have evolved in nature for millions of years. However, depending on the specific protein, there may be useful functions, such as mechanical toughness, while other critical features may be more limiting, such as cell compatibility or a broader range of mechanical properties. Silk proteins, as a building blocks for biomaterials construction, combine a unique properties of high mechanical performance and overall biocompatibility. This has led to their use in artificial vascularized tissues, nerve guides and functional soft/hard scaffold and recently silkworm silk has received Food and Drug Administration approval for expanded biomaterials device utility. Yet this wonder-material is not without its own challenges. These include the extreme shear sensitivity of silk fibroins and their propensity to aggregate upon extraction and thus it requires more biologically sensitive processing routes. Our research addresses these fundamental limitations by exploring a platform technology, based on microfluidics, that unlocks investigation of unstable fibroins, as well as other aggregation-prone proteins, processing and routes towards the use of material in contact with cells enabling us to explore possible applications in biomedicine.



References:

1 *T.O. Mason, U. Shimanovich*. Adv.Matter.* ***2018****, 30, 1706462*
2 *U. Shimanovich, D. Pinotsi, et al. Macromol.Biosci.* ***2018****, 17000295*
3 *U. Shimanovich, F. Ruggeri, et al. NatComm.* ***2017****, 8, 15902*
4 *A. Levin, T.O. Mason, T.P.J. Knowles*, U. Shimanovich*. Isr.J.Chem.* ***2017****, 57, 1-6.*
5 *Y. Song, U. Shimanovich, et al. NatComm.* ***2016****, 7, 12934.*

Measuring EGFR-mediated gene expression at a single molecule resolution in Drosophila tissues

Aprotim Mazumder

TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research,Hyderabad, India.

Two current major directions of our laboratory lie in studying DNA damage responses (DDR) and EGFR-mediated cell proliferation and differentiation. DDR is intimately linked to the cell cycle, and recently we have developed imaging-based methods for studying cell cycle dependent DDR and associated chromatin level changes. While I will talk briefly about these, in this talk I will emphasize the methods we have recently developed our group for studying gene expression at a single molecule resolution in primary Drosophila tissue like larval wing and eye imaginal discs (1). Distinct expression of EGFR pathway genes simultaneously in the same tissue are observed that cannot be detected by standard in situ hybridization techniques. Using these approaches we are currently investigating EGFR-mediated cell proliferation and differentiation in the larval eye disc. Together these studies are leading us to uncover how the interplay of positive and negative regulators of the EGFR pathway is critical for photoreceptor differentiation.

References:

1. *Pasnuri, N., Khuntia, P. and Mazumder, A.* ***2018*** *Mech Dev, 153, 10-16.*

T-cell microvilli as activation hubs

Shirsendu Ghosh[1], Vincenzo Di Bartolo[2], Liron Tubul[1], Eyal Shimoni[3], Elena Kartvelishvily[3], Sara W. Feigelson[4], Ronen Alon[4], Andres Alcover[2] and Gilad Haran[1]*

[1]*Department of Chemical Physics, Weizmann Institute of Science, Rehovot 76100, Israel*

[2]*Lymphocyte Cell Biology Unit, INSERM U1221, Department of Immunology, Institut Pasteur, Paris 75015*

[3]*Chemical Research Support, Weizmann Institute of Science, Rehovot 76100, Israel*

[4]*Department of Immunology, Weizmann Institute of Science, Rehovot 76100, Israel*

When T cells encounter cognate peptide-MHC complexes on antigen presenting cells they respond within seconds. How such a fast response involving multiple proteins is orchestrated in very short periods of time has long been disputed. We show that the T-cell receptor (TCR) complex, its co-stimulatory proteins and key signaling proteins are all localized on thin, flexible protrusions on the T-cell surface called microvilli. We further show that the TCR complex is anchored to the microvillar actin cytoskeleton by members of the ezrin-radixin-moesin protein family. Disruption of these anchors disperses TCR molecules over the whole cellular surface. T cells thus use their microvilli as signaling hubs, on which they actively pre-organize all proteins necessary for the earliest transmission of activation signals.

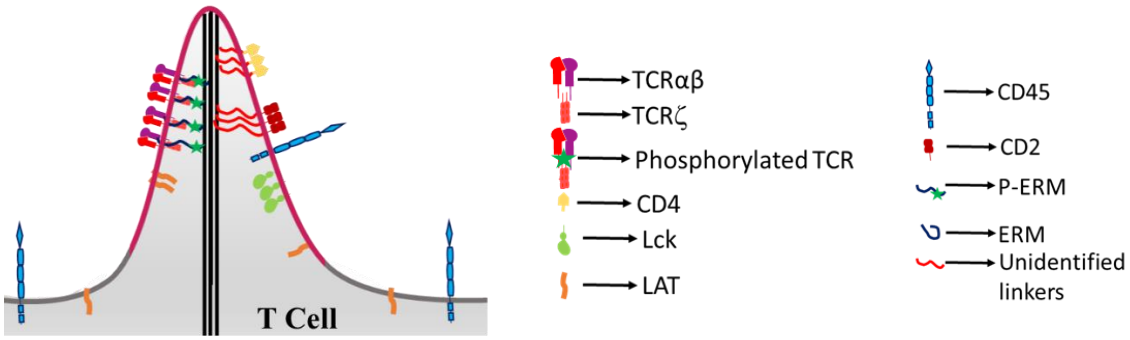


Figure 8: Model for immune-response protein organization on the T-cell membrane on resting state of T cell.

Understanding 3D-domain-swapping in proteins

Shachi Gosavi

National Centre for Biological Sciences, Tata Institute of Fundamental Research, Bengaluru, India

In 3D-domain-swapping, two or more identical protein monomers exchange structural elements at a hinge loop and fold into dimers or multimers whose units are structurally similar to the original monomer. Although domain-swapping is common and is used to build protein assemblies in nature, it is not well understood. Using simulations, we show that the specifics of local energetic interactions of the hinge-loop modulate domain-swapping in the naturally domain-swapping protease inhibitor, stefin-B. Introducing this hinge-loop and the associated energetics into monellin, a protein structurally similar to stefin-B but which does not domain-swap, causes it to domain-swap in simulations. We then tested these simulations by structurally characterizing several mutants of monellin.

References:

1. *Mascarenhas, N. M., Gosavi, S., Prog. Biophys. Mol. Biol. 128, 113* ***2017****.*
2. *Mascarenhas, N. M., Gosavi, S., J. Phys. Chem. B 120, 6929* ***2016****.*

Mechanotransduction in muscle nuclei: signals affecting epigenetic response and DNA replication

Talila Volk

Department of Molecular Genetics, Weizmann Institute of Science, Rehovot, Israel

In Mature contractile muscle fibers are unique because in contrast to non-migratory cells their multiple nuclei are exposed to mechanical forces which vary due to contractile/relaxation waves. The mechano-transducer Linker of Nucleoskeleton and Cytoskeleton (LINC) complex physically connects the cytoskeleton with the nucleoskeleton through a set of KASH proteins, that bind both cytoskeletal proteins at the outer nuclear membrane and SUN proteins at the inner nuclear membrane. SUN proteins further associate with nuclear lamina proteins, chromatin binding proteins as well as the nuclear pore complex.

Using Drosophila larval muscles as a an experimental model, we analyze the molecular signaling pathways transduced by the LINC complex into the muscle nuclei, and affect the epigenetic state of the chromatin. Furthermore, by following the behavior of muscle nuclei during individual muscle contraction, we were able to extract biophysical characteristics of the nuclei and evaluate the differences in forces applied on the nuclear membrane in wild type and LINC mutant muscles. Overall our studies reveal novel aspects in the nuclear mechanotransduction pathway that will finally enable to elucidate the molecular basis for an array of human diseases associated with impaired transmission of mechanical inputs into the nucleus.

Metabolic inputs and protein domains in physiology aging

Ullas Kolthur-Seetharam

Department of Biological Sciences, Tata Institute of Fundamental Research, Mumbai, India

Ability of cells and organisms to sense and respond to environmental cues is vital for their survival. Specifically, sensing metabolic inputs becomes vital given that metabolism drives all cellular processes. Although considered as a set of mundane biochemical reactions, metabolic pathways are known to encode information. Particularly metabolite driven modifications on several proteins, across compartments, have emerged as key determinants of protein structure/function. Sirtuins are a family of evolutionarily conserved NAD-dependent protein deacylases. Work from our lab and others have revealed that they are crucial for linking metabolic status to cellular/organismal physiology. They are key determinants of processes such as cell proliferation/death/differentiation, stress response, mitochondrial functions and aging mechanisms. Despite much being known about the phenotypes associated with mutants, interplay between metabolic states and their functions still remain elusive.

Organismal physiology is maintained by a complex interplay between multitude of pathways and molecular factors. Providing directionaility to processes specifically in response to inputs from metabolism seems daunting given that metabolic status is a continuum and dynamically modulated in a spatio-temporal manner. In this talk, I will highlight some of recent work, which have led us to discover how evolution has selected seemingly disarrayed components vis-à-vis metabolite fluctuations and disordered regions to create specificities in terms of protein functions. Such interplay provides the ability to expand phenotypic outputs and dynamic switching of physiological states.

Reversible chemical tools for timing and probing biology

Ankona Datta

Department of Chemical Science, Tata Institute of Fundamental Research, Mumbai, India

Small molecules and ions are key players in biological regulation and signaling processes. Dynamic changes in molecular and ionic distributions are functionally relevant and hence essential for driving life. Chemical probes that can track small molecules and ions in living systems will help us record 'molecular motion pictures' revealing essential life processes. Changes in molecular distributions under pathophysiological conditions can also be tracked by using these probes. The major challenges in small molecule detection are: How do we detect dynamic concentration changes? How do we distinguish between chemically similar species that might have very distinct biological functions? And finally, what strategies can allow efficient translation of *in vitro* detection assays into living systems? In our group, we use coordination chemistry and molecular recognition insights to build designer probes that can address these challenges. Optical imaging is our modality of choice because of its high sensitivity and spatiotemporal resolution for live imaging. By engineering molecular motifs spanning the range from proteins to small peptides and synthetic macrocycles we have developed reversible sensing strategies for *in vivo* molecular sensing.[1-3] Our forays into sensor development have not only led to sensitive chemical probes but have also enhanced our understanding of chemical selectivity principles. Using insights obtained from our fundamental sensor design endeavors we have therefore also initiated applied directions in the development of strategies for early disease diagnosis and routes for targeted chelation therapy.[4] In this talk, I will highlight our probe design principles and recent results on sensing signaling lipids and developing selective binders for metal ions in living systems.

References:

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Unraveling the determinants that confer dependence on the chaperonin GroEL for folding

Amnon Horovitz

Dept. of Structural Biology, Weizmann Institute of Science, Rehovot, Israel

Chaperonins are molecular machines that assist protein folding by undergoing ATP-driven conformational changes (1). They consist of two back-to-back stacked oligomeric rings with a cavity at each end where protein folding can take place under protective conditions. The GroE chaperonin system in *Escherichia coli*, which comprises GroEL and its co-factor GroES, can assist in the folding *in vitro* of a wide range of proteins. *In vivo*, however, GroEL interacts with only ~250 *E. coli* proteins (2) of which ~60 are "obligatory" clients (i.e. they require GroE assistance even under normal conditions). Attempts to predict the GroE dependence of proteins using various structure- and sequence-based features have been unsuccessful. It has remained unclear, therefore, why some proteins with very similar sequences and structures differ in their GroE dependence. In my talk, I will describe experiments (3, 4) using GFP as a model system that show that both local (i.e. frustration) and global (i.e. topology) properties of protein determine GroEL dependence.

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Probing charge transfer states in macromolecules using ultrafast Raman spectroscopy

Jyotishman Dasgupta

Department of Chemical Sciences, Tata Institute of Fundamental Research, Colaba, Mumbai, India

Charge transfer (CT) states provide an escape route for strongly bound electrons and holes to encode functional chemistry in macromolecular systems. From fuel synthesis in natural photosynthesis to functional materials for photovoltaic devices, the efficiencies of all these light-triggered processes critically depend on tuning the energy, spatial extent and lifetime of the CT states. In this talk, I will describe our efforts to spectroscopically probe these states using set of Ultrafast Raman techniques. Information on photoactivated structural dynamics and spatial delocalization of these states will be discussed in the context of electron transfer in protein Azurin and covalently attached donor-acceptor molecular entities.

Controlling the self-assembly – reality and illusion?

Nidhi Aggarwal, Ulyana Shimanovich

Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot,Israel

Self- assembly is a key principle for the existence of viral capsids, pathogenic amyloids, gels and functional amyloids. These molecules look different at the molecular level yet the main driving forces for their existence are the interactions of amino acids within a single protein molecule and between different protein molecules. It is a well-documented fact that amyloids are responsible for various pathogenic conditions viz. cancer and neurodegeneration. Alongside, these pathogenic amyloids exist, model systems like silk that provide ample opportunities to understand and unravel the mechanism of formation and control of self –assembly of amyloids. Combining the findings of ability of diphenylalanine and benzoylated diphenylalanine to form nanotubes and spheres respectively with silk, we designed silk derived peptides with increased content of aromatic amino acids. Our findings from aggregation kinetics, AFM, TEM and FT-IR reveals the striking differences in their morphology, their possible mechanisms and hydrogen bonding abilities.

Sensing across scales: biosensors, fluorescent probes and natural light sensing

Akash Gulyani

Institute for Stem Cell Biology and Regenerative Medicine (inStem), inStem-NCBS-CCAMP biocluster, Bengaluru, India

I will present our comprehensive and multi-faceted approach of sensing dynamics across scales,with an emphasis on developing new measurements and sensing approaches. I will highlight our work towards generating new, generally applicable biosensors for visualizing cellular dynamics. We have developed fluorescent biosensors based on engineered protein ‘binders’ that recognize 'active' signaling proteins or conformations in live cells. Our approach is general and is compatible with multiple readouts in the cell. Our new biosensor for a specific Src family kinase, Fyn reveals fascinating compartmentalization of signaling activities inside the cell. Biosensor imaging reveals that Fyn activity is spatially localized, pulsatile and is subject to cross-talk between cell adhesion receptors and growth factor receptors (receptor tyrosine kinases RTKs). Here, I will also present the development of new mitochondrial probes and dyes help visualize unexplored patterns of mitochondrial activity and dynamics in live cells. These new probes specifically report on the local environment at the mitochondria and enable new inquiries in the regulation of cell state. More broadly, I will place these findings in our overall efforts to develop new measurements for biology. Here, I will briefly discuss our new discoveries in the natural light sensing, and how natural light sensing can be used for studying regeneration as well as neural processing.

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A synthetic protein system connects molecular structure to mesoscale phenotypes of phase separation in vivo

Emmanuel Levy

Department of Structural Biology, Weizmann Institute of Science, Rehovat,Israel

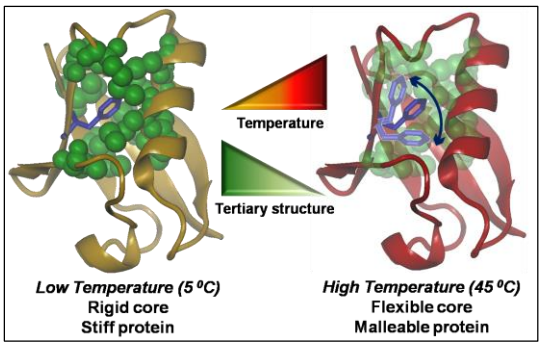
Phase-separation is emerging as a fundamental organizational process of living matter. In this process, the molecular structure of components translates into mesoscale properties of condensates such as their phase-diagram, material state, or composition. Dissecting this relationship in vivo for natural condensates is, however, difficult because it requires a precise knowledge of their composition and regulation by the cell. This limitation motivates us to use synthetic biology to shed light on principles of phase separation in vivo. We engineered two homo-oligomeric proteins that phase separate upon interacting intermolecularly, forming mesh-like assemblies. Uniquely, we revealed the phase diagram of this system in vivo. Increasing the valency or the interaction affinity between the proteins enhanced their phase-separation and made the condensates more rigid, as predicted. Using this system, we subsequently explored synergistic effects between phase separation and cellular processes: quiescent cells enhanced phase-separation of our system, despite not affecting the affinity between its constituent proteins. This minimal system provides a well-controlled molecular toolkit to model mesoscale assembly from first principles, and potentially for designing advanced biomaterials and scaffolds.

Mechanistic origins of proteins malleability

Sri Rama Koti Ainavarapu

Department of Chemical Sciences, Tata Institute of Fundamental Research, Colaba, Mumbai,India

Despite the growing interest in the thermal softening of proteins, the mechanistic details of it are far from understood. β-Grasp proteins have globular shape with compact structure and they are mechanically resilient. Although previous studies showed that temperature can perturb the protein mechanical stability, the structural changes leading to the lowered mechanical resistance are not known. Here, we investigated the temperature dependent mechanical stability of ubiquitin and small ubiquitin-related modifier 2 (SUMO2) using single-molecule force spectroscopy (SMFS) and the corresponding conformational changes using ensemble experiments.



SMFS studies on SUMO2 estimate a decrease in the spring constant of the protein from 4.50 to 1.35 N/m upon increasing the temperature from 5 to 45 °C which correlated with a decrease in tertiary structure suggesting a correlated the importance of the intramolecular interactions at the protein core along with the β-clamp or mechanical clamp in providing the mechanical resistance as well as in modulating the protein stiffness.[1] Ubiquitin has a conserved salt-bridge connecting the α-helix to a loop between the β3 and β4 strands. We inserted a Trp (L43W) at the protein core within 5Å of the above mentioned salt bridge (K27-D52) as a reporter of the micro environment of the protein. Circular dichroism and fluorescence anisotropy studies showed that the ubiquitin core is conformationally rigid in the temperature range 5-55 °C. Disrupting the salt-bridge by a double mutation K27A/D52L, increased the conformational flexibility of the protein core at 5 °C which also gradually increased with temperature up to 55 °C. These results also suggest that the core flexibility of Ubiquitin K27A/D52L mutant lacking the salt-bridge resembles SUMO2 to an appreciable extent. Furthermore, a more severe salt-bridge mutation of ubiquitin (K27M/D52L) replacing Lys with Met to mimic SUMO2, showed that the protein's core is highly flexible even at 5 °C and devoid of any tertiary structure. Our studies on ubiquitin and SUMO2 suggest that the conserved salt-bridge of ubiquitin family proteins plays an important role in determining protein conformational flexibility.

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Serotonin – a regulator of neuronal mitochondrial energetics and biogenesis

Sashaina E. Fanibunda[1,2], Sukrita Deb[1], Babukrishna Maniyadath[1], Ashok. D. B. Vaidya[2], Ullas Seetharam-Kolthur[1*], Vidita A.Vaidya[1*]

[*]Equal Senior Corresponding Authors

[1] Department of Biological Sciences, Tata Institute of Fundamental Research, Mumbai, India
[2] Medical Research Centre, Kasturba Health Society, Mumbai, India

Serotonin (5-HT) modulates neuronal differentiation, growth and synaptic plasticity, however it's influence on mitochondrial physiology in neurons is largely unknown. In cortical cultures, 5-HT treatment evoked an increase in mitochondrial biogenesis, with enhanced mtDNA levels, increased expression (mRNA and protein) of specific mitochondrial markers, and increased mitotracker staining. We also observed that 5-HT treatment of cortical neurons increases cellular ATP levels and enhances basal as well as maximal respiration. The effects of 5-HT were mimicked by the $5\text{-}HT_{2A}$ receptor agonist, DOI, which enhanced mtDNA and ATP production. Pretreatment with a $5\text{-}HT_{2A}$ receptor selective antagonist MDL100,907 or cortical neurons cultured from $5\text{-}HT_{2A}$ receptor knockout mice showed a complete blockade of the effects of 5-HT on mitochondrial biogenesis/ function. We examined the role for SIRT1, a key regulator of mitochondrial biogenesis, in mediating the effects of 5-HT. In cortical cultures derived from SIRT1 knockout mice or treated with the SIRT1 inhibitor EX-527, 5-HT failed to elicit an increase in mitochondrial biogenesis/function. We also observed a robust induction of PGC-1α following treatment with 5-HT or the $5\text{-}HT_{2A}$receptor agonist, DOI. PGC-1α is known to influence the transcription of the mitochondrial transcription factor (TFAM), which was upregulated by both 5-HT and DOI. Notably, the increase in PGC-1α and TFAM levels preceded the increase in mtDNA and ATP levels, demonstrating that 5-HT may influence mitochondrial physiology through modulation of mitochondrial biogenesis in neurons. In cortical neurons 5-HT decreased cellular ROS levels and enhanced anti-oxidant enzymes SOD2 and catalase, indicating a potential role in buffering cellular stress. We show that pretreatment with 5-HT has a neuroprotective effect in primary cortical neurons buffering excitotoxic and oxidative stress evoked by kainate and H_2O_2 respectively. Our results highlight the important influence of 5-HT in regulating neuronal mitochondrial physiology.

Supported by TIFR intramural funding to VV and UK

How fast are functional motions of proteins?

Gilad Haran

Chemical and Biological Physics Department, Weizmann Institute of Science, Rehovot, Israel

The catalytic mechanisms of complex biological machines may involve a combination of chemical steps and conformational transitions. The latter are oftentimes hidden to traditional biochemical investigations, but can be exposed by single-molecule experiments. Single-molecule FRET (smFRET) is an ideal tool to probe the conformational dynamics accompanying functional dynamics of biological machines (1). We recently discovered that functional motions can be very fast, occurring on the microsecond time scale.

Our first experiment involved the domain closure reaction of the enzyme adenylate kinase from *E. coli* (2). Surprisingly, we found that the bound enzyme opens and closes its domains much faster than the unbound enzyme, and two orders of magnitudes faster than the turnover rate of the enzyme! This exciting finding, which radically deviates from previous observations on adenylate kinase, led us to suggest that multi-substrate enzymes use numerous cycles of conformational rearrangement as a means to optimize the mutual orientation of their substrates for reaction.

We also studied the functional dynamics of the disaggregation machine ClpB from *T. Thermophilus*. This machine is comprised of six identical subunits arranged as a barrel. A coiled-coil domain resides on the outside surface of each subunit, and this domain has been implicated as the switch of the machine, to which the co-chaperone DnaK binds. We found that the coiled-coil domain resides in two conformational states, which interchange on the microsecond time scale, making it a continuous, tunable switch. Further, a complex network of allosteric interactions involving the coiled-coil domain, the protein substrate-binding site and the ATP-binding sites was revealed.

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Guiding self-organized developmental patterns

Vijaykumar Krishnamurthy

International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru, India

The development of organisms starting from their zygotic state involves a tight integration of biochemical signaling and mechanical forces that eventually pattern and shape the resulting embryo. However, developmental patterns seldom form spontaneously--instead they are controlled by regulatory biochemical interactions that provide molecular guiding cues. Often, these cues involve mechanical forces and flows. How do mechanical forces enter developmental patterns? How do these guiding cues lead to controlled biological pattern formation?. We will show that cell-polarity establishment in the one-cell-stage *C. elegans* embryo is an example of a guided mechanochemical pattern. By coupling a mass-conserved Turing-like reaction–diffusion system for polarity proteins to an active-gel description of the actomyosin cortex, we reveal a transition point beyond which feedback ensures self-organized polarization, even when cues are removed. Notably, the system switches from a guide-dominated to a feedback-dominated regime well beyond this transition point, which ensures robustness. Together, these results reveal a general criterion for controlling biological pattern-forming systems: feedback remains subcritical to avoid unstable behaviour, and molecular guiding cues drive the system beyond a transition point for pattern formation. Towards the end, we will speculate on how the very same mechanical forces can control the shape the embryo during development.

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Thermostable cytochrome P450- Stability and catalytic properties

Abhijit Mondal, Mriganka Das, Shibdas Banerjee, Sandeep Goyal, Dwaipayan Dutta Gupta and Shyamalava Mazumdar

Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai

CYP175A1 is a thermostable cytochrome P450 from *Thermus thermophilus*. The natural substrate of this enzyme is still not known. Our group is involved in developing biocatalytic systems based on this thermostable enzyme, that can catalyse mono-oxygenation of variety of compounds. We have studied the biocatalytic activities of CYP175A1 on different substituted polyaromatics, and the effect of the substituent on the reaction was determined. The results showed that the enzyme first acts as a peroxygenase to convert these substrates to the corresponding aromatic alcohols, which subsequently undergo in-situ oxidative dimerization by the peroxidase-type activity of CYP175A1. Furthermore, we investigated the origin of thermostability of the enzyme and the role of the prosthetic group using multi-wavelength circular dichroism spectroscopy at different temperatures. The results show that weak non-bonding interactions such as hydrogen bonding and metal coordination play critical role in imparting high thermostability of the overall structure of the thermostable enzyme, CYP175A1. The thermostability of the tertiary structure of the active site of the enzyme was also shown to depend on the nature of binding of the metal cofactor to the protein matrix.

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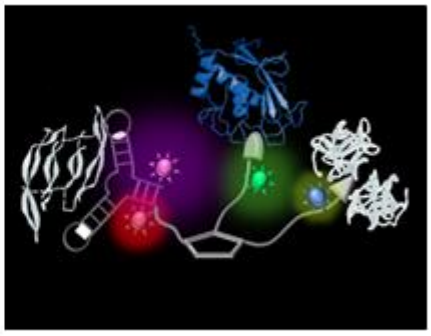
Molecules that generate 'fingerprints': a new class of fluorescent probes for medical diagnosis and chemical biology

David Margulies

Department of Organic Chemistry, Weizmann Institute of Science, Rehovot, Israel

Our group has recently developed a new class of molecular sensors, termed 'combinatorial fluorescent molecular sensors', which mimic the function of cross-reactive sensor arrays (the so-called chemical "noses/tongues").[1-5] In this talk I will explain how these pattern-generating probes could expand the fluorescent toolbox currently used to detect and image proteins. Specifically, I will show how such systems can be used to identify combinations of specific protein families within complex mixtures and to discriminate among isoforms in living cells, where macroscopic arrays cannot access.[4] The way by which these molecule-size 'noses' can be used to track several binding interactions simultaneously and be generated by self-assembly[5] will also be discussed.



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Protein disorder and function

Sudipta Maiti

Department of Chemical Sciences, Tata Institute of Fundamental Research

Central dogma of biology states that for a protein, sequence determines structure, which in turn determines function. This model is not directly applicable to intrinsically disordered proteins, which have little or no structure, yet have defined functions (sometime toxic functions, as in some amyloids). We are trying to understand the basis of the functions of two such proteins/peptides: amyloid beta (related to Alzheimer's disease), and Amylin (related to Type II diabetes). We are probing the roles played by the ordered and disordered parts of these molecules in their interactions with cell mimics and living cells, using several new optical tools / strategies which we have developed.

Separation of enantiomers by their enantiospecific interaction with achiral magnetic substrates

Koyel Banerjee-Ghosh, Oren Ben Dor, Francesco Tassinari, Eyal Capua, Shira Yochelis, Amir Capua, See-Hun Yang, Stuart S. P. Parkin, Soumyajit Sarkar, Leeor Kronik, Lech Tomasz Baczewski, Ron Naaman, Yossi Paltiel

Department of Chemical and Biological Physics, Weizmann Institute of Science

Chiral molecules are the building blocks of life. Therefore, enantio-separation is a very important process in the pharmaceutical and chemical industries. Currently, the separation process is complex and expensive. However, in nature this process is efficient. It is commonly assumed that recognition and discrimination of chirality, both in nature and in artificial systems, depend solely on spatial effects. However, recent studies have suggested that charge redistribution in chiral molecules manifests an enantio-specific preference in electron spin orientation. We therefore reasoned that the induced spin polarization may affect enantio-recognition through exchange interactions. We showed experimentally that the interaction of chiral molecules with a perpendicularly magnetized substrate is enantio-specific. Thus, one enantiomer adsorbs preferentially when the magnetic dipole is pointing up, whereas the other adsorbs faster for the opposite alignment of the magnetization. The interaction is not controlled by the magnetic field per se, but rather by the electron spin orientations, and opens prospects for a distinct approach to enantiomeric separations.

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Protein Dynamics as a marker to sense and regulate protein-protein interactions

Ravi Venkatramani

Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai

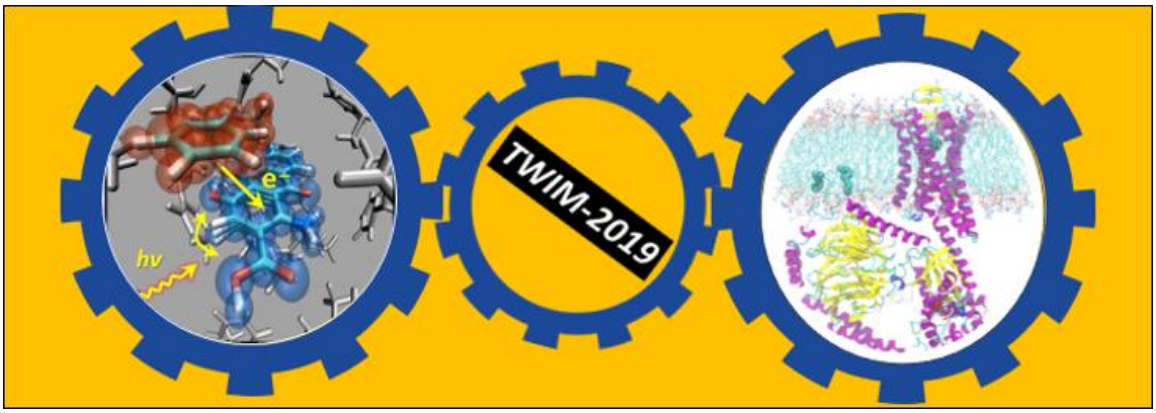
A major effort in our research group is the computational study of protein dynamics and assessing its importance for biological function. In this talk I will present examples where equilibrium protein dynamics acts as a molecular level descriptor to either distinguish or regulate protein-protein interactions. The equilibrium dynamics of ubiquitin, a post-translational molecular tag, regulating diverse cellular processes in eukaryotes, is exquisitely sensitive to its complexation state and can resolve non-covalent interactions with protein partners with similar binding modes. In CDK1, an essential kinase which dictates cell-cycle progression in eukaryotes, an active site post-translational modification alters protein dynamics to allosterically regulate interactions with Cyclin-B essential for kinase activity.

Interaction Meeting on Materials, Chemistry, and Biology

Posters

Venue: HBA Foyer

Presentation Schedule:
Odd # Posters (Tue Jan 15th 2-3:30 pm)
Even # Posters (Thrs Jan 17th 2-3:30 pm)



#	Presenter	Dept/Inst	Poster title
1	*Sandhya Koushika*	*TIFR-DBS*	*Faster is not better: injury signaling mediated cytoskeletal control of functional axon regeneration*
2	*Shrabasti Bhattacharya*	*TIFR-DCS*	*A tale of two proteins: similar structure but different dynamics*
3	*Sayani Das*	*TIFR-DCS*	*Manganese sensor diaries: stumbling upon a mercury sensor and what we learn from it!!*
4	*Mohd Taher*	*TIFR-DCS*	*Enzyme design for novel catalysis: logical way of directed evolution*
5	*Rajasree Kundu*	*TIFR-DCS*	*Design and development of optical sensors for imaging signal mediating phospholipids*
6	*Sravanthi Nadiminti*	*TIFR-DBS*	*Liprin-α/syd-2, a pre-synaptic active zone protein, controls neuronal protein trafficking at the cell body*
7	*Vidur Sabharwal*	*TIFR-DBS*	*Ubiquitination dependent regulation of the neuronal synaptic vesicle motor kinesin-3/unc-104*
8	*Keertana Venkatesh*	*TIFR-DBS*	*Reversals can mitigate local traffic jams to maintain cargo flow in axons*
9	*Amruta Vasudevan*	*TIFR-DBS*	*Motor levels and microtubules regulate how cargo navigate branch points in neurons*
10	*Souvik Modi*	*TIFR-DBS*	*Mitochondrial positions in c. Elegans axons corelate with spontaneuous calcium sparks and influence behavioural responses*
11	*Amitava Chandra*	*TIFR-DCS*	*Cell permeable optical probes for phosphatidylserine*
12	*Arup Kundu*	*TIFR-DCS*	*Probing singlet fission in all-trans-lycopene aggregates*
13	*Sunandita Paul*	*TIFR-DCS*	*Towards light induced generation of carbocation inside supramolecular cavity*
14	*Babukrishna Maniyadath*	*TIFR-DBS*	*Molecular interplay between epigenomic regulators modulates oscillatory gene expression during feed-fast cycles*
15	*Harshita Kaul*	*TIFR-DBS*	*Sirt1 is essential for meiotic progression, coupling of recombination and synapsis*
16	*Namrata Shukla*	*TIFR-DBS*	*Understanding signalling kinetics of fasted and fed insulin response: role of acetylation in modulating insulin-igf signalling (iis)*

17	*Sanjoy Paul*	*TIFR-DCS*	*Directional flexibility of protein from its crystal structure by combining elastic network model and method of error propagation*
18	*Nita Ghosh*	*TIFR-DCS*	*Elucidating the reaction co-ordinate for charge transfer dynamics in organic donor acceptor framework*
19	*Ananya Rakshit*	*TIFR-DCS*	*Cu(ii) chelators attenuate copper induced oxidative stress in vivo.*
20	*Ankita Das*	*TIFR-DCS*	*Hammering on a c-h bond with light inside a nanocage*
21	*Ravinder Kumar*	*TIFR-DCS*	*Molecular breadboard circuits: basis circuits and conformations*
22	*Krishna Kant*	*TIFR-DCS*	*Understanding the regulation of protein-protein interaction in cdk1:cyclin-b protein complex*
23	*Imon Mandal*	*TIFR-DCS*	*Charge transfer transitions associated with charged amino acids: sensitive to protein dynamics and aggregation*
24	*Purna Gadre*	*TIFR-DBS*	*Somatic EGFR signaling defines the rate of germ cell divisions in drosophila testis*
25	*Tushna Kapoor*	*TIFR-DBS*	*Acto-myosin assembly in somatic cells bundles mature spermatids heads, facilitating sperm release in drosophila testis*
26	*Pranali Patil*	*TIFR-DBS*	*Axonal transport of functionally distinct cargos is differentially modulated by neuronal activity in chordotonal neurons of drosophila*
27	*Kaustav Khatua*	*TIFR-DCS*	*Water soluble chemical probes for tracking mn(ii)*
28	*Anirban Das*	*TIFR-DCS*	*Xeno-nuclei enable protein-specific modulation of order-disorder transition*
29	*Mona Gupta*	*TIFR-DCS*	*Mechanical properties of ubiquitin complexed with structurally homologous ubiquitin binding domains*
30	*Barun Kumar Maity*	*TIFR-DCS*	*Role of order and disordered regions of abeta40 oligomers in multistep toxicity pathway*
31	*Anustup Chakraborty*	*TIFR-DCS*	*Unfolding of proteins in solutions : a computational study on ubiquitin*
32	*Jagjeet Singh*	*TIFR-DBS*	*Kinesin-1 facilitates maintenance of stable lipid droplet-endoplasmic reticulum contacts*
33	*Simli Dey*	*TIFR-DCS*	*A receptor-independent lipid mediated membrane pathway for serotonin action*

34	*Ankur Gupta*	*TIFR-DCS*	*The role of lipid ordered and disordered phases in determining the conformation and affinity of toxic oligomers to the membrane*
35	*Tathagata Nandi*	*TIFR-DCS*	*Comparing the folding-unfolding pathways of sumo proteins with their structural homologue ubiquitin*
36	*Priya Yadav*	*TIFR-DCS*	*Circular permutant in azurin - creating new termini for pulling along diferent directions*
37	*Khurshid Ahmad*	*TIFR-DCS*	*Computational determination of f19-l34 binding energy for amyloid beta :understanding aggregation and toxicity*
38	*Souvik Ghosal*	*TIFR-DCS*	*Tuning photoselection of sp2-carbon centered oxidative functionalization in water-soluble nanocages: towards the evolution of artificial photo-enzyme*
39	*Sahil Kumar*	*TIFR-DCS*	*Tuning peptide scaffolds for selective phospholipid detection*
40	*Arpan Dey*	*TIFR-DCS*	*A single-molecule method to characterize the conformation of individual oligomers of amyloid proteins*
41	*Aditya Chhatre*	*TIFR-DBS*	*Lis1 regulates cortical actin dynamics during phagocytosis*
42	*Vicky*	*TIFR-DCS*	*Finding binding partners for intrinsically disordered proteins by measuring fast fluctuations with fluorescence cross correlation spectroscopy*
43	*Sutanuka Manna*	*TIFR-DCS*	*Assessing the limitations of TDDFT in describing optical UV-visible backbone-sidechain charge transfer transition in proteins*
44	*Abhijit Mondal*	*TIFR-DCS*	*A biological catalysis by reconstituted heme proteins*
45	*Debanjana Das*	*TIFR-DCS*	*Copper-binding induced structural transitions in a small peptide derived from azurin*
46	*Srikant Ojha*	*TIFR-DBS*	*Phosphatidic acid mediates secretion of VLDL from hepatocytes*
47	*Aasna Parui*	*ACTREC*	*Allosteric regulation of serine protease htra2*
48	*Abhinandan Ambastha*	*TIFR*	*Selective coupling of photonic defect states in modulated P3HT films*