India of the 21st Century is headed towards knowledge economy, which is expected to bring changes in the economic scenario. In this context, we are ushering a new education system in science and technology.

Amongst the many initiatives of the country is the establishment of the Indian Institutes of Science Education and Research (IISERs). These autonomous research institutes have been set up at five locations across India, one of them in Pune, by the Ministry of Human Resource Development, Govt. of India with the primary goal of integrating high quality research with undergraduate teaching to improve science education in India and to enhance the number and quality of future academic as well as industrial researchers of the country.

The model of education at IISER Pune (http://www.iiserpune.ac.in) is concept-based and inquiry-driven, as opposed to the more traditional content-based models. IISER Pune offers a 5-year BS MS dual degree program, Integrated-PhD programs for bachelor level students, and PhD programs for Master's level students.

In the shortest time possible, we have set up one of the best-equipped research facilities in the country at IISER Pune. Faculty members are carefully chosen for their research accomplishments, promise and teaching proficiency. While the identity of individual disciplines is maintained, we have physicists, chemists, biologists and mathematicians working shoulder to shoulder without any departmental (or compartmental) structure. One of the greatest strengths of IISER Pune is this interdisciplinary ambiance. At IISER Pune, we also aim to integrate natural sciences with social sciences and humanities in knowledge production and education. The whole ambiance is very academic and energy levels are high. There is a great enthusiasm amongst faculty members and students to pursue high quality research: together, they investigate questions in science that lie beyond the boundaries of conventional thinking.
Scanning Electron Microscopy image of cadmium sulphide nanotubes
(Image: Shouvik Datta's Group)
NONLINEAR DYNAMICS AND COMPLEX SYSTEMS

Natural systems are highly complex since their dynamics involve a large number of units with highly nonlinear interactions among themselves and with the environment. We analyze how the dynamics of such connected systems can be suppressed due to interaction with environment. We propose that this mechanism provides for the first time a physical model for Alzheimer’s disease, where due to the induced activity on certain proteins called amyloid beta, the normal neuronal activity will be suppressed.

We have recently introduced a novel coupling scheme for synchronizing nonlinear chaotic systems where the delay in coupling is varied within a reset interval. This has lead to a novel error dynamics and Lyapunov exponent computations. This introduces a new method for synchronizing time delay systems and has relevance in applications like secure communication.

We have developed methods for quantifying complexity with relevant measures computed from the observed time series. A few parameters identified to characterize the Multifractal spectrum serve as better quantifiers for diagnostic purposes for data like EEG and ECG. A complete analysis of the light curves from all the states of the black hole system, GRS 1915+105 is done using these quantifiers.

SELECTED PUBLICATIONS


THEORETICAL PARTICLE PHYSICS

According to our current understanding, there are four fundamental forces in Nature. Quantum Yang-Mills theory provides a remarkably accurate description of three — electromagnetic, weak and strong — of these four forces. The fourth force, gravity, is classically well understood thanks to the general theory of relativity. However, we still lack a consistent quantum mechanical description of the gravitational force.

My research is aimed at understanding this apparent incompatibility between general relativity and quantum mechanics. Themes of current interest include

1. Efficient methods to compute correlation functions in conformal field theories.
2. Origin of divergences in quantum field theories.
3. Perturbative relations between gravity and gauge theory: using perturbative ties between gravity and Yang-Mills theory to understand ultra-violet behavior in gravity theories.
4. Ultra-violet properties of N=8 supergravity.

SELECTED PUBLICATIONS


1. ASTROPHYSICS AT LOW RADIO FREQUENCIES

I focus on astrophysical phenomena which are best studied at low radio frequencies, largely with the Giant Metre-wave Radio Telescope (GMRT) near Pune. These include an eclectic mixture of radio halos and relics in galaxy clusters, AGN feedback in galaxy clusters, absorption line spectra of quasars and other objects in the early Universe, steep spectrum radio sources, pulsars, etc. In the past I have worked on gravitational lensing, and radio galaxies and Lyman alpha galaxies at high redshift. Recently, I developed a technique to excise man-made radio frequency interference from radio telescope data which has resulted in a significant improvement in the quality of imaging.

SELECTED PUBLICATIONS


2. BIOLOGICAL DIVERSITY: RESEARCH AND CONSERVATION

I am interested in research on and conservation of the rich biological diversity in India. I initiated and lead the Eaglenest Biodiversity Project, which is inventorying the fauna of Eaglenest sanctuary in Arunachal Pradesh and helping in its conservation. My research in this field involves delineating the geographical distribution of diversity across Arunachal and investigating the factors responsible for the same. This work has resulted in the discovery of several new species including a spectacular bird species new to science.

SELECTED PUBLICATIONS


STRING THEORY AND HOLOGRAPHY

Of the four fundamental forces of Nature, gravity is the most ubiquitous and also the least understood. Einstein’s theory of relativity successfully describes classical gravity but breaks down at extremely small length-scales when probing the quantum nature of gravity. Quantum gravity has been the holy grail of theoretical physics and is essential for understanding the deep questions about the origin of the universe and unravelling the mysteries of black holes.

String theory is the most successful attempt at a theory of quantum gravity. One of the most intriguing ideas arising from research in string theory is the Holographic Principle which states that in a quantum gravity theory all physics within some volume can be described in terms of some theory on the boundary. This revolutionary proposal was put on firm footing by the AdS/CFT correspondence. AdS/CFT is a conjectured equivalence or duality between two apparently unrelated theories, one a theory of gravity living in a negatively curved Anti de-Sitter (AdS) spacetime and the other a conformal field theory (CFT) living on its boundary.

The primary goal of my research has been to understand the Holographic Principle by looking to generalise it to different situations which go beyond standard AdS/CFT. My current main research programme aims to understand aspects of holography in flat spacetimes. I am also interesting in the recent formulations of a holographic connection for higher spin theories and its potential link to the tensionless limit of string theory.

SELECTED PUBLICATIONS


Ashna received her PhD in Physics from UGC-DAE Consortium for Scientific Research in Indore, followed by a postdoctoral stint at the Tata Institute of Fundamental Research (TIFR), Mumbai, India. In 2006, she moved to the Liebniz Institute for Solid State and Material Research at Dresden, Germany as a Marie Curie Fellow. Subsequently, she worked at the Department of Materials at Oxford University, UK before joining IISER Pune in December 2011.

**ASHNA BAJPAI**  
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**MAGNETISM, NANO-SPINTRONICS, STRONGLY CORRELATED ELECTRONIC SYSTEMS**

I work in the field of experimental condensed matter physics and my core area of research is the magnetism and electron transport in strongly correlated electronic systems.

My current research interests pertain to the investigation of multifunctional magnetic oxides and their potential applications in the field of spin electronics. I am presently working on the encapsulation of some functional magnetic materials inside carbon nanotubes (CNT). Coupling the functionality of the nano-scale magnetic materials with that of CNT is highly desired for a diverse range of future applications. This is particularly relevant in the field of spintronics, where magnetic field, electric field and possibly strain guided applications for magnetically functionalized nanotubes can give rise to novel nano-spintronic devices. I am currently investigating electric transport properties of individual CNTs, filled with a magnetoelectric /spintronic oxide Cr$_2$O$_3$. Here we observe some novel current induced structural changes taking place inside the core of the nanotube, such as the transformation of the continuous polycrystalline filling into the regular shaped beads and eventually nano-scale single crystals.

**SELECTED PUBLICATIONS**


Arijit Bhattacharyay obtained PhD from Indian Association for the Cultivation of Science (IACS), Kolkata, India. He then pursued postdoctoral work at TU Darmstadt, Germany; Padova University, Italy; and Warwick University, UK before joining IISER Pune in 2008.

**STATISTICAL PHYSICS, COMPLEX SYSTEMS**

My research interest is in the broad area of complex systems. A part of my work concerns understanding localized patterns formed near instability boundaries. There are numerous models of pattern formation existing, and, near the instability boundaries, the dynamics of such systems are very rich. Interestingly, at instability boundaries, the dynamics of such apparently different models are universal, and, therefore, a general understanding of pattern forming instabilities is possible. Complex Ginzburg-Landau equations are mostly studied in the context of pattern formation near instability boundaries. Such a dynamical system also applies to superconducting-to-normal phase transition in a one-dimensional superconductor. Presently, I am working on localized amplitude modulations observed in the resistive regime of a one-dimensional superconductor.

The other part of my research interest so far has been diverse and in the area of application of statistical physics tools to bio-physical problems. To name a few, I have worked on quantitative genetics, protein folding, self-assembly etc. Presently, I am working on modeling active transport of bacterium and similar systems to understand basic minimum ingredients required for symmetry breaking and directional transport as shown by these entities.

**SELECTED PUBLICATIONS**


Apratim Chatterji completed PhD in 2002 from Indian Institute of Science (IISc), Bangalore, India with Prof Rahul Pandit. He took up postdoctoral work initially at the Kurt Binder group in Germany, and later at University of Toronto, Canada and at the Soft Matter and Biophysics group in Research Center in Juelich, Germany. He joined IISER Pune in January 2009.

SOFT MATTER PHYSICS AND STATISTICAL PHYSICS

Soft Matter is the physics of interacting macromolecules. The defining characteristic of such systems is that the interaction energy between the constituent molecules is of the order of thermal energy. Therefore, soft matter systems show large response under external perturbations such as shear flow fields or electric field, i.e., these systems have very low elastic moduli. The basic building blocks of soft matter systems can be broadly classified as: (a) Colloidal particles (Brownian particles whose size can vary from nm to microns); (b) Polymers (from a physicists perspective: long chains undergoing Brownian motion); (c) Amphiphilic molecules capable of self assembly.

In the recent past I have been investigating the dynamics of charged colloidal suspensions and star-polymer solutions. Hydrodynamic interactions between the macromolecules are incorporated using multiscale modeling and simulation techniques which enables us to span over multiple length and time scales. I have contributions in the development of hybrid simulation techniques such as coupled Molecular Dynamics-Lattice Boltzmann (MD-LB) simulations as well as MD-Multi-Particle Collision dynamics (MD-MPC). Currently, I am working on the phenomenon of charged colloidal electrophoresis, the rheology of micellar systems and colloids/polymer in extensional flow.

SELECTED PUBLICATIONS


Harsh Chaturvedi completed BE in Electronics and Communication with First class with distinction from Visvesvaraya Technological University, Belgaum, India (2003) and PhD from University of North Carolina, Charlotte, USA (2008). He joined IISER Pune in 2009.

**DEVICE FABRICATION BASED ON FUNCTIONALIZED NANOMATERIALS LIKE SINGLE WALLED CARBON NANOTUBES**

The goal of bottom-up technology is to realize functional machines by directed structural assembling of individual molecules. My research focuses on following themes: Nanoscale Structures, Novel Photon induced Phenomena and Controlled Molecular Assembly. We aim to understand and develop the phenomena associated with “optically induced doping” of nanotubes. Essentially, we aim to selectively bind supramolecular charge transfer molecules to structures like nanotubes and nanowires with high aspect ratio for enhanced sensitivity and effective charge separation such that upon their optical excitation, the molecules will transfer electrons or holes onto the nanoparticle. This doping will, in turn, affect the electronic and vibrational states of the nanoparticles. It is this phenomenon that we will study fundamentally and exploit for applications based on the optoelectronic elements. We believe that the unique electrical, optical, and mechanical properties of these assemblies will lead to novel biological and optical sensors, devices and composite materials. Charge separation in these supramolecular devices may be effectively exploited for fabricating efficient solar and photovoltaic cells. Molecular hybrid system will be characterized using spectroscopic (absorption and Raman) and microscopic techniques (AFM, SEM). Optical effects such as photon enhanced aggregation will be explored further, to develop it as a viable technique for controlled and directed assembly of nanoparticles into functional devices. Devices will be fabricated using e-Beam lithography and conventional photolithography.

**SELECTED PUBLICATIONS**


OPTO-ELECTRONIC PROPERTIES OF SEMICONDUCTOR NANO-MATERIALS AND DEVICES

1) What happens to the electrical dielectric response of a material medium or a laser diode when it starts to emit light or even starts lasing? Conventional techniques like DLTS etc are only useful to study material junctions held under reverse bias and cannot be used directly with their usual interpretations under high forward bias where depletion approximation need not be valid because of the presence of a large number of injected charge carriers. We are currently asking (Bansal and Datta, 2013) - whether we can we still understand the condensed matter physics of light emitting medium using electrostatics approximation only? Is population inversion necessary for lasing? etc.

2) Do we need to revisit the Bohr exciton radius? Bohr exciton radius is the characteristic size to observe quantum confinement effects at the nanoscale. Is the usual 'electrostatic' interaction of electron-hole bound pair sufficient (arXiv: 1105.2205) to describe optical transitions involving 'hot' excitons? Does it modify in presence of strong dispersions of dielectric response near a resonant absorption? In our experiments, we see significant departure from the usual limiting form of dielectric screening (\(\varepsilon\)) of coulomb interactions of 'hot' excitonic resonance in the region of strong dispersion at energies much above the fundamental band gap. We predict optimum size window of semiconductor nanoparticles for efficient usage in nano-photovoltaic devices.

3) What causes directionally asymmetric self-assembly of cadmium sulfide (CdS) nano-tubes with high optical quality under capillary flow mediated chemical reactions in porous alumina 'nano-reactor': We are exploring whether chemo-hydrodynamic origin of convective interfacial instability of multi-component liquid-liquid reactive interface and surface charge controlled diffusion are competing for sustained nucleation of CdS nano-tubes at the edges of porous nano-channels (Varghese and Datta, 2012). We are also studying the physics of fluorescence blue-shifts in nano-tubes having diameters much larger than the Bohr exciton radius of CdS and the origin of stoichiometric imbalance of Cadmium and Sulfur on the surface! We are interested to understand how confinement affects the entropic changes associated with the fluid flow inside such 'nano-reactor'?

4) How electronic defects behave at the nano-scale: Free energy redistribution and entropic changes associated with charge capture & charge emission processes by electronic defects were shown (Datta et al., 2008) to trigger configurational relaxations in neighborhood of these defects. Due to its small effective size and large surface to volume ratio, such configurational modifications of electronically and optically active defects can be significantly different in nano-materials and devices as compared to their bulk counterparts.

SELECTED PUBLICATIONS


Low dimensional systems at nanometer length scale have unique properties. The electrons in these systems are confined to one or more dimensions. This gives rise to a variation in the density of states of the systems. My research is focused on the investigation of low dimensional systems using ultra high vacuum scanning tunneling microscopy (STM). The high spatial resolution of STM provides real space images with atomic resolution. With scanning tunneling spectroscopy performed using STM at low temperature (4.2 K), the enhanced energy resolution at low temperature allows a direct measurement of the local electronic properties of these systems. The atomic scale structure and electronic information provides an insight into the quantum phenomena and interactions in these systems. My spatially resolved STM imaging and spectroscopy studies on graphene, the two dimensional form of carbon, have helped unravel the charge inhomogeneities in graphene. Another area of my interest is to use STM as an active tool for STM manipulation to bring out a change in the atomic scale structure of the assembly of atoms and molecules deposited on a conducting surface. The change in structure is then followed by spectroscopy measurements to test the fundamental properties of atoms and molecules at the atomic level for nanoelectronic and spintronic device applications.
C V Dharmadhikari received his PhD degree from University of Pune, India in 1979 and was a postdoctoral fellow at University of Chicago, USA until 1984. He then joined University of Pune as a faculty and served as the department head for Physics and Instrumentation Science. He joined IISER Pune as a visiting faculty in December 2011.

**SURFACE SCIENCE, SCANNING PROBE MICROSCOPY**

My work involves development of a whole range of Scanning Probe Microscopes and their application to the investigation of a host of problems at the frontiers of surface science, thin films and nanoscience. My current research interests are in the following areas.

- Photon emitting STM (PESTM), Low current STM operating in field emission mode for imaging nanostructures/nanobiostructures
- Contact mode/Non-contact mode current imaging using AFM
- Force spectroscopy of colloidal systems
- AFM imaging using piezoelectric/piezoresistive cantilevers
- Noise analysis of tunneling and field emission current fluctuations
- Electron transport across nanostructures
- Synthesis of nanostructures using SPM

**SELECTED PUBLICATIONS**


CALCULUS ON FRACTALS, NONLINEAR DYNAMICS

Fractals are often too irregular to have any smooth differentiable structure defined on them and render the methods and techniques of ordinary calculus powerless or inapplicable. Ordinary calculus does not equip us to handle problems such as fractal time random walks, anomalous diffusion, dynamics on fractals, fields of fractally distributed sources etc., by setting up and solving ordinary differential equations. Setting up a general framework and formalism to address these issues is highly desirable but very challenging goal.

The need to use fractional derivatives and integrals was recognized in this context. However, fractional derivatives are nonlocal operators and not always suitable to handle the local scaling behavior; e.g., the behavior of fractal functions. This difficulty was circumvented by renormalizing fractional derivatives and constructing local fractional operators. A particular success of this approach was the demonstration of the striking fact that fractal functions can be differentiated up to an order (fractional) determined by the Holder exponent of the function (or dimension of its graph). In particular, Weierstrass’s nowhere differentiable function was shown to be differentiable up to order (2-d), if d is the box dimension of its graph.

Fractional Fokker Planck and Diffusion Equations were written using this construction. New exact solutions of Chapman-Kolmogorov equations were obtained by solving such fractional equations. These solutions correspond to sub-diffusive processes and are suitable to deal with a class of hindered diffusions. A systematic development of calculus on fractal subsets of real line involving integrals and derivatives whose orders are precisely the dimensions of those fractals was carried out. Sobolev spaces on fractal subsets of the real line were constructed. The calculus developed retains much of the simplicity of ordinary calculus.

The calculus on fractals provides a powerful tool to pose new questions which could not be formulated earlier. Thus, e.g., one can ask: what is equation of motion for a particle moving in a fractal medium so that the support of friction is a fractal. Another example is an equation for anomalous diffusion.

SELECTED PUBLICATIONS

Mukul Kabir received his PhD in Physics from the S N Bose National Center for Basic Sciences, Kolkata, India in 2006. Soon after he joined Massachusetts Institute of Technology as a postdoctoral associate, and subsequently promoted to senior postdoctoral associate, which he has held till late 2011. Before joining IISER Pune, he was a Visiting Assistant Professor at the S N Bose National Center for Basic Sciences, Kolkata.

MATERIALS MODELING AT DIFFERENT LENGTH- AND TIME-SCALES

Our main interest evolves with predictive multi-scale materials modeling, which requires bridging theories at the different length- and time-scales with careful information transfer. The approach can be divided into three major steps: (1) Understanding the complex energy landscape (thermodynamics) via quantum chemical calculations; (2) Understanding the microscopic kinetic mechanisms via transition-state based theories; and (3) Studying the macroscopic properties at larger spatial and temporal scales via statistical sampling of the (microscopic) unit kinetic processes. This enables us to predict macroscopic properties from microscopic fidelity.

Application wise, we have a special interest in the fundamental challenges toward sustainable energy, which includes the issues in structural materials, catalyst design for water oxidation, and material design for hydrogen storage. Thus, we have been closely studying the defect thermodynamics, and their microscopic kinetics in the technologically important alloys at the operating conditions relevant to nuclear reactors. We are also investigating the catalytic role of Mn₃O₄Ca-complex (observed in Photosystem II) in water splitting.

We are also interested in various other problems including topological defect formation and activation in fullerene and carbon nanotube, which are important to understand the microscopic growth, fusion, and mechanical properties of these carbon nanostructures. Spin crossover in transition metal cyanide, shape dependence of quantum confinement in semiconductor nanocrystals, and manipulating edge magnetism in graphene flakes are some other active fields of research that we are currently involved in.

SELECTED PUBLICATIONS


Avinash Khare did his PhD in 1971 from Saha Institute of Nuclear Physics, Kolkata, India in Theoretical Elementary Particle Physics. After spending two years in University of Tokyo, Japan as a postdoctoral fellow, he joined Institute of Physics, Bhubaneswar, India as a faculty member in 1975. He served in the institute for 36 years in different positions and retired as a Senior Professor in 2010. He moved to IISER Pune in January 2011 as a Raja Ramanna Fellow of the Department of Atomic Energy, Government of India.

**HIGH ENERGY PHYSICS, LOW DIMENSIONAL FIELD THEORY, SUPERSYMMETRIC QUANTUM MECHANICS, NONLINEAR DYNAMICS**

Over the last 45 years of my research career, important results have been obtained in several areas of physics. By now 230 papers have appeared in refereed journals, several of these have got more than 100 citations. Some of the important results obtained are (i) constructed $\phi^2-\phi^4-\phi^6$ field theory as a model for structural phase transition. Obtained several exact solutions of this model (as well as double sinh-hyperbolic Gordon equation including exact expression for free energy at several temperatures in the thermodynamic limit (ii) predicted accurately the splittings of the P levels of the charmonium and the bottomonium systems before they were experimentally measured (iii) discovered the charged vortex solutions in abelian Higgs model with Chern-Simons term in 2+1 dimensions, which was the first example of (extended) anyons in field theory. This work has lead to host of developments in the field (iv) obtained the third virial coefficient of anyon gas and also studied many other properties of anyons (which are particles in 2+1 dimensions obeying fractional statistics (v) did several important works in the area of Supersymmetric Quantum mechanics including exactness of Supersymmetry inspired WKB approximation, showed how to obtain eigenfunctions algebraically for shape invariant potentials (SIP) and did classification of SIP with translation (vi) discovered new identities for Jacobi elliptic functions which have already appeared in Mathematica as well as in Chapter 22.7 and 22.9 of Abromowitz-Stegun and also on Internet at "http://dlmf.nist.gov/22 (vi) have written two monographs published by World Scientific, Singapore, entitled: (1) *Fractional Statistics and Quantum Theory* (2) *Supersymmetry in Quantum Mechanics* (with F. Cooper and U.P. Sukhatme).

**SELECTED PUBLICATIONS**


NANOSCIENCE, PHOTOVOLTAICS

Our group is engaged in the synthesis using different physical and chemical routes and analysis of a large variety of nanoparticles. The materials of our interest include II-VI semiconductors, metals like gold, silver, iron, cobalt, ferrite particles etc. We have also developed particles in different sizes and shapes to tune optical and magnetic properties. Various core-shell and polymer composites also have been developed. High strength aerogels and some other porous materials, anodized alumina templates (AAO) also have been developed. Soft lithography techniques have been developed and some nanoparticles have been patterned. Besides developing nanomaterials and carrying out basic investigations we have demonstrated the use of some of these materials as field emitters, biosensors etc. Recently gold nanorods with high aspect ratio have been used in laser welding of the tissues. Some of our recent work on doped and undoped CdSe showed that these nanoparticles exhibit room temperature ferromagnetic like behavior. Our group is currently engaged in developing solar cells using Quantum Dots.

SELECTED PUBLICATIONS


T S Mahesh obtained his PhD in 2004 from Indian Institute of Science (IISc), Bangalore, India. He was a postdoctoral fellow at Massachusetts Institute of Technology, Cambridge, USA and later a Humboldt Fellow at Dortmund University in Germany before joining IISER Pune in 2007.

**NUCLEAR MAGNETIC RESONANCE AND QUANTUM INFORMATION PROCESSING**

Nuclear Magnetic Resonance (NMR) has wide ranging applications such as structure-function analysis of molecules, medical diagnosis and Quantum Information Processing (QIP). Coherent superposition of quantum bits allows QIP to tackle certain mathematical problems and simulation of quantum dynamics that are intrinsically difficult otherwise.

NMR enables us to simulate QIP by treating spin states of atomic nuclei in bulk matter as quantum bits. Long lasting nuclear spin coherences and excellent control techniques help us to carry out hundreds of logic gates and implement most complex quantum algorithms to date.

Our research focuses on building solid-state architectures for spin-based QIP, achieving larger quantum registers, experimental implementation of quantum algorithms, development of techniques to control spin dynamics with high fidelity, and designing novel NMR experiments.

**SELECTED PUBLICATIONS**


\(^{1}H\) NMR spectra of chloroform displaying particle-like and wave-like behaviors of protons on applying a transformation equivalent to the Mach-Zehnder Interferometer (http://lanl.arxiv.org/abs/1112.3524)
Sunil Mukhi earned his BSc from St Xavier’s College, University of Bombay and PhD in Theoretical Physics from the State University of New York at Stony Brook, USA. After spending about two years at ICTP, Trieste, Italy as a postdoctoral fellow, he joined TIFR, Mumbai in 1984 and worked there for the next 28 years, becoming Senior Professor in 2009. He was the first Dean of Graduate Studies of the TIFR Deemed University and later the Chair of the Department of Theoretical Physics. He has joined IISER Pune in 2012.

STRING THEORY AND QUANTUM FIELD THEORY

My research has centered on fundamental properties of string theories and model quantum field theories with supersymmetry. Early work provided evidence for the conformal invariance of supersymmetric sigma models now known to describe the world-sheet dynamics of strings. This was followed by a study of the topological properties of supersymmetric field theories and their solitonic states using index theorems. Mathematical features of 2d conformal field theories on the plane and on higher genus surfaces were extensively analysed. Noncritical strings were formulated via topological black hole backgrounds and matrix models. New dualities in M-theory were discovered along with nonperturbative properties of F-theory, BPS states such as string networks, and orbifold and orientifold compactifications. My most recent work found novel properties of highly supersymmetric 2+1 dimensional field theories describing multiple membranes in M-theory. I have co-authored a textbook on Advanced Mathematical Methods in Physics, edited three Conference Proceedings and guided five Ph.D. students.

SELECTED PUBLICATIONS


Sunil Nair did his PhD at the Inter University Consortium for DAE Facilities, Indore followed by a brief postdoctoral stint at the Tata Institute of Fundamental Research (TIFR), Mumbai, India. In 2005 he moved to the Max Planck Institute for Chemical Physics of Solids at Dresden, Germany as a Humboldt Fellow. Subsequently, he worked in the Clarendon Laboratory at the University of Oxford, UK as a Marie Curie Fellow. He joined IISER Pune in July 2011.

**STRONGLY CORRELATED ELECTRON SYSTEMS**

My primary research interests lie in the field of strongly correlated electron systems, which exhibit a plethora of novel properties as a function of external control parameters like temperature, electric or magnetic fields and pressure. The primary quest is to identify novel phenomena and phases, and to understand their microscopic origins. This is usually accomplished by measurements which probe the spin and the charge degrees of freedom. Experimental probes which I have relied on for this purpose have been linear and nonlinear magnetic susceptibilities, DC magnetization, high field magnetoresistance, the Hall effect, and x-ray and neutron scattering. Systems which I have investigated during the course of my research career include magnetoresistive, and charge ordered manganites, heavy fermion superconductors, spin glasses, and multiferroic transition metal oxides. Since a rigorous investigation of these complex systems warrants the use of sensitive physical property measurement techniques, a continuous focus of my research work has been the development of low temperature measurement techniques to accomplish this task. With this area of research being fuelled by the synthesis of novel materials, I am also actively involved in the synthesis of new materials with improved, or tailor-made properties.

In IISER Pune, I aim to establish a research program which combines all of these above mentioned interests. Of particular interest would be the investigation of new oxide and intermetallic systems, where strong electronic correlations manifest themselves in the form of striking physical properties.

**SELECTED PUBLICATIONS**


Nair, S. and Nigam, A.K. (2008). Re-entrant canted antiferromagnetic state in the Mn site substituted manganite La_{0.64}Sr_{0.36}Mn_{1-x}Cr_{x}O_3. *Europhysics Letters* 84:37008.

Rajaram Nityananda was a research scholar at the National Aerospace Laboratory, Bangalore (1969-1975) before joining the Raman Research Institute where he spent nearly 25 years working in the areas of theoretical physics and astrophysics. He was a professor at the National Centre for Radio Astrophysics, Tata Institute of Fundamental Research, Pune until early 2013 when he joined IISER Pune.

**OPTICS, STATISTICAL PHYSICS, DATA ANALYSIS, APPLICATIONS IN ASTRONOMY**

My work on optics has covered propagation in liquid crystals, polarisation and geometric phase, and gravitational lenses, i.e., the bending of light from very distant objects by masses encountered on its way to us, which has consequences like multiple and distorted images and is a useful tool in astronomy. Another theme related to optics is the recovery of information from data obtained from telescopes which are subject to loss of information and noise, using statistical and other techniques. More recently, I have worked on some aspects of separating the desired signals in radio telescopes from undesired, usually man-made disturbances (known as RFI or radio frequency interference).

The dynamics of galaxies involves a large number of interacting particles and comes under the purview of statistical physics, but with many features unique to gravitating systems. I have worked - with colleagues - on some aspects of galaxy dynamics.

One of my major current interests is the teaching of physics and conveying new concepts beyond the classroom to students including through articles in journals like Resonance.

**SELECTED PUBLICATIONS**


Shivprasad Patil obtained his PhD from University of Pune, India. He was a postdoctoral fellow at Wayne State University, USA and Instituto Microelectronica de Madrid CSIC, Spain before joining IISER Pune in 2008.

NANO-MECHANICS OF BIOMATERIALS

Nanotechnology has spawned significant new ideas which may lead to another industrial revolution. The device fabrication from few molecules with a bottom-up approach requires understanding of basic processes such as dissipation, lubrication at molecular scale and interaction between single molecules. On the other hand, nature uses the architecture and interaction at molecular scales to perform certain tasks that human technology has not been able to achieve so far. The nano-mechanics lab of IISER Pune uses single molecule techniques such as atomic force microscope (AFM), optical tweezers and fluorescence correlation spectroscopy (FCS) to understand mechanical response of biomaterials. This includes lipid bi-layers and single protein molecules under controlled stress. The group develops above-mentioned techniques for quantitative information of the forces involved. In particular, we combine the spatial resolution of probe microscopic techniques with temporal resolution of optical spectroscopy to develop new methods to unravel mechanistic details of single molecule processes.

In order to gain insight into functioning of biomaterials, not only the molecules that constitute the material, but the water within or around them is also of significant interest. As a model system, we probe the mechanical response of water films which are less than a nm thick and are confined by rigid walls. We have recently established that the rate of formation of these films plays an important role in determining their mechanical response. This response varies from elastic solid-like to Newtonian fluid-like analogues to glassy transitions. Our group is now developing new techniques to measure the mobility of such molecularly confined water.

SELECTED PUBLICATIONS


G V Pavan Kumar obtained his PhD from the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Subsequently, he was an ICFO Fellow at the Institute of Photonic Sciences, Barcelona and postdoctoral fellow at Discovery Park, Purdue University, USA. He joined the faculty of Physics and Chemistry at IISER Pune in May 2010.

**PLASMONICS, RAMAN SCATTERING, NANO- AND BIO-PHOTONICS**

The theme of our inter-disciplinary research is to understand interaction of light with materials and molecules at micro- and nano-scales. We are interested in questions such as:

- How does light interact with matter smaller than its wavelength?
- How to create an efficient optical antenna with nanomaterials?
- How to create electromagnetic hot-spots for Raman scattering?
- What happens to structure of illuminated biomolecules near metallic surfaces?
- How to optically detect single non-fluorescent molecule or nanoparticle?
- How to harness lithography procedures and material synthesis to develop nano-optical devices?

To find solutions to these problems, we focus on developing experimental and theoretical methods of plasmonics, Raman microscopy, optical trapping, opto-fluidics and near-field optics. We employ both bottom-up and top-down approaches to fabricate nanomaterials.

**SELECTED PUBLICATIONS**


Umakant Rapol received his PhD from Indian Institute of Science (IISc), Bangalore, India in 2003. He was a postdoctoral researcher at the Ecole Normale Superieure, Paris (France) and Universitaet Innsbruck, Innsbruck (Austria) from 2003 to 2005. During 2005-2009, he worked at General Electric Global Research Center in Bangalore and joined IISER Pune in September 2009.

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ATOMIC PHYSICS, QUANTUM OPTICS AND APPLIED QUANTUM OPTICS

My research interests are in the area of atomic physics and quantum optics. Special emphasis is on developing new platforms for entangling isolated particles, precision spectroscopy, quantum information processing, and high-sensitivity detection of environmental perturbations. These new platforms will be developed using a combination of a variety of techniques from ultra-cold and dense sample of neutral atoms, plasmonic arrays, ultra-high quality factor optical cavities and ions trapped in electro-dynamic traps.

Initial research direction is toward creating ultra-strong electromagnetic coupling between neutral atom pairs using localized plasmonic arrays. These experiments will utilize ultracold-dense samples of neutral alkali atoms prepared at temperatures and densities close to quantum degeneracy. High-sensitivity perturbation detection will have immense technological applications in the monitoring biochemical processes and interactions in biological assays and imaging. Parallel efforts are focused on developing ion traps with novel architectures for next-generation quantum computers. These trapped ion systems will also be used for precision measurements of forbidden atomic transitions which have significant technological applications including atomic clocks and variation of fundamental physical constants.

SELECTED PUBLICATIONS


M S Santhanam received PhD in 1999 from Physical Research Laboratory/Gujarat University, Ahmedabad, India. He was with IBM Research Division for 3 years and later took up a Guest Scientist position at Max Planck Institute for the Physics of Complex Systems, Dresden, Germany. Since 2005 he was a Reader at Physical Research Laboratory, India before joining IISER Pune in 2008.

**COMPLEXITY: CHAOS AND ITS QUANTUM MANIFESTATIONS, EXTREME EVENTS AND THEIR STATISTICS**

Many nonlinear systems display chaos in the classical sense, which imply sensitivity to initial conditions. This is manifested in the spectral statistics of the quantum counterparts and is a signature of chaos in quantum mechanics. One of my research interests is to study directed motion in quantum chaotic systems. Typically, directed motion implies breaking of relevant spatio-temporal symmetries and non-zero mean velocity even with vanishing net forces. The broad idea is to be able to control the direction and magnitude of directed currents in few body chaotic systems including those of nano dimensions.

Many natural and socio-economic processes, for example, earth quakes, temperature records, stock market dynamics display long memory such that the correlations do not decay in finite time. My current research focuses on various questions associated with the extreme value statistics of such long memory processes such as the distribution of recurrences of extreme events.

**SELECTED PUBLICATIONS**


**MAGNETISM AND SUPERCONDUCTIVITY**

My research interests revolve around understanding the bulk properties of solids at low temperatures and often under the influence of external stimuli, such as, electric and magnetic fields and/or pressure. Currently, I am interested in geometrical frustration where unusual ground states arise due to the competing nature of magnetic interactions; magnetic properties of low-dimensional quantum magnets (spin-chains and spin-ladders) and the anisotropic heat transport in these low-dimensional magnets. Very recently, I also got myself interested into iron-based superconductors which show rather unconventional magnetic and superconducting order parameters interplay. In my lab we investigate these materials in their pure and single-crystalline form. The single-crystals are grown using a four-mirror infrared image furnace and magnetic and transport properties are measured using a cryogen-free physical properties measurement system capable of simultaneous temperature and magnetic field variations.

**SELECTED PUBLICATIONS**


Prasad Subramanian received his PhD from George Mason University, USA in 1997. Following this, he held postdoctoral positions at the Solar Physics branch of the Naval Research Laboratory, Washington, DC, USA and the Inter-University Centre for Astronomy and Astrophysics, Pune before joining the faculty of the Indian Institute of Astrophysics, Bangalore, India in 2006. He has been on the faculty of IISER Pune since 2008.

PLASMA ASTROPHYSICS – SOLAR CORONAL PHYSICS, BLACK HOLE ACCRETION

My research interests range from solar physics to black hole accretion, within the overall framework of plasma astrophysics. They span black hole accretion disks, jets from Active Galactic Nuclei and microquasars, radio emission from the Solar corona, Solar Coronal Mass Ejections (CMEs) and their terrestrial effects. I use a combination of semi-analytical theory and analysis of data from ground and space-based instruments.

With regard to Solar Physics, I am interested in the dynamics and basic energetics of solar CMEs and in the manner in which their effects are manifested in the near-Earth space environment. The physics of radio emission from the solar corona and the scattering of radio waves due to turbulence in the solar corona also interest me.

In relation to black hole accretion disks, I am interested in the microphysical viscosity mechanisms which enable accretion. I am also interested in the physical mechanisms that result in flares of TeV emission from jets that emanate from such accretion disks.

SELECTED PUBLICATIONS


Suneeta Vardarajan received a BSc (Hons) degree in Physics from St Stephen’s College, Delhi and an MSc in Physics from Indian Institute of Technology (IIT) Madras and did her PhD from the Institute of Mathematical Sciences, Chennai, India. Her subsequent past positions have been as a Humboldt Fellow at the University of Munich (Germany), a fellow of the Pacific Institute of Mathematical Sciences at the University of Alberta, a research fellow at the University of New Brunswick, and Assistant Professor at University of Alberta (Canada) before joining IISER Pune in July 2010.

MATHEMATICAL PHYSICS, GRAVITATION AND RELATIVITY

My research interests lie at the interface of physics and mathematics. I am mainly interested in questions that arise in theoretical physics (particularly relativity and black holes) and their connections to geometry. Mathematical physics is an area that has seen many dynamic developments recently (particularly, insights from physics which have led to new mathematics), and I like to constantly expand my boundaries and explore emerging interface areas. Some of my work in the last few years has been on Ricci flow, which is a partial differential equation describing a flow of geometries, and was used to prove the Poincare conjecture in mathematics. This flow equation appears in physics as a renormalization group flow (which arises when a physical system is viewed at different scales) for a class of quantum field theories. In a special case, this flow also describes the flow of a fluid through a porous medium. These connections lead to insights both in the relevant physical models and in the geometry of Ricci flow.

Some of the themes I am currently working on include the classical and quantum stability of black holes and stability of special solutions to the porous medium flow. Another area of interest is in models of three-dimensional quantum gravity – which attempt to unify gravity and quantum mechanics in three space-time dimensions, and provide valuable lessons for quantizing gravity in four dimensions.

SELECTED PUBLICATIONS


Here \( \Pi \) is a cuspidal automorphic representation with a Shalika model, i.e., \( \Pi \) is transfroded from...
Baskar Balasubramanyam completed his PhD from Brandeis University, USA in 2007. In 2007-08, he was a postdoctoral fellow at the Center for Advanced Study in Mathematics at the Ben-Gurion University of the Negev in Israel. Following this, he was a Bateman Instructor at California Institute of Technology, USA during 2008-10. He has been with IISER Pune since September 2010.

MODULAR FORMS AND GALOIS REPRESENTATIONS

My research interests are in Number Theory. A modular form is essentially a function defined on the complex upper half-plane (everything above the real axis) that behaves in a good way under transformations of certain 2x2 matrices with integer entries. The expansion at infinity of such a function gives us a power series whose coefficients have interesting arithmetic properties. An important example of numbers that arise in such a way is the Ramanujan Tau function \( \tau(n) \). In order to understand these coefficients, it is useful to consider an object attached to it called the L-function (these are generalizations of the Riemann zeta function).

A Galois group is a set of permutations of roots of an irreducible polynomial. For example, complex conjugation permutes the roots of \( x^2 + 1 \). It is possible to represent such permutations by matrices. One of the problems in Number Theory is to try and understand the Galois group by studying its representations. One can also attach L-functions to Galois representations and in some cases modular forms and Galois representations are related through their L-functions.

SELECTED PUBLICATIONS


Rabeya Basu received her PhD from Tata Institute of Fundamental Research (TIFR), Mumbai, India in 2007. She then undertook postdoctoral work initially at Harish Chandra Research Institute, Allahabad and later as an NBHM Fellow at the Indian Statistical Institute, Kolkata, India. She was in IISER Kolkata as an assistant professor before joining IISER Pune in 2010.

UNITARY WHITEHEAD GROUP

From the late 1950s to the early 1970s several attempts were made to generalize classical groups by constructing a theory which does not depend on the invertibility of 2. In 1966-67, Antony Bak resolved this problem by introducing form rings and form parameter. I am working on recent development of Bak’s general quadratic (unitary) groups.

SELECTED PUBLICATIONS


Chandrasheel Bhagwat obtained Bachelor of Science in Mathematics from Fergusson College, Pune in 2003 followed by Master of Mathematics at Indian Statistical Institute, Bangalore in 2005. He completed PhD in Mathematics from Tata Institute of Fundamental Research (TIFR) Mumbai, India in 2011 and spent a few months as a post-doctoral fellow at IISER Pune. He has received the DST-INSPIRE faculty award and research grant in 2011 and has joined IISER Pune in March 2012.

**NUMBER THEORY, REPRESENTATION THEORY AND SPECTRAL THEORY OF SYMMETRIC SPACES**

The interplay between arithmetic, spectral theory and geometry was studied by mathematicians like Selberg, Maass, and Sunada among many others. From the last few years, I have been working on the study of arithmetic aspects of the spectral theory and geometry of symmetric spaces. My thesis work involved proving various analogues of the classical number theoretic results in the context of symmetric spaces. I am also interested in the study of analytic properties of the Zeta functions associated to a rank one locally symmetric space, which encode a lot of spectral and geometric data. They can be considered as the spectral counterparts of the Dedekind zeta functions associated to number fields. I would like to look at some of the ‘inverse problems’ on locally symmetric spaces with the aid of the Zeta functions mentioned above.

In a joint work with Prof C S Rajan and Dr Supriya Pisolkar, we have established some results which relate the notions of weak commensurability (introduced by Prasad and Rapinchuk) and representation equivalence of arithmetic lattices in Lie groups. These notions are in turn related to the geometry and spectral theory of the locally symmetric spaces defined by them.

My recent work with Prof Raghuram establishes period relations for the tensor product of motives which, together with the celebrated Deligne’s conjecture, predict the results of a similar nature about the special values of Rankin-Selberg L-functions and Dirichlet L-series. In future, I would like to work on some the problems associated with special values of L-functions.

**SELECTED PUBLICATIONS**

Bhagwat C. and Raghuram A. Ratios of periods for tensor product motives (Submitted).


Diganta Borah received his PhD from the Indian Institute of Science (IISc), Bangalore, India in 2010 and was a Research Associate there until 2011. He joined IISER Pune in January 2012.

**SEVERAL COMPLEX VARIABLES**

Much of my current work focuses on the study of the intrinsic properties of a Kähler metric, the so called Robin metric, on smoothly bounded pseudoconvex domains in $C^n$, $n>1$. This metric was constructed by N. Levenberg and H. Yamaguchi using the Robin function that arises from the Green function associated to the standard sum-of-squares Laplacian in $C^n$.

**SELECTED PUBLICATIONS**


Anisa Chorwadwala received her PhD from the University of Mumbai in 2007. Following this, she held postdoctoral positions at the Institute of Mathematical Sciences (IMSc), Chennai; The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy; and the Tata Institute of Fundamental Research (TIFR), Mumbai. She has been on the faculty of IISER Pune since April 2011.

**SHAPE OPTIMIZATION PROBLEMS**

My research work falls mainly in the following two branches of Mathematics: Partial differential equations and Riemannian geometry. I work on shape optimization problems including isoperimetric problems. A typical shape optimization problem is to find a shape which is optimal in the sense that it minimizes a certain cost functional while satisfying given constraints. In many cases, the functional being minimized depends on the solution of a given partial differential equation defined on the variable domain.

We have solved some shape optimization problems for a class of doubly connected domains over Rank-one symmetric spaces of non-compact type. Here the functionals to be optimized were the energy functional and the principal frequency associated with the Dirichlet boundary value problem and the Dirichlet Eigenvalue problem respectively, for both linear as well non-linear operators, namely the Laplacian and the p-Laplacian.

**SELECTED PUBLICATIONS**

- Anisa M. H. C. and Mahadevan, R. A shape optimization problem for the $p$-Laplacian (Submitted).
MATHEMATICAL STATISTICS

My current research is on (i) bounds for the reliability and expected life of coherent systems whose components have lifetimes belonging to certain well established aging classes of probability distributions such as the IFRA class and the NBUFRA class, (ii) modeling the probability distributions of parallel and k-out-of-n systems where the distributions are modified due to load sharing at the epoch of every component failure and (iii) nonparametric tests for testing the constancy or the equality and proportionality of fatality rates of emerging epidemics at one or more locations.

SELECTED PUBLICATIONS


Pranay Goel received his PhD in Physics at the University of Pittsburgh, USA. His postdoctoral work was carried out at the Mathematical Biosciences Institute, The Ohio State University, and at the Laboratory of Biological Modeling, NIDDK, National Institutes of Health, USA. He joined the Mathematics and Biology faculty at IISER Pune in 2009.

**DYNAMICAL SYSTEMS MODELING OF MULTISCALE PHENOMENA IN BIOLOGY**

Dynamical processes in biology naturally span several systems and multiple scales, both in space and in time. We are interested in studying the dynamical behavior of biological processes through mathematical modeling to complement experimental understanding. My research focuses primarily on theoretical neuroscience, cardiac dynamics and diabetes. Each of these areas is rich with issues that arise from a fundamental need to develop theoretical frameworks, and to handle multiscale dynamics within those.

Our understanding of glucose-stimulated insulin secretion from the pancreatic endocrine tissue, the islets of Langerhans, has developed considerably over the last three decades. Much of my recent work has been related to analyzing some newly proposed models of islet voltage oscillations (called “bursting”) that implicate both ionic as well as metabolic activity as being jointly responsible for function. Simultaneously, we are also interested in modeling and analysis of data collected from patients diagnosed with Type 2 diabetes. This is joint work with researchers at the University of Pune and K. E. M. Hospital, Pune.

Although we are a dry lab, since such research is highly interdisciplinary in nature, we collaborate extensively with experimentalists.

**SELECTED PUBLICATIONS**


Anindya Goswami received his PhD from Indian Institute of Science (IISc), Bangalore, India in 2008. Following this, he held postdoctoral positions at the Universiteit Twente in Enschede, The Netherlands; INRIA in Rennes, France; and Technion in Haifa, Israel before joining IISER Pune in 2011.

**STOCHASTIC CONTROL – GAME THEORY, MATH FINANCE, QUEUING NETWORKS, RENEWAL PROCESSES**

I am exploring various topics in Applied Probability. Those include generalization of Black-Sholes-Merton PDE for options in semi-Markov modulated market, Föllmer Schweizer decomposition of an unattainable contingent claim, equilibrium of non-cooperative semi-Markov game under ergodic cost, optimal control under risk sensitive cost, portfolio optimization, large deviation limit, fluid limit in queuing network, PDE techniques in stochastic control and differential games etc.

I use Markov models, filtering techniques, stochastic calculus, infinitesimal generator for semigroup of operators, mild solution technique for parabolic equations, viscosity solution method for HJB/HJI equations, stability analysis of numerical schemes for solving PDE or IE., convergence of value iteration schemes, marginalization technique in rare event simulation for hybrid processes, martingale formulation for Markov processes etc.

**SELECTED PUBLICATIONS**

Atar, R., Goswami, A. and Shwartz, A. Risk-sensitive control for the parallel server model (Submitted).


Ayan Mahalanobis obtained his PhD from Florida Atlantic University, Boca Raton, USA in 2005. He was then a Visiting Assistant Professor at the Stevens Institute of Technology, New Jersey, USA for a few years before joining IISER Pune in 2009.

**PUBLIC KEY CRYPTOGRAPHY**

I work at the intersection of pure mathematics (group theory) and public key cryptography. Cryptography, especially public key cryptography, is the backbone of a modern society. It serves us with the required tools for online transactions and trading, i.e., online commerce.

My research aims to find new cryptographic primitives and to build secure protocols from that. We look for groups in which the discrete logarithm problem is secure. My recent work has shown that the group of non-singular circulant matrices over a finite field has some properties that make them attractive over the discrete logarithm problem on a finite field. This new finding has opened a new avenue in research of public key cryptography.

**SELECTED PUBLICATIONS**

Shah, J. and Mahalanobis, A. A new guess-and-determine attack on the A5/1 stream cipher (Submitted).

Mahalanobis, A. The ElGamal cryptosystem over circulant matrices (Submitted).

Mahalanobis, A. The MOR cryptosystem and extra-special p-groups (Submitted).

Mahalanobis, A. The automorphism group of the group of unitriangular matrices over a field (Submitted).


**SOUMEN MAITY**  
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Soumen Maity received a PhD from the Theoretical Statistics & Mathematics Unit at Indian Statistical Institute, Kolkata, India in 2002. He has postdoctoral experience from Lund University Sweden; Indian Institute of Management (IIM) Kolkata, India; and University of Ottawa, Canada. Prior to joining IISER Pune in 2009, he served as an assistant professor at Indian Institute of Technology (IIT) Guwahati and Indian Institute of Technology (IIT) Kharagpur, India.

**COMBINATORICS  COVERING ARRAYS, CRYPTOGRAPHY, AND EXTREMAL SET THEORY**

I am mostly interested in combinatorial problems. More specifically, I have been working on covering arrays on hypergraphs, construction of cryptographically important Boolean functions, and extremal set theory.

**Covering Arrays on Hypergraphs**: Covering arrays are combinatorial structures which extend the notion of orthogonal arrays and have applications in the realm of software and circuit testing. A covering array of strength three is an array with the property that any three rows are qualitatively independent. A covering array is optimal if it has the minimum number of columns among covering arrays with the same number of rows. We work on upper and lower bounds on the size of covering arrays on hypergraphs based on hypergraph homomorphism.

**Cryptography**: Boolean functions are used as nonlinear combining functions in LFSR based stream ciphers. A Boolean function is said to be resilient if its output leaks no information about its input values. My research in this area presents some strategies to modify the bent functions, by toggling some of its outputs, in getting a large class of 1-resilient functions with very good nonlinearity and autocorrelation.

**Extremal Set Theory**: Given a finite set X, the general problem in extremal set theory asks how large or small a family of subsets of X can be if it satisfies certain restrictions. Two core concepts in extremal set theory are intersecting families and shadows. The main results for intersecting families are the Erdos-Ko-Rado and Hilton-Milner theorems, and the principal result for shadows is the Kruskal-Katona theorem. By defining suitable notions of “intersecting” and “shadow” we intend to find remarkable analogs of these theorems for other structures such as multisets, permutations, set partitions, etc.

**SELECTED PUBLICATIONS**


ALGEBRAIC GEOMETRY

My research can be divided into three categories: intersection theory, derived categories, and T-varieties.

Intersection Theory
In intersection theory, one defines invariants of algebraically defined geometric spaces in terms of how the spaces lying on the given space intersect each other. One can study those invariants to determine deep geometric properties of the space.

Derived Category
Given a variety (a type of algebraically defined geometric space), one can define another algebraic object called derived category. It is known that a lot of the geometric properties of the space translate to algebraic properties of the derived category.

T-Variety
While studying an object one many times first determine its group of symmetries. The same holds for varieties. When the group of symmetries contain a torus, one can, with some additional hypothesis describe a variety purely in terms of some combinatorial data. Currently I am working on such varieties.

SELECTED PUBLICATIONS


Rama Mishra has obtained her PhD from Indian Institute of Technology (IIT) Bombay, India in 1994. She spent a few years with Harish Chandra Research Institute, Allahabad and Indian Statistical Institute, Delhi as postdoctoral fellow and then served as a faculty at IIT Kharagpur and IIT Delhi for several years. She worked as a JSPS fellow at Osaka City University, Japan for one year and as a visiting faculty at Boise State University, USA before joining IISER Pune.

LOW DIMENSIONAL TOPOLOGY

For a reasonably long period of time my research focused around the Polynomial representation of long knots. It was motivated by the issue of settling a long lasting conjecture of Abhayankar. We established the equivalence between polynomial isotopic classes of long knots with the ambient isotopic classes of classical knots. Thus the entire knot theory can be done over polynomial knot category. I am trying to compute some numerical knot invariants such as unknotting number through polynomial knot theory.

Quantum topology is one of the emerging research areas. Many knot invariants naturally arise through nice matrix algebra representation of interesting quantum groups. They have been related to several models in statistical mechanics. I would like to explore some models that are related to Singular knot theory.

I am also interested in classical knot invariants and their application in mathematics and biological sciences. My joint work with Prof Louis Kauffman on A nodal parity invariants of knotted rigid vertex graphs, discusses the application of this invariant on protein folding classification.

SELECTED PUBLICATIONS

After getting a BTech in Computer Science and Engineering from Indian Institute of Technology (IIT) Kanpur, Raghuram moved to Mathematics and got a PhD in Mathematics in 2001 from the Tata Institute of Fundamental Research (TIFR), Mumbai, India. He held postdoctoral positions at University of Toronto, Canada and TIFR, Mumbai, India and visiting assistant professorships at Purdue University and University of Iowa, USA. He was at Oklahoma State University, USA as an associate professor before joining IISER Pune in 2011.

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NUMBER THEORY, REPRESENTATION THEORY AND AUTOMORPHIC FORMS

My research has been partially funded by the National Science Foundation, USA, and the Alexander von Humboldt Foundation, Germany. My group is currently studying the arithmetic properties of special values of automorphic L-functions.

The earliest prototype of a special value of an L-function is the classical formula by Euler which says that the sum $\sum 1/n^2$ of reciprocals of squares of all positive integers is $\pi^2/6$. More generally, suppose $M = \{a_n\}$ is a sequence of numbers coming from some interesting data, for example, $a_p$ can be the number of solutions of an equation modulo a prime $p$, then a guiding principle in modern number theory says that to study the sequence $M$ one should study the L-function $L(s, M) = \sum a_n/n^s$. One can glean much information about the sequence $M$ by studying first the analytic properties, and second the arithmetic properties of $L(s, M)$.

The Langlands program, considered by many as a grand unifying principle in modern mathematics, bridges different areas of mathematics, like geometry (elliptic curves), number theory (Galois representations) and representation theory (automorphic forms). The central theme making these bridges possible is the notion of an L-function.

Our work uses the results and techniques of the Langlands program to prove theorems about special values of various L-functions. These values encode within them a lot of arithmetic and geometric information of the objects to which the L-functions are attached. In earlier work stemming from my thesis, we have also studied the representation theory and harmonic analysis of p-adic groups.

SELECTED PUBLICATIONS


CONJUGACY QUESTIONS AND REPRESENTATION THEORY OF GROUPS

Conjugacy questions in group theory have been of interest for its connection with the representation theory and they have not been understood very well for Algebraic Groups over arbitrary field. Usually groups are difficult objects and one studies them via their representations to get better understanding.

Let $G$ (e.g. $GL_n$) be an algebraic group defined over a field $k$. We denote the $k$ points of $G$ by $G(k)$ (e.g. $GL_n(k), SL_n(k)$ etc.). An element $t$ of $G(k)$ is said to be real if it is conjugate to its own inverse in $G(k)$. I have been concerned with finding real elements in algebraic groups. Very interestingly often it relates to finding strongly real elements (the elements which are product of two involutions in $G(k)$).

Apart from studying structure of real elements in Algebraic Groups over $k$, I also looked at many examples such as linear groups, orthogonal groups, symplectic groups and the groups of type $G_2$ to get better understanding of the problem. Finding real elements helps in the understanding of real characters of the group which in turn give information about those complex representations of the group which are either orthogonal or symplectic.

SELECTED PUBLICATIONS


Kaneenika Sinha completed her PhD from Queen’s University, Canada in 2006. She has held postdoctoral fellowships at University of Toronto, University of Alberta and Mathematical Sciences Research Institute, Berkeley. She was an assistant professor in IISER Kolkata before joining IISER Pune in December 2012.

**KANEENIKA SINHA**  
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**ANALYTIC NUMBER THEORY, HARMONIC ANALYSIS AND ARITHMETIC GEOMETRY**

My primary research work is concerned with extremal functions in Fourier analysis, equidistribution of Fourier coefficients of modular cusp forms, Eichler-Selberg trace formula and arithmetic of modular curves. Modular forms play an extremely important role in number theory and their Fourier coefficients carry fundamental information about points of elliptic curves over finite fields, values of the partition function, class numbers and representations of integers by quadratic forms. They are essential tools in addressing many fundamental problems in Mathematics, like Fermat’s Last Theorem. Modular forms are a special case of automorphic representations and lead to the Langlands program, a theme that drives much of the twenty first century research in number theory and representation theory. My research program focuses on the behavior of the Fourier coefficients of normalized Hecke eigenforms and their connections with Jacobian varieties of modular curves.

My research program in number theory heavily draws ideas and techniques from various mathematical areas, like harmonic analysis and arithmetic geometry. The problems pursued by me are posed in the language of algebra and geometry, where as the techniques used in resolving them come from harmonic analysis. Moreover, a comprehensive understanding of these questions necessitates approaching them from a representation-theoretic point of view.

**SELECTED PUBLICATIONS**


Steven Spallone received his PhD from the University of Chicago, USA in 2004. Afterwards he did postdoctoral work at the Max-Planck Institute in Bonn, at Purdue University, and at the University of Oklahoma, USA. He also visited the Tata Institute of Fundamental Research (TIFR) Mumbai, India. He joined the faculty of IISER Pune in July 2012.

**REPRESENTATION THEORY AND CANONICAL FORMS**

A basic theme in representation theory for a topological group is the duality between the geometry of the group and its spectral theory. In one project, I study arithmetically interesting representations called “discrete series” using this duality. I attempt to write their multiplicities in terms of measures over conjugacy classes of p-adic groups.

In another project, I study representations of isometry groups of quadratic forms, notably those induced from a stabilizer P of a nondegenerate subspace. I show that relationships between such representations are illuminated by first decomposing P into two subgroups M and N, and then by finding canonical forms for the conjugation action of M on N.

To introduce another project, consider square matrices, with entries modulo a cubefree integer. I study the question of when two such matrices are conjugate. I have also written some papers regarding when two germs of dynamical systems fixing a point are conjugate, in the p-adic setting.

**SELECTED PUBLICATIONS**


Perspective view of a new structurally flexible metal organic framework
(Image: Sujit Ghosh’s Group)
STRUCTURAL FEATURES AND RING CURRENT EFFECTS IN \( \pi \) CONJUGATED MACROCYCLES

Ever since the discovery of benzene, understanding ring current effects has been a challenge due to several factors. A main impediment is to generalize the correlation between topology and the strength of \( \pi \) electron delocalization with respect to length of the cyclic system.

An important aspect of our research is to design and synthesize conjugated macrocycles to study the effect of structure on delocalization of \( \pi \) electrons. We have chosen isophlorin, an unstable anti-aromatic structure postulated by Woodward, as a model to synthesize 10\( \pi \) isophlorinoids. Macrocycles varying from 20\( \pi \) to 40\( \pi \) electrons were found to be stable and characterized to understand the effect of electron delocalization. It has been observed that 4n\( \pi \) systems with strong electron withdrawing substituents resist oxidation to form (4n+2)\( \pi \) systems. Since all these molecules have a near planar geometry, as characterized in solution and solid states, they exhibit ring current effects. Also, they show strong C-H...F inter-molecular hydrogen bonding, in solid state, leading to impressive supramolecular structures. The 40\( \pi \) octa furan macrocycle is the largest anti-aromatic molecule to be characterized in solid state.

SELECTED PUBLICATIONS


Nirmalya Ballav obtained his PhD from the University of Calcutta in 2005. Before joining IISER Pune in April 2011, he was a research associate at the Applied Physical Chemistry Department of the University of Heidelberg, Germany from 2005 to 2008 and worked as a senior postdoctoral fellow at Laboratory for Micro- and Nanotechnology at Paul Scherrer Institute (ETH domain), Switzerland from 2008 to 2011.

**Nirmalya Ballav**  
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SURFACE MOLECULAR NANOSCIENCE AND MATERIALS CHEMISTRY

We like to play with molecules on the surface – specifically scoring with the help of self-assembly phenomena. Surface is a beautiful playground for chemists, physicists, biologists, material scientists and theoreticians. Our main research activities are in these areas: i) self-assembled monolayers (SAMs); ii) metal-organic coordination networks (MOCNs); and iii) molecule-substrate spin interfaces.

In order to understand characteristic molecular behavior on the surface, we employ spectro-microscopy-theory correlation approach by combining lab-based X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and density functional theory (DFT). Besides, we do Synchrotron research involving X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) spectroscopy. We use self-assembled monolayers as molecular templates for the fabrication of micro- and nanopatterns of biological relevance including chemical/morphological gradients by applying electron-beam lithography (EBL) technique. In view of designing functional materials originating from the hybridization of organic and inorganic components, we are also interested in core-shell conducting polymer nanocomposites (PNCs). Specifically, polyaniline (PANI), polythiophene (PTh) and polypyrrole (PPy) will be taken into consideration. As for the inorganic counterparts we use metallic and magnetic nanoparticles (MNPs), fullerenes (C60), carbon nanotubes (CNTs), nano-clay, and mixed valence oxides.

We are open to national and international collaborations.

**SELECTED PUBLICATIONS**


Sudipta Basu obtained his PhD in Chemical Biology in 2006 from Max-Planck Institute for Molecular Physiology in Dortmund, Germany. He worked as a postdoctoral fellow in Harvard Medical School, USA prior to joining IISER Pune in January 2012.

TARGETING ONCOGENIC SIGNALING PATHWAYS BY CHEMICAL NANOBIO TECHNOLOGY TOWARD NEXT-GENERATION THERAPEUTICS

In multicellular organisms, biological signal transduction pathways regulate key functions such as survival, growth, differentiation and metabolism. These signaling pathways are almost invariably altered/hijacked in different diseases including inflammatory diseases, asthma, neurodegenerative diseases, obesity, diabetes and cancer. It is now increasingly clear that signals (extracellular or intracellular) propagate through a tangled network of interconnecting proteins and cascades rather than through independent linear route. As a result, a disease state is rarely a consequence of an abnormality in a single signaling pathway, but reflects various signaling processes that interact in a complex network. Hence the futuristic strategy in effective drug discovery is to perturb the 'disease-causing network' instead of 'disease-causing pathway'.

My laboratory focus is to address these challenges by merging 'chemical biology' and 'nanotechnology' to develop novel program in “chemical nanobiotechnology”, where the understanding of biology will inspire the design of novel chemical structures that are spatiotemporally displayed to a cell using integrated nanotechnology platforms. In “chemical nanobiotechnology”, the nano-platform itself will be the active agent(s), which will (a) perturb (inhibit or activate) multiple signaling pathways to understand and target signaling crosstalk and (b) control the spatio-temporal dynamics of signaling networks in diseased states which will lead to the next generation therapeutics.

SELECTED PUBLICATIONS


MEDICINAL CHEMISTRY: KINASE AND mTOR INHIBITORS; TOTAL SYNTHESIS OF NATURAL PRODUCTS & SYNTHETIC METHODOLOGY

There is an ever-increasing body of data implicating PI3K signaling pathways in tumor growth, angiogenesis, metastasis and resistance to apoptosis. Phosphatidylinositol-3 kinases (PI3 kinases) are important in controlling various aspects of the malignant phenotype, including proliferation, survival/apoptosis, adhesion/mobility, angiogenesis and also cell size.

However, deregulation of kinase function has been implicated in other disorders, including immunological, neurological, metabolic and infectious disease. This has generated considerable interest in the development of small molecule kinase inhibitors for the treatment of these disorders.

Currently, our research is focused on the synthesis of small molecule inhibitors based on rational drug design approach and in-silico molecular modeling for more potent inhibitors to target PI-3 kinase gamma and mTOR. Our group is also working on the total synthesis of bioactive natural products and developing newer synthetic methodologies.

SELECTED PUBLICATIONS


Boomi Shankar obtained his PhD from Indian Institute of Technology (IIT) Kanpur, India in 2004. He did his postdoctoral research from University of Illinois at Urbana-Champaign, USA and University of Liverpool, UK (2004–2007). He was previously employed as an Assistant Professor at IIT Guwahati (April 2008–November 2010) and has joined IISER Pune in December 2010.

**R BOOMI SHANKAR**

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**MAIN GROUP AND ORGANOMETALLIC CHEMISTRY**

My lab focuses on the development of molecular systems derived from the elements of Groups 13, 14 and 15 and their applications in materials chemistry and catalysis. Some of the topics studied in my current research group include the following.

1. Use of cyclic and acyclic building blocks containing P-N, B-N, P-O and Si-O motifs for constructing molecules with novel cage, cluster and framework structures.

2. Developing dendrimer like inorganic scaffolds as supports for electro and photo active molecules for applications in opto-electronic devices.

3. Use of peripherally functionalized cyclic and cage like molecules as capping ligands for stabilizing metallo-supramolecular ensembles and nanomaterials and their utility in catalysis.

4. Applications of metal complexes derived from inorganic heterocyclic rings as catalysts for various organic transformations.

**SELECTED PUBLICATIONS**


Our group focuses on designing and synthesizing organic compounds for controlled generation of reactive species. These compounds have applications as tools for chemical biology but also have potential therapeutic applications. We have initiated a research project on selective and controlled delivery of gaseous reactive sulfur species, sulfur dioxide (SO₂). We have developed a new class of thiol-mediated prodrugs of sulfur dioxide with tunable rates of sulfur dioxide generation. Several of these compounds also have shown high potency in inhibiting growth of *Mycobacterium tuberculosis*, the causative agent of tuberculosis which affects millions each year.

We have also been working on development of new organic sources of reactive oxygen species (ROS) including superoxide anion and hydrogen peroxide, which are generated during immune response to combat pathogens. We have developed several new scaffolds with scope for tunable ROS generation and we found several new compounds that are good inhibitors of leukemia cell proliferation. Our group also works on new methodologies for site-directed delivery of nitric oxide (NO) prodrugs. Specifically, we are looking at new strategies to target hypoxic tumours, which are characterized by a bioreductive environment.

**SELECTED PUBLICATIONS**


Srabanti Chaudhury did her PhD at the Indian Institute of Science, Bangalore (2004-2008) and took up postdoctoral work at Rice University (2008-2009); University of Texas at Austin (2009-2010); and Los Alamos National Laboratory (USA), (2010-2012) in USA. She has joined IISER Pune in June 2013.

**THEORETICAL BIOPHYSICS**

Biological processes at the cellular level take place in heterogeneous environments and involve only a few molecules at a time. Such processes are intrinsically stochastic. My research will involve some of such biological processes and investigate how the randomness and stochasticity that is intrinsic to their dynamics can be characterized and treated mathematically. I am utilizing approaches based on principles of equilibrium and time dependent statistical mechanics, reaction rate theories, and molecular dynamic simulations. Such studies can provide us greater insight to the role of stochastic fluctuations and the effect of different biological parameters on the dynamic and kinetics of the systems.

**SELECTED PUBLICATIONS**


Jeetender Chugh received his doctorate in Physical Chemistry from Tata Institute of Fundamental Research (TIFR), Mumbai in 2008 for research on NMR investigations on large protein assemblies and method developments. Before joining IISER Pune in April 2013, Dr Chugh was a post-doctoral fellow and Lecturer at the University of Michigan where he discovered a new class of switches that are significantly smaller and orders of magnitudes faster than the other known class of RNA switches.

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STRUCTURE AND DYNAMICS OF NUCLEIC ACIDS AND INTERACTING PROTEINS BY NMR SPECTROSCOPY

Research in our lab is focussed on various aspects of solution NMR including theoretical design and experimental implementation of new NMR experiments to probe the biophysical characteristics of RNA and proteins; understanding functional aspects of non-coding RNAs; and structural biology of microRNAs and their regulation in various disease settings.

SELECTED PUBLICATIONS


Aloke Das obtained his PhD in Laser spectroscopy in supersonic jet in 2002 from Indian Institute of Technology (IIT) Kanpur, India. He was a postdoctoral fellow at Purdue University and jointly at Lawrence Berkeley National Laboratory and Louisiana State University in USA before joining IISER Pune in 2007.

**LASER SPECTROSCOPY OF BIOMOLECULES IN THE GAS PHASE**

Our group is focused on molecular level understanding of weak non-covalent interactions responsible for the stabilization of specific structures of biomolecules (protein, DNA etc.) as well as biological recognition processes like protein-protein, protein-DNA, protein-carbohydrate and protein-ligand interactions. We are also interested in understanding the mechanism of urea-induced protein denaturation in the microscopic level. We would like to study as well the role of amino acid sequence in protein folding or misfolding. Presently, we are involved in studying the structures of mixed dimers and trimers consisting of aza-aromatic molecules present in the backbones of aromatic amino acids.

We study structures of isolated molecules as well as molecular complexes in the gas phase using UV (Ultraviolet) and IR (Infrared) laser based spectroscopic techniques combined with quantum chemistry calculations. We perform the spectroscopy experiments using a home-built REMPI (Resonantly Enhanced Multiphoton Ionization) jet-cooled Laser-Desorption Time of Flight Mass spectrometer. In principle, we measure mass selected electronic and infrared spectra of molecular systems in isolated gas phase using UV and IR lasers.

**SELECTED PUBLICATIONS**


CheMical Biology of nuCLEIC acids and PePTides; DNA nanosCience

Research in our group for more than a decade is focused on rational design of a novel class of DNA mimics PNA analogues, incorporating chiral, non-chiral conformational constrains and cationic substituents in backbone to make them bind differentially to DNA/RNA, promote cell entry and be bioviable. These attributes would make them good candidates for the development of nucleic acid targeted therapeutic and diagnostic agents. Recently, we have shown that PNAs carrying methylene amino side chains on backbone exhibit regio- and stereo-specific effects on both DNA/RNA binding and on cell uptake properties of derived PNAs.

Another project involves synthesis of a series of 4-aminoproline containing collagen mimics that form highly stable triple helices that are stable to collagenase in order to develop scaffolds for tissue engineering. Aminoproline polypeptides have been shown to undergo switching from novel beta structure in hydrophobic solvent to PPII conformation in water. The alignment of cationic lysine capped nanoparticles on anionic DNA template in combination with electron source such as ferrocene would enable generation of conducting molecular wires and exploiting the DNA sequence dependent self-assembly of these systems may lead to design of molecular circuits.

Selected publications

COMPUTATIONAL MATERIAL SCIENCE

Research in our group involves exploring novel physics and chemistry of materials at the nanoscale using theoretical tools. In particular, we are interested in how properties (e.g. structural, electronic, vibrational, magnetic and chemical) change upon reducing size or lowering dimensionality (particularly in the nano-scale) and how changes in these properties affect the phenomena associated with these low dimensional (e.g. nanowires, nanotubes, surfaces and clusters) materials. To address such issues we perform first principles calculations using quantum mechanical density functional theory (for ground state properties), density functional perturbation theory (for vibrational properties) and time dependent density functional theory (for excited state properties).

Using the above methods, we try to achieve the following goals: (a) understand aspects of chemical bonding and microscopic couplings that are essential to the specific properties of materials, (b) obtain information about the atomistic structure and electronic states which are often hard and sometimes inaccessible to experiments and (c) design new materials and/or modify existing materials to yield materials with desired properties. We are primarily interested in materials with applications in heterogeneous catalysis, photovoltaic cells, and hydrogen storage.

Although we mainly use theoretical tools, we collaborate strongly with experimental groups.

SELECTED PUBLICATIONS


Sujit Ghosh obtained his PhD from Indian Institute of Technology (IIT) Kanpur, India in 2006. He then spent three years at Kyoto University, Japan as a JSPS and CREST postdoctoral fellow before joining IISER Pune in 2009.

**FUNCTIONAL SUPRAMOLECULAR CHEMISTRY**

My work focuses on design, synthesis, structural characterization and functional studies of self-assembled supramolecular materials based on organic-inorganic hybrid compounds and also small organic molecules based self-assembled structures for crystal engineering, molecular recognition etc.

Organic-inorganic hybrid materials also known as porous coordination polymers (PCP) or metal-organic frameworks (MOF) that are self-assembled by coordination of suitable metal ions/clusters with predesigned organic building blocks are of great interest for their potential applications in gas storage, separations, sensors, and catalysis. We seek to correlate structural features with physical properties and to design synthetic methods to prepare functional materials and to tune their structures and properties.

**SELECTED PUBLICATIONS**


HYBRID PEPTIDE FOLDAMERS: SYNTHESIS, STRUCTURE AND APPLICATIONS

Research in my group focuses on the design and synthesis of non-natural peptides and miniproteins composed of \(\omega\)-amino acids and their applications in pharmaceuticals and material science. Shown here are a few \(\omega\)-amino acids that we use in our research.

In the past few years, \(\omega\)-peptides composed of non-natural amino acids emerged as very promising tools in medicinal chemistry. Higher homologues of \(\omega\)-peptides form unique, stable secondary structures such as helices, sheets and turns. Our research will focus on understanding the behavior of supersecondary structures composed of \(\omega\)-peptides. These non-natural structural motifs may present new systems for testing the rules of protein folding and structural stabilization, while also providing an excellent opportunity for the design of biomimetic structures with practical applications in the areas of pharmaceuticals and material science. We are currently developing hybrid peptide foldamers to inhibit the HIV-1 fusion process.

We use 2D-NMR, X-ray and CD to analyze the structures of designed peptides and ITC (Isothermal Titration Calorimetry) to study the protein-protein and enzyme-substrate interactions.

SELECTED PUBLICATIONS


THEORETICAL STUDIES OF ULTRAFAST PHOTOINDUCED MOLECULAR PROCESSES

Photoinduced or light initiated processes constitute a large class of phenomena in nature. Several of these phenomena occur at the ultrafast or femtosecond timescale and play important roles in living organisms and in atmospheric phenomena. The detailed mechanistic understanding of such processes is of basic scientific interest and is also important for its technological implications in solar-based renewable energy devices, particularly the conversion of solar energy to chemical energy.

The general theme of our research is theoretical investigation of photoinduced molecular phenomena using quantum chemistry and nuclear dynamics methods. We have formulated a theory for modeling ultrafast dynamics in photoinduced proton-coupled electron transfer (PCET) reactions, which are common in energy conversion processes in living organisms and in devices like dye-sensitized solar cells. The studies provide insight into the interplay between the solvent dynamics and the electron-proton transfer for these types of processes. In addition, these studies illustrate how the coupling between the electron-proton transfer and the solvent dynamics can be tuned by altering the solute and solvent properties. The investigation of hydrogen/deuterium isotope effects suggests unusual trends for ultrafast photoinduced PCET as compared to regular PCET reactions.

SELECTED PUBLICATIONS


PHOTOPHYSICS AND BIOPHYSICS

My research interests span the following areas.

(a) Excited state photophysics of flavins: Flavins are heterocyclic molecules whose electronic properties allow them to serve as versatile electron donors and acceptors in a bewildering variety of biological roles. They are the chromophores of the biological flavoproteins and blue light absorbing photoreceptors. The function of the flavoproteins and these blue light photoreceptor proteins critically depends on the cofactor (Flavin adenine dinucleotide (FAD) or flavin mononucleotide (FMN) or riboflavin (vitamin B2)) present within it. Thus, exploring excited state photophysics of the FAD, FMN and riboflavin may give new insight into the photochemistry and function of flavoproteins and photoreceptors proteins.

(b) Charge transfer, electron transfer, proton transfer, energy transfer and isomerization reactions in microheterogeneous and biologically relevant systems, in ionic liquids, and in supramolecular environment using different spectroscopic techniques.

(c) Solvation dynamics near the active site of bio-molecules using fluorescence as a tool.

(d) Protein-drug, DNA-drug, RNA-drug interactions study using various spectroscopic techniques.

SELECTED PUBLICATIONS


CHEMICAL GLY COSYLATION

Glycosylation is a process in which a glycosyl donor and a glycosyl acceptor react to form an O-glycosidic bond at the anomeric position. My group has discovered propargyl and methyl glycosides to behave as glycosyl donors in the presence of gold(III) catalysts. Further studies on these glycosyl donors enabled to show that they are orthogonal to other known glycosyl donors and facilitate synthesis of several interesting glycoconjugates that could be utilized to probe either biological pathways or to make glycomaterials. Recently, glycopolymers and glycopolypeptides were synthesized by exploiting salient features of gold catalyzed glycosylations and free radical or ring opening polymerizations. The current interest in the group is to identify a more efficient strategy for synthesizing oligosaccharides and glycoconjugates in a rapid manner.

Another area of interest in my group is to exploit sugar-based scaffolds for diversity oriented synthesis of small molecules. In this direction, many contemporary reactions were performed on sugar scaffolds to obtain natural product-like, oxygen-rich, chiral and multi-cyclic frameworks. 'Click' chemistry has been exploited for synthesizing a library of small molecules and a novel ligation procedure was developed in our group for the synthesis of pseudo-oligosaccharides and amino acid glycoconjugates in an effective manner. In collaboration, we design, synthesize and show the function of the ligand by capping with nanoparticles and/or mesoporous materials.

SELECTED PUBLICATIONS


SYNTHETIC POLYMER CHEMISTRY AND NANOMATERIALS

Recent developments in polymer science provide wide opportunities in designing new polymeric structures for applications in molecular electronics and biological systems. Our research group primarily focuses on developing new synthetic polymers and self-assembled organic nano-materials to understand the fundamental aspects of macromolecular system and to explore their applications in chemical and biological sensors, targeted drug delivery of medicines, and opto-electronics such as photovoltaics and light emitting diodes. Self-assembled molecular template approach for conducting polymer nano-materials, development of new bulky supramolecular π-conjugated materials for electronic devices, melt transurethane reaction-a new green chemical approach for hazardous polyurethanes and PEG-based triblock copolymers for drug-delivery are some of the research projects which are currently engaged in the research group.

SELECTED PUBLICATIONS


M Jeganmohan obtained his PhD from the National Tsing Hua University, Hsinchu, Taiwan in 2005. He was a postdoctoral fellow at National Tsing Hua University, Taiwan and later at Ludwig-Maximilians-Universitat, Munich, Germany before joining IISER Pune.

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**ORGANOMETALLIC CHEMISTRY, ASYMMETRIC SYNTHESIS AND NATURAL PRODUCT SYNTHESIS**

The development of highly efficient, easily accessible and environmentally friendly methods to construct carbon-carbon and carbon-hetero bonds is always an ultimate goal in organic synthesis. Metal catalyzed or metal mediated reactions have been well-recognized as a powerful synthetic tool in organic synthesis.

Our research is mainly focused on developing new synthetic methodologies by using transition metal complexes and main group metal reagents. We investigate metal catalyzed or metal mediated coupling, cyclization, addition and C-H bond activation reactions, particularly by using less expensive and non-toxic metals such as Fe, Mn, Co, Ni, Cu, Ru and Pd. By employing metal complexes and chiral ligands, the investigation of chiral reactions will be in consideration. In the mean time, total synthesis of natural products and biologically active molecules by using metal catalyzed C-H bond activation as a key step will be pursued.

**SELECTED PUBLICATIONS**


Jeet Kalia received his bachelors and masters education at Indian Institute of Technology (IIT) Kharagpur, India. He obtained his PhD in Biochemistry in 2008 from the University of Wisconsin–Madison, where he worked in the laboratory of Prof Ronald Raines. He then moved to the laboratory of Dr Kenton Swartz as a National Institute of Neurological Disorders and Stroke (NINDS) competitive postdoctoral fellow at the National Institutes of Health (NIH) where his research focused on ion channel biology. He has joined IISER Pune in June 2013.

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CHEMICAL BIOLOGY OF LIPIDS AND ION CHANNEL PROTEINS

Research in the Kalia laboratory is intrinsically interdisciplinary, and lies at the interface of chemistry and biology. We utilize diverse tools ranging from synthetic chemistry and molecular biology to electrophysiology and protein chemistry to address problems in ion channel biology, lipid biology, and bioconjugation.

A major thrust area of the group is the development of activity-based probes and small molecule modulators of ion channel proteins that could ultimately have therapeutic applications and serve as mechanistic probes. Ion channels are membrane proteins expressed in all cell types and are extremely important for life. Our group is developing small molecule modulators of TRP and voltage-activated channels. In addition to utilizing these compounds as candidates for drug development, we study the detailed mechanism of action of these compounds on their target ion channels by utilizing electrophysiological techniques, providing insights into the mechanism of opening and closing of these fascinating molecular machines.

Another major focus of the laboratory is developing chemical biology-based approaches to study lipids. There are thousands of lipids in cells, most with undefined function. One reason why lipids remain poorly understood as compared to proteins and nucleic acids is that powerful tools available to study them in cells are lacking. We aim to address this urgent unmet need by developing new technologies to label lipids in cells with synthetic, tailor-made chemical handles, thereby endowing them with desired properties. These approaches will be applied to elucidate facets of lipid and membrane biology, including understanding the role of lipids in ion channel function.

Our third major interest is in developing novel methods of bioconjugation—a term that refers to the chemical derivatization of biomolecules. Site-specific bioconjugation techniques facilitate a host of applications, including protein labeling with affinity tags and fluorophores, development of protein-based therapeutics, and protein immobilization. We are interested in developing synthetic organic compounds and ligation methods for site-specific protein bioconjugation.

SELECTED PUBLICATIONS

Shabana Khan obtained her PhD from IIT Delhi in 2008. After spending nine months in Bharat Petroleum Corporation Limited, India as a senior scientist, Dr Khan worked with Prof Herbert Roesky in University of Göttingen, Germany from 2009 to 2011 as a postdoctoral fellow supported by Deutscher Akademischer Austausch Dienst. She then worked with Dr Manuel Alcarazo at Max Planck Institut für Kohlenforchung as a postdoctoral fellow before joining IISER Pune in March 2013.

**SILICON BASED FRUSTRATED LEWIS PAIRS AND THEIR REACTIVITY TOWARD SMALL MOLECULES**

Frustrated Lewis pair (FLP) is a combination of a Lewis acid and a Lewis base where the simple adduct formation is precluded due to steric demand. In 2006 Stephan et al showed a phosphine-borane FLP combination could reversibly bind H₂ under near ambient conditions. Recent work has extended the list of H₂ activation by FLP systems to include borane complexes of carbenes, amines, and phosphines. Apart from these, there are some other exciting reactions shown by FLPs including the addition to small molecules such as CO₂, NO, alkenes, alkynes, dienes, diynes, azides, and P₄ and cleavage of several bonds such as C-H, B-H, C-O etc.

One of the major limitations of FLP chemistry is its huge dependence on classical P- or N-based Lewis bases in conjunction with polyfluorinated boranes/alanes. In order to expand the ranges of Lewis bases in FLP recently, N-heterocyclic carbenes (NHCs) have been employed in FLP framework in combination with boranes.

The discovery of N-heterocyclic silylenes and functionalized silylenes and their exploitation as σ-donor ligands to form adduct with boranes and metal carbonyls evidenced that they also have potential to resemble NHC. Therefore, it is highly desirable to explore silylenes in FLP which may lead to the discovery of a range of interesting new applications. Our target is to synthesize novel silicon based FLPs and utilize them to activate small molecules.

**SELECTED PUBLICATIONS**


CARBOHYDRATE MIMICS: FROM STRUCTURAL PROBES TO DIAGNOSTIC TOOLS

While carbohydrate-protein interactions are involved in a large number of biological processes, the structure-activity relationships of carbohydrates for specific interaction with proteins are still poorly understood. It has become evident that defined glycan patterns are responsible for binding to a particular protein and modulating its biological activity. However, monomeric binding affinities for carbohydrate–lectin interactions are typically in the milli- to micromolar range and are difficult to quantify in vivo.

Our research will mainly focus on developing a set of rules for understanding and predicting synthetic molecules that will mimic and modulate carbohydrate-protein interactions. By designing molecules that display extraordinarily high affinity to specific lectins, we will be able, not only to evaluate the crucial parameters for protein-receptor recognition, but also to turn off their function and probe their roles in cell biology. So far, two promising strategies emerged for improving the binding affinity: (1) multivalent presentation of carbohydrates (2) carbohydrate-carbohydrate recognition in a lanthanide dependent manner. Currently our group seeks to develop new tools to strengthen carbohydrate-protein interactions and to translate them into early diagnosis and therapeutic approaches.

SELECTED PUBLICATIONS


RADIATION CHEMICAL STUDIES OF ORGANIC AND BIOLOGICALLY IMPORTANT MOLECULES

Pulse radiolysis is a powerful technique for the generation of radicals of choice in known yields in dilute aqueous solutions (≤ 1 mM) and is ideal for studying kinetics and spectroscopy of short-lived intermediates. Further, the ease of using quantum chemical methods has provided complementary information to accurately predict the site of radical attack. Thus, pulse and steady state radiolysis in combination with theoretical calculations has become a powerful tool in the formulation of detailed mechanisms of free radical reactions.

Our group has been involved in radiation chemical studies of both organic and biologically important molecules using these techniques.

SELECTED PUBLICATIONS


Pankaj Mandal obtained his PhD from the Indian Institute of Science (IISc), Bangalore, India in 2005. He was a postdoctoral fellow at Kansas State University and Rowland Institute at Harvard, USA before joining IISER Pune.

**TERAHertz SPECTROSCOPY**

We are trying to explore the “Terahertz (THz) gap” in the electromagnetic spectrum, which became accessible only recently and opens new avenues of probing matter at ultrafast time scales and at the nanoscale. THz frequencies, typically 0.1 to 10 THz (3 to 330 cm⁻¹), span the range of low-energy excitations in electronic materials, low-frequency vibrational modes of condensed phase media, and vibrational and rotational transitions in molecules. Hence this is a key spectral range for probing fundamental physical interactions as well as practical applications with great technological promise for security and medical imaging. Specifically, we use time-resolved THz spectroscopy to study the carrier and spin dynamics in nanoparticles and hydrogen-bond dynamics in solvated biomolecules. THz spectroscopy is ‘the ideal’ technique to probe the above dynamical processes because the time scales related to them are in the picosecond (10⁻¹²) range which corresponds to THz frequency (10¹² Hz).

Currently, we are pursuing the following problems:

1. Probing multiple exciton generation (MEG) and carrier dynamics in semiconductor nanocrystals by time-resolved THz spectroscopy (TRTS)
2. THz induced spin dynamics and magnetization dynamics

**SELECTED PUBLICATIONS**


Arnab Mukherjee obtained his PhD from the Indian Institute of Science (IISc), Bangalore, India in 2005. He was a postdoctoral fellow at Ecole Normale Superieure, Paris, France and University of Colorado, Boulder, USA before joining IISER Pune.

COMPUTATIONAL CHEMISTRY & BIOPHYSICS

We apply computational methods to study free energy landscape and reaction mechanisms in biological systems using classical, and combined classical and quantum chemical (QM/MM) molecular dynamics (MD) simulations and various Monte Carlo methods. Presently we focus primarily on the mechanism of intercalation of anthracycline type of anti-cancer drugs into DNA and RNA. This intercalation process has enormous significance in terms of their clinical activity since these drugs after intercalating into a DNA stop its replication leading to the cell death.

We have recently shown (using a detailed free energy landscape of intercalation process) that the intercalation involves mainly two steps: first step involves binding in the minor groove of the DNA in a diffusion-limited process, and the second step is the activated intercalation into DNA. We are working in this interesting area to understand the general mechanism of this intercalation process and we pose the following questions: do all drugs follow the same mechanism? What is the effect of DNA sequence? Is there any dynamical role? What are the relevant thermodynamic properties of each of the ingredients involved in the intercalation process?

Apart from intercalation, we are interested in the following areas: (i) protein DNA interaction (e.g., topoisomerase-DNA interaction, DNA-ligase/DNA interaction) (ii) water dynamics around DNA and drug/DNA systems (iii) role of water entropy in binding processes (iv) protein folding and dynamics using all-atom and coarse-gained models and bio-informatics techniques.

SELECTED PUBLICATIONS


Angshuman Nag completed his PhD in Chemistry in 2009 from Indian Institute of Science (IISc), Bangalore. Subsequently, he was an IISc centenary postdoctoral fellow in Bangalore for a year, followed by his second term (2010-2012) as a postdoctoral fellow at University of Chicago, USA. He joined IISER Pune in October 2012.

**ANGSHUMAN NAG**

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**COLLOIDAL SEMICONDUCTOR NANOCRYSTALS: DOPING, LIGHTING AND OPTOELECTRONICS**

Overall idea of our research is to develop functional inorganic materials using solution processed nanocrystalline modules. Semiconductor nanocrystals, also known as Quantum Dots (QDs), provide unique size-dependent electronic and optical properties along with solution processibility, and thus, constitute ideal building blocks for realizing macroscopic functional materials. Specifically, the group is involved in the following activities.

**Colloidal Synthesis:** II-VI, III-V and III-VI semiconductors, heterostructures, and doped nanocrystals; also reduced graphene oxide.

**Surface Modification (All-Inorganic Nanocrystals):** Development of inorganic ligands for nanocrystal surface to enhance inter-nanocrystal electronic coupling, and decorating nanocrystal surface with transition metal ions for luminescence, magnetic, charge transport and catalytic properties.

**Solid State Reactions:** Few-layer inorganic graphene (BN and BCN), films of new material using solution processed nanocrystal precursors.

**Spectroscopy:** Excited state and steady state optical spectroscopy are used to elucidate photophysical phenomena, whereas X-ray Photoelectron Spectroscopy (XPS) and Extended X-Ray Absorption Fine Structure (EXAFS) are used for advanced characterization.

**Optoelectronic Applications:** Light emitting devices (LEDs), transparent conductors, and field effect transistors (FETs) are prepared using colloidal nanocrystals. Solution processed and flexible devices.

**SELECTED PUBLICATIONS**


SYNTHESIS OF SAFER ANTIFUNGAL COMPOUNDS

In view of the need to develop novel anti-fungal compounds to counter the resistance and the side effects associated with currently available drugs and to ensure environmental safety, it is increasingly becoming essential to develop not only new chemical classes of compounds but also to identify novel targets or novel biological pathways that can be disrupted resulting in effective control of fungal pathogens. This will lead to safer new anti-fungals.

In pursuit of this we have selected chitin synthase as our initial target because of its presence in all fungi, essentiality in the survival of fungi and most importantly, its absence in either humans or plants. To make it safer, libraries of several molecules based on carbohydrate scaffold incorporating nucleic acids and peptides have been prepared of ~sixty compounds.

In order to get these molecules several specific reactions such as Click reaction and Pausen khand reaction, IMDA reaction, Enyne metathesis reaction, Barbier reaction have been often used. A new method for the glycosidation of nucleoside has been developed and extensively used to introduce the bases into the scaffolds. Many of these compounds have shown encouraging activity using specifically developed haploin sufficiency assay. Appropriate chemical modifications are in progress.

SELECTED PUBLICATIONS


Mrinalini Puranik has recently moved to IISER Pune from the National Centre for Biological Sciences (NCBS) Bangalore, India. She did her doctoral work at the Indian Institute of Science (IISc), Bangalore followed by postdoctoral work at Princeton University, USA.

**DESIGN PRINCIPLES OF PROTEINS: STRUCTURE, FUNCTION AND DYNAMICS**

A majority of cellular processes do ultimately arise from protein-protein, protein-nucleic acid, and protein-lipid interactions. Deconstructed to a molecular level, these interactions are governed by rates of enzymatic catalysis and allosteric control of access to interaction sites. Therefore, a strategy underlying drug design is modulation of the function of proteins. Eco-friendly industrial processes rely on our ability to develop enzymes designed for specific chemical catalysis of small molecules. To attain these goals it is critical to understand the fundamental design principles of natural proteins. Natural enzymes can achieve turnover rates of $10^{14}$ while designed enzymes rarely achieve 1% of this rate. Clearly, we still do not have sufficient understanding to modulate desired properties with the required specificity for target proteins. Particularly less understood is the role of protein dynamics in governing function.

We are using innovative approaches that combine spectroscopic, biochemical and computational strategies to understand the design principles of proteins with high spatial and temporal resolution. Proteins being studied in the lab are: protein-nucleic acid complexes involved in purine metabolism, ATP homeostasis and DNA repair. These fascinating proteins have the ability to catalyze many types of substrates. We aim to understand how catalytic efficiency and protein plasticity coexist. We are also measuring the dynamics of proteins relevant to the chemical step of the catalysis.

**SELECTED PUBLICATIONS**


Vaidhyanathan Ramanathan gained his PhD in Chemistry from Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India, working with Prof C N R Rao and Prof S Natarajan. He then joined the group of Prof M J Rosseinsky at the University of Liverpool, where he investigated the magnetic properties of Co oxide-hydrides, and chiral metal–organic frameworks (MOFs). Before joining IISER Pune in 2012, he worked with Prof George Shimizu investigating the proton conduction and gas capture applications of MOFs.

My research interests include designing and developing porous solids for application in CO₂ capture and in capture and separation of other industrially valuable gases. Another major focus of the research work would be to engineer and optimize these gas capture and separation processes in larger scales that could serve as prototypes for industrial scale captures. Other areas of interest pertain to developing chiral solids for heterogeneous enantio-separation and catalysis.

Other research interests target at developing hierarchy of inorganic-organic solids capable of exhibiting properties ranging from insulating to semi conducting to conducting. They would be engineered for their potential application in fuel cells, solar cells and other areas of alternate energy.

**SELECTED PUBLICATIONS**


Srivatsan received his PhD in Bioorganic Chemistry from the Indian Institute of Technology (IIT) Kanpur, India in 2003. He was an Alexander von Humboldt fellow at University of Bonn (Germany) and a postdoctoral fellow at University of California, San Diego, USA. He joined IISER Pune in November 2008.

**CHEMICAL BIOLOGY: NUCLEIC ACID CHEMISTRY**

Our group is focused on developing tools for assessing biological events utilizing contemporary nucleic acid functions and synthetic biology by bringing together synthetic organic chemistry, biophysics and biochemistry. Also, our research is directed towards designing functionalized nucleic acids that would self assemble into nano-architecture and exhibit extraordinary metal assisted enzymatic activity as well as electrical/magnetic properties.

Site-Specific Labeling of Nucleic Acids: Several RNA motifs that regulate enzyme activity and interact with viral proteins as well as small molecules are being vigorously investigated as potential therapeutic targets. Consequently, numerous tools have been developed to advance the understanding of protein-RNA interaction and the discovery of potential inhibitors. Our research program is focused towards developing new protocols to site-specifically label nucleic acids with functions that can be employed in investigating nucleic acid structure, dynamics and recognition processes.

Functionalized DNA Directed Self-Assemblies: The scope of DNA as material composite could be greatly augmented if DNA molecules could be chemically tuned with additional functionalities apart from predictable Watson-Crick pairing. For example, nucleic acids can be chemically modified to possess additional hydrogen bonding acceptor and donor pairs, π-stacking interaction and coordination sites for metal ions. Such systems could possibly form 2D and 3D architectures and exhibit extraordinary metal assisted enzymatic activity as well as electrical/magnetic properties.

**SELECTED PUBLICATIONS**


Pinaki Talukdar obtained his PhD from the Department of Organic Chemistry, University of Geneva, Switzerland in 2005. Following this he did postdoctoral research at Department of Chemistry, University of Illinois at Urbana-Champaign, USA. He then worked as a Senior Research Scientist at AMRI Global, Hyderabad and Institute of Life Sciences, Hyderabad before joining IISER Pune in 2009.

**CHEMICAL BIOLOGY: FROM SMALL MOLECULES TO SUPRAMOLECULES**

Research in our group is focused in the broad area of chemical biology. We are interested to design organic small molecules to supramolecules for structural and functional studies.

A. Synthetic methodology: The research in this area is aimed to develop new methodology for synthesizing small molecule natural product library and, unnatural amino acid library, etc.

B. Fluorescent Probes: Our research is focused on developing fluorescent probes for detection of biological analytes and cell imaging. Recently, we have developed a fluorescent thiol probe for selective detection of biological thiols and demonstrated its application in live cell imaging.

C. Ion channels: We are working on the synthesis of ion channel forming molecules aiming to control gating and selectivity using external ligands. We use the fluorescence based vesicle leakage assay for studying ion channel formation in large unilamellar vesicles (LUVs). Ligand-gating, ion selectivity and molecular recognition are main objectives behind the design of these functional supramolecules.

**SELECTED PUBLICATIONS**


Arun Venkatnathan obtained his PhD in Chemistry from Indian Institute of Technology (IIT) Bombay, India in 2001. He then worked as a postdoctoral fellow at University of California, Los Angeles and later at University of Utah and at the Pacific Northwest National Laboratory, USA before joining IISER Pune in July 2008.

THEORETICAL AND COMPUTATIONAL CHEMISTRY, COMPUTATIONAL MATERIALS SCIENCE

Research in my group involves use of Molecular Dynamics simulations to characterize structure and dynamics of various polymer membranes as electrolytes in fuel cells. We also investigate structure, energy, thermodynamic stability and spectral properties of clathrate hydrates using density functional theory.

SELECTED PUBLICATIONS


MULTIFUNCTIONAL MAGNETIC NANOPARTICLES

Nanostructured magnetic materials have received a great deal of attention because of the fascinating physical phenomena associated with them as well as their significance for several diverse and important applications. My research group focuses on the development of various low temperature techniques to synthesize high quality monodisperse magnetic nanoparticles and study them for their novel magnetic behavior. We further develop strategies to fabricate these tiny particles into large scale stable 2D assembly. The fact that these magnetic nanoparticles respond to external magnetic fields allows the biomolecules to be tagged and detected magnetically. This enables some exciting new approaches towards targeted drug delivery, magnetic fluid hyperthermia, bioseparation and biodetection. In this direction, we aim to couple magnetic nanoparticles with targeting agents, therapeutic drugs and other functional probes. With systematically tunable size and high magnetic response of these multifunctional magnetic nanoparticles, we focus on the generic approach to achieve stable dispersion of magnetic nanoparticles in both aqueous and non-aqueous media by appropriate surface functionalities. An effort is also devoted to synthesize multifunctional hybrid nanoparticles for their excellent antibacterial properties.

SELECTED PUBLICATIONS


Whole brain immunofluorescence of the zebrafish olfactory epithelium and olfactory bulb. NPY (green) is found in a population of the olfactory sensory neurons in the epithelium whose projection form the olfactory nerve. The latter eventually terminates in specific glomeruli in the olfactory bulb (marked by SV2 - red) (Image: Ajinkya Deogade and Aurnab Ghose)
Collins Assisi completed his BSc from the University of Mumbai and MSc in Physics from the Department of Physics in Pune University, India. Following a PhD in Complex Systems in 2005 at the Center for Complex Systems and Brain Sciences in Florida Atlantic University, he moved to The Salk Institute, La Jolla, California and University of California, Riverside for postdoctoral research in Computational Neuroscience. He has joined IISER Pune in August 2012.

COMPUTATIONAL NEUROSCIENCE

Animals can rapidly detect changes, characterize, and navigate a constantly changing environment. The richness of this milieu is reflected in the variety of dynamic patterns that neuronal networks can generate. The goal of my research is to study how cellular and network properties constrain the generation of these spatiotemporal patterns and determine their functional role. My work addresses this broad goal within the context of two paradigmatic systems, the hippocampus and the olfactory system.

**Spatial navigation and the hippocampus** Place cells and grid cells in the hippocampus generate patterns of activity that reflect the animal’s position in its environment. Distinct units respond at different locations forming a patchwork that covers the entire space. As the animal moves through space, groups of cells are sequentially activated. Retaining this spatial and temporal organization then provides a neural instantiation of the memory of a path traversed. My research looks at the role of network structure in the formation of these representations.

**Olfactory information processing** A study of olfaction offers the promise of insight into a successful and perhaps optimal biological algorithm for processing complex information. The representation of an odor is transformed as it traverses multiple layers of the olfactory system. My research examines the mechanisms and the computational advantages underlying these transformations in the olfactory system. I construct and simulate detailed and idealized models of neuronal networks to understand the peculiarities of these systems while also abstracting broad principles underlying information processing in the brain.

**SELECTED PUBLICATIONS**


Chaitanya Athale obtained his PhD in Biology in 2003 from the University of Heidelberg, Germany with a magna cum laude. He was a postdoctoral fellow at MGH-MIT (Boston, USA) and EMBL (Heidelberg, Germany) before joining IISER Pune in 2009.

**SELF ORGANIZATION AND CELL MORPHOGENESIS**

Cellular morphogenesis is governed by a combination of genetic and physical processes. Self-organization that relies on collective non-linear local interactions that depend on energy flows to produce emergent behavior. Our lab aims to study such self-organized collective behavior of molecules in cell-polarization and decision-making and their role in organogenesis.

At the smallest scale we are studying the motor dependent movement of centrosomal asters and their apparent guidance towards chromatin. Currently we are both preparing an *in vitro* reconstitution system as well as simulating the interaction between chromosome positions and microtubule pushing. At a higher spatial scale we are examining the role of cell division and DNA replication in bacterial cell size and shape determination.

**SELECTED PUBLICATIONS**


NAGARAJ BALASUBRAMANIAN
Assistant Professor
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Nagaraj Balasubramanian did his BSc and MSc in Microbiology from the University of Bombay and PhD in Biochemistry from the Cancer Research Institute, Tata Memorial Center, India. He did his postdoc at the University of Miami and then at University of Virginia, USA. He was a Research Assistant Professor at the University of Virginia before joining IISER Pune as a Ramalingaswami Fellow in 2010.

CELL ADHESION AND TRAFFICKING

Most cells in the human body depend on their ability to attach to the extracellular matrix (ECM) to grow, survive and migrate. Signaling pathways controlling these functions are regulated by integrin mediated adhesion to confer anchorage dependence. Cancer cells overcome this regulatory control to become anchorage independent and acquire their unique growth and survival advantage. This coupled with their ability to migrate and undergo metastasis contributes to cancer mortality. Understanding how adhesion regulates growth, survival, migratory signals and how transformed cells overcome this regulation is important to our knowledge of how cancers are caused and eventually treated.

Integrin mediated adhesion is seen to regulate caveolar endocytosis (del Pozo et al., 2005) and RalA & Arf6 exocyst dependent exocytosis (Balasubramanian et al., 2007, 2009) to drive anchorage dependent Erk, Akt and Rac signaling (del Pozo et al. (2004) Science 303:839). The lab focuses on understanding how caveolar endocytosis and exocyst function is regulated in normal and cancer cells. We are also interested in studying how trafficking pathways are differentially regulated in 2D vs 3D matrices.

SELECTED PUBLICATIONS


MACROMOLECULAR TRANSPORT AND LONG DISTANCE SIGNALING IN PLANT DEVELOPMENT

Plasticity is an important phenotypic disposition of plants as they adapt to the environment. In this regard, plant’s vascular system, the so called main highway in plants, plays a crucial role in the delivery of nutrients to distantly located organs. The phloem, one of the components of plant vascular tissue, functions as a conduit and constitutes the major long-distance route in this highway. Recent discoveries suggest that the phloem translocation stream not only transports photoassimilates, hormones, amino acids and proteins but also ferries information macromolecules such as mRNAs, small RNAs (miRNAs) and RNPs that could transfer information and control the gene regulatory network in the target organs.

Homeobox genes are ubiquitous in plants and are involved in plant growth and development. RNA regulatory networks are also implied to control a large number of plant developmental pathways and micro RNAs (miRNAs) are found to be one of the key components in this network as they target a large number of genes. My primary research interest is on potato homeobox genes (KNOX/BELs) and miRNAs in response to various environmental cues such as photoperiod, biotic and abiotic stress responses. Their role as information macromolecules in long distance signaling is also our research interest. We explore a combination of bioinformatics and molecular approaches to investigate the functions in this regard.

SELECTED PUBLICATIONS:

Deepak Barua completed his PhD in Biology from Syracuse University, USA in 2003. He was a postdoctoral fellow at the University of Toledo and at Harvard University, USA before joining IISER Pune in 2008.

**PLANT PHYSIOLOGICAL ECOLOGY**

A major question concerning evolution and adaptation includes how organisms respond to changing environments. There is tremendous diversity in plant responses to the environment and in the underlying traits and mechanisms. Broad goals of my research are to characterize such variation, identify traits and interactions among traits, understand how this translates to variation in performance, and test how variation in performance influences population persistence and adaptation in complex ecological environments.

Using an integrated approach, my lab is examining the adaptive significance of natural variation in plant responses to temperature. This includes a survey of thermotolerance in populations adapted to diverse environments, investigation of the underlying mechanisms, and its relationship to geographic distribution.

Other work in the lab investigates patterns in plant phenology - e.g. timing of germination and flowering. Phenology is extremely sensitive to the environmental, and is an early indicator of changes in vegetation dynamics in response to climate change. Work on plant phenology is currently being conducted at sites in the Northern Western Ghats and the Eastern Himalayas.

**SELECTED PUBLICATIONS**


Akanksha Chaturvedi received her PhD from ICGEB, New Delhi, India and took up postdoctoral research at the Laboratory of Immunogenetics, National Institute of Allergy and Infectious Diseases (NIAID), NIH, USA. She joined IISER Pune in January 2013.

INTEGRATION OF ADAPTIVE AND INNATE RECEPTOR SIGNALING IN B CELLS

Antibodies are essential in providing protection against many infectious agents. Antibody responses are initiated by B cells that recognize and respond to foreign antigens through antigen-specific B cell receptors (BCRs). In addition to the BCRs, B cells also express various germline encoded innate immune system receptors, Toll like receptors (TLRs) that recognize highly conserved motifs present in microorganisms. This dual expression allows B cells to not only sense antigen but also survey their environment for danger signals associated with the presence of pathogens. How the BCR and TLRs function independently of one another is known in considerable molecular details. We know little about the mechanisms that integrate BCR and TLRs signaling at subcellular and molecular levels. Although both BCR and TLRs initiate signal independently, in response to antigens and PAMPs, B cells are able to integrate both antigen-specific and danger signals into a qualitatively and quantitatively unique molecular response.

The goal of my lab is to determine the cellular and molecular mechanism by which B cells integrate BCR and TLR signaling to modify and tailor antibody responses. In addition, we also plan to understand how inappropriate B cell activation by TLRs potentially results in autoimmunity and even tumorigenesis.

SELECTED PUBLICATIONS


MOLECULAR PHYLOGENY, EVOLUTIONARY GAME THEORY AND THEIR IMPLICATIONS IN BIOLOGICAL CONSERVATION

Molecular phylogeny explores the evolutionary relationships among organisms. Coupled with molecular dating and biogeographical distribution, molecular phylogeny can reveal the patterns of evolution, phylogeographical distribution and phylogenetic endemism. Such patterns could be helpful in species management and conservations. I work on the molecular phylogeny, phylogeography and evolution of freshwater fishes and amphibians of the Western Ghats and their implications in species conservation. Our work has challenged several current paradigms in systematics and taxonomy of freshwater fishes and amphibians and has contributed to baseline information for the assessment of several taxa in IUCN Redlist of Threatened Species.

I also work in theoretical evolutionary biology using 'Game Theory' framework. While my work till date has explored the evolution of social norms and sanctions in social dilemmas, I am more inclined towards studying complex real life conflicts of interests. I am currently developing models in sustainable resource management and resolution of conflicts and their application in biological conservation.

SELECTED PUBLICATIONS


Sutirth Dey obtained PhD from Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India in 2007 and joined IISER Pune as an Assistant Professor. His non-academic interests include dramatics and movies.

**POPULATION BIOLOGY**

I study the factors that determine how population sizes change over time and space, using a combination of mathematical modeling and laboratory experiments. I also plan to investigate the various micro-evolutionary forces that impact the genetic architecture of laboratory populations. Current research themes in the lab include:

Effects of localized perturbations on fragmented populations: Due to its practical implications, stabilizing fragmented populations is a major area of research in conservation biology. Theoretical studies predict that localized perturbations (i.e. adding or killing some individuals in particular subpopulations) would stabilize the dynamics of fragmented populations. However, the first experimental study seeking to verify these predictions indicated that the effects of simple localized perturbations on stability are negligible. In that case, how should one perturb a fragmented population, such that its stability properties can be altered? What are the various factors that are expected to play a role in determining the dynamics of fragmented populations under perturbation? Questions like these have prompted us to launch a series of experiments aimed at investigating the effects of perturbations in spatially structured and unstructured populations. Currently, Council of Scientific and Industrial Research (CSIR), India is sponsoring us through an extra-mural project, to investigate the effects of perturbation on metapopulation dynamics.

Effects of migration rate on metapopulations: How does migration rate affect the dynamics of metapopulations? How does it interact with subpopulation growth rate to produce the observed dynamics? What affects the synchrony among subpopulations? We are investigating these questions through simulations and laboratory experiments on *Drosophila melanogaster*.

**SELECTED PUBLICATIONS**


**CHROMATIN BIOLOGY AND EPIGENETICS**

The global chromatin organizer SATB1 has emerged as a key factor integrating higher-order chromatin architecture with gene regulation. Studies in recent years have unraveled the role of SATB1 in organization of chromatin “loopscape” and its dynamic nature in response to physiological stimuli. At genome-wide level, SATB1 seems to play a role in organization of the ‘transcriptionally poised’ chromatin, the part of chromatin that contains genes that are actively involved in specific cellular processes. A major emphasis is on studying epigenetic modifications, the heritable changes that influence gene function without changing DNA sequence. We are particularly interested in studying the implications of these phenomena towards development and differentiation of cells. We are also interested in studying the global regulatory networks and the dynamic interplay of various cis and trans regulatory elements that dictate patterns of gene expression. The outcome of these studies would be important towards understanding the biology of diseases such as infectious diseases, cancer and other complex disorders.

**Model systems and ongoing projects**

Recently, the repertoire of model systems used in our laboratory has been expanded to enable addressing specific questions in epigenetic regulation. Thus, the centre has now employed a wide spectrum of model systems such as yeast, C. elegans, Drosophila and zebrafish in addition to mouse and human cells. Using these, we are actively engaged in addressing the following:

1. To understand the principles and mechanisms of evolution of epigenetic regulation.
2. To investigate complex and dynamic processes including transcription, gene regulation, cell proliferation, self-renewal, regeneration and interrelationships between these processes.
3. To understand the role of SATB1 in Wnt signaling during early development.
4. To study the dynamics of epigenetic modifications in human cell types and uncover its potential association with environment and complex human diseases.

**SELECTED PUBLICATIONS**


Aurnab Ghose obtained his PhD from the Beatson Institute for Cancer Research, UK. He was a postdoctoral fellow at the Department of Cell Biology, Harvard Medical School, USA before joining IISER Pune in 2008.

NEURONAL CONNECTIVITY: GENESIS AND FUNCTION

Accurate neuronal connectivity underlies the proper functioning of the nervous system. Our laboratory investigates the development and function of neuronal circuits.

We are interested in exploring the cellular and molecular logic of axonal guidance and synapse formation using genetic, biophysical and high-resolution live imaging approaches. Regulation of cytoskeleton dynamics is critical for growth cone based motility of axons and initiation of synaptogenesis. A major area of focus is the characterization of the molecular mediators of cross-talk between the actin and microtubule polymer systems.

Mechanical forces provide an important mechanism for integration in morphogenesis and may provide a faster alternative to biochemical signaling in neurons, which typically have high aspect ratios. Another interest in our laboratory is to investigate the biomechanics of neurons and the physiological relevance of mechanical signal propagation. We are developing new tools to quantitatively study the role of mechanical tension in the development of neuronal circuits.

Specific connectivity patterns impinge on functional outputs of neuronal circuits. We are currently identifying molecularly defined circuits regulating simple behaviours and aim to study the development of connectivity within these systems.

SELECTED PUBLICATIONS


BIOLOGICAL SEQUENCE ANALYSIS

One aspect of my research is related to building algorithms for analyzing high throughput sequencing data. In particular, I am interested in finding binding sites for transcription factors that regulate gene activity and finding clusters of transcription factor binding sites.

Another part of my research is on correlating genotypes with phenotypes. I develop methods that can be used to associate a genotype (sequence data) with phenotype (physical traits) while taking the phylogenetic history of the organisms under consideration into account. I am mining datasets of mutational history implied by phylogenetic trees for concurrent changes in phenotype and genotype among lineages to identify candidate loci for phenotypic traits.

Recently, we developed a human histone infobase http://www.iiserpune.ac.in/~coee/histome which is a compilation of information about human histone variants, sites of their post-translational modifications and about various histone modifying enzymes.

SELECTED PUBLICATIONS


Krishanpal Karmodiya completed his PhD in Biology from Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR), Bangalore, India in 2008. He was a postdoctoral fellow at the Institut de Génétique et de Biologie Moléculaire et Cellulaire (IGBMC), Strasbourg, France before joining the Center of Excellence in Epigenetics at IISER Pune in 2012.

EPIGENETICS AND TRANSCRIPTIONAL CONTROL IN PLASMODIUM

My research focuses on the human malaria parasite *Plasmodium falciparum*, with the goal of improving our understanding of the parasite's epigenetic and transcriptional regulation. These are underexplored areas in malaria parasites, which control vital virulence processes such as host cell invasion and cytoadherence.

Specific aims of my research include:

- Identification and characterization of novel transcriptional regulators in *Plasmodium* using mass spectrometry.
- Application of Next Generation Sequencing (NGS) approaches to map direct target genes for these transcriptional regulators.
- Investigation of mode of action of these transcriptional regulators.

SELECTED PUBLICATIONS


Saikrishnan Kayarat did his BSc in Physics at University College, Thiruvananthapuram followed by Integrated PhD in Biological Sciences from the Indian Institute of Science, Bangalore, India. Subsequent to postdoctoral work at Cancer Research, UK, he joined IISER Pune as a Wellcome Trust-DBT Intermediate Fellow in 2010.

**Structural Biology**

Fundamental cellular processes rely on protein machines that use energy to perform specific tasks. Often, this involves orchestration of activities of various functional domains of the protein molecule. The principal aim of my research is to gain insights into the working of such complex protein molecules by studying their structure in atomic detail.

One of the model systems chosen for this study is nucleoside triphosphate (NTP) dependent restriction-modification (R-M) enzymes. In general, these enzymes bind to a specific DNA sequence, perform sequence-specific methylation (modification), translocate DNA by hydrolysis of NTP and nucleolytically cleave it (restriction). Modification of host DNA protects it from restriction, while unmodified foreign DNA (eg. bacteriophage DNA) is cleaved. The molecular basis of this fascinating interplay and regulation of activities of the R-M enzymes is not well understood. Using X-ray crystallography and other tools of structural biology, a molecular framework for the function and regulation of NTP-dependent R-M enzymes will be elucidated. The findings of the project will help unravel how the enzymes perform and coordinate their varied activities, and will also facilitate the understanding of how other complex protein machines involved in nucleic acid transactions work.

**Selected Publications**


Mayurika Lahiri did her PhD from University of Wolverhampton, UK. She spent her postdoctoral years first at Tufts University, USA and then at MGH Cancer Center, Harvard Medical School, USA. She joined IISER Pune in 2008.

**GENOMIC INTEGRITY AND DNA DAMAGE**

Research in my lab focuses on the use of biochemical and molecular techniques in human cell culture systems to better understand the DNA damage response mechanisms of cells to maintain genome stability. Damage response mechanisms include cell cycle checkpoint arrest, DNA repair and apoptosis. Understanding the key processes involved in the maintenance of genomic integrity is critical in the prevention, diagnosis and treatment of a number of human pathologies, including cancer.

One avenue that the lab is currently engaged in studying is the signal transduction pathways in breast cancer cells after nitric oxide [NO] production and the role played by NO in breast cancer invasion and metastasis.

Another avenue of research the lab is focused on is studying the effects of N-nitroso compounds on eliciting the cell surveillance pathway. N-nitroso compounds have been known to cause DNA damage but their exact mechanism of action is yet to be deciphered.

My lab is also interested in investigating the role of the DNA damage surveillance pathways in the development of oral cancers.

**SELECTED PUBLICATIONS**


BIOMOLECULAR 3D STRUCTURE MODELING

The broad aim of our research is to accurately model the 3D structures of proteins and their complexes. To this end, we combine experimental observations, statistical knowledge and the laws of physics to develop computational methods in structural biology. Using the modeled 3D structures, we investigate the function of the modeled proteins/complexes. While the methods are broadly applicable, they are tested on particular systems of interest, often in close collaboration with experimentalists. Our research gives detailed information of cellular processes and hence impacts research on human health, nutrition and biology as a whole. The models we build utilize spatial restraints, such as distances, angles, volumes etc. that are taken from template structures, extracted from experimental data, deduced using computational tools, or from a combination of the above. Our computational tools identify appropriate sources of spatial restraints (http://mspc.bii.a-star.edu.sg/click) and characterize the local environments and functions of the modeled structures (http://mspc.bii.a-star.edu.sg/depth). Besides predicting/modeling the 3D structures of proteins, protein-ligand (small molecule), protein-protein and protein-DNA/RNA complexes, we are now developing methods to design these molecules and complexes.

SELECTED PUBLICATIONS


BIOPHYSICS OF SYNAPTIC TRANSMISSION IN NORMAL FUNCTION AND PATHOLOGICAL STATES

Our broad goal is to understand the contribution of each of the molecular pathways involved in synaptic transmission to higher level function. The approach in our lab is to devise realistic biophysical computational models of these sophisticated neural components that allow for ‘In-Silico’ experiments and make testable predictions.

**Calcium hypothesis of Alzheimer’s Disease (AD):** Calcium is a key molecule in synaptic transmission that finely orchestrates all forms of memory. In a rare inherited form of AD it is seen that the intracellular calcium signal is modified. As a basis of cognitive dysfunction, this project aims to quantify each of the cascades involved in changing the calcium signal.

**Modeling astrocyte–neuron signaling:** More recently, the idea that astrocytes, the non-neuronal cells of the brain too play a role in information processing is gaining traction. Astrocytes release a variety of gliotransmitters like glutamate, Adenosine Triphosphate (ATP) and D-serine in response to neuronal activity ensuring multiple levels of interaction with neurons. This project aims to develop computational models of glutamate and ATP release from astrocytes and investigate its effects on neuronal networks.

**SELECTED PUBLICATIONS**


Gayathri Pananghat did her Integrated MSc in Chemistry and Biological Sciences from Birla Institute of Technology and Science, Pilani, and PhD from the Indian Institute of Science, Bangalore. After a brief stint at IISER Pune as visiting faculty, she worked at MRC Laboratory of Molecular Biology, Cambridge, UK for her postdoctoral research. She joined IISER Pune as INSPIRE Faculty from April 2013.

**STRUCTURE AND MECHANISM OF CYTOSKELETAL MOTILITY SYSTEMS**

Cell motility is a fundamental process in biology. In many organisms, movement is mediated by appendages like cilia, flagella and pili. In addition, motility is also driven by the dynamics of assembly of cytoskeletal filaments, as in eukaryotic cell crawling. Research in bacterial cell biology has identified a few novel modes of motility based on the bacterial cytoskeleton. My research focus is to understand the molecular mechanism of motility using these as model systems.

Cytoskeleton-based motility is an example of how the dynamic assembly of macromolecules, in response to environmental cues, leads to movement. I plan to use the techniques of structural biology (mainly X-ray crystallography and cryoelectron microscopy) and single-molecule fluorescence microscopy to study the structure and dynamics of assembly of the macromolecular complexes involved in motility, thus capturing the assemblies at both spatial and temporal resolutions.

A long-term objective of the research is to compare and contrast different systems of motility based on their molecular mechanism and bring out unifying features between bacterial and eukaryotic cell motility, thus understanding the basic principles of cell motility. The fundamental nature of the research has potential to establish significant links in the evolution of cytoskeletal systems across the different domains of life.

**SELECTED PUBLICATIONS**


MEMBRANE BIOLOGY, VESICULAR TRANSPORT

Clathrin-mediated endocytosis (CME) is the major route of vesicular transport of membrane proteins (referred to as cargo) from the plasma membrane. CME is a complex phenomenon involving the co-operative action of a diverse set of endocytic proteins. It is initiated by the budding of clathrin-coated pits (CCPs) on the membrane and their scission leads to the release of clathrin-coated vesicles (CCVs) into the cytoplasm. In order for CME to be productive, CCP budding and cargo sorting into CCPs must be temporally linked events so that only cargo-laden CCVs are generated. Mechanisms by which this is achieved remain largely unknown.

My research is aimed at understanding how endocytic proteins manage cargo sorting and packaging into budded CCPs. We employ a bottom-up approach of reconstituting partial reactions en route to CCV formation on supported bilayers displaying a variety of membrane proteins as cargo. The overall objective is to arrive at a mechanistic description of CME with an obligatory focus on developing novel technologies that enable monitoring cargo recognition and sorting, membrane budding, and fission processes.

SELECTED PUBLICATIONS


Thomas Pucadyil received his PhD at the Centre for Cellular and Molecular Biology, Hyderabad, India. Subsequent to a postdoctoral training at The Scripps Research Institute, La Jolla, USA, he joined IISER Pune in October 2010.
Raghav Rajan completed his PhD in neuroscience with Dr Upinder Bhalla at the National Centre for Biological Sciences, Bangalore, India in 2006. He did his postdoctoral research in neuroscience with Dr Allison Doupe at the University of California at San Francisco, USA and joined IISER Pune in 2013.

RAGHAV RAJAN
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NEUROBIOLOGY OF MOVEMENT INITIATION

Movements are ubiquitous in our lives. With extensive repetition every day, even complex learned movement sequences like speech become automatic and we hardly notice initiating them. The importance of movement initiation is more apparent in diseases like Parkinson's disease, where movement initiation becomes difficult. Yet, how the brain initiates learned movement sequences and why movements fail to initiate in disease conditions remains poorly understood. In my lab, we use the zebra finch, a songbird, as a model system to understand how the brain initiates learned movement sequences.

Songbirds are a well-studied animal model for learned motor sequences. The learned song sequence of an adult zebra finch comprising of a stereotyped song sequence of acoustic elements, has many parallels to human speech. My postdoctoral research on song initiation suggested that adult zebra finches “warm-up” with a variable number of short introductory vocalizations before initiating their song sequence. Using various techniques to record and manipulate the activity of individual neurons in awake singing birds, current research in my lab is focused on examining the neural processes that underlie this “warm-up”, with the goal of understanding how the zebra finch brain initiates the learned song sequence.

SELECTED PUBLICATIONS


ROLE OF LIPIDS IN THE ORIGIN OF LIFE

The fundamental question of how life originated is one of the greatest scientific mysteries. In particular, the processes by which polymers capable of catalysis and replication emerged and propagated on early Earth are still elusive. Plausible prebiotic mechanisms have been described that result in biologically important monomers. These are required to synthesize complicated molecules like nucleic acids and peptides. However, it is still unclear what relevant processes might have enabled the formation of complex mixtures of such oligomers. Therefore, an important question we hope to answer is: what plausible processes allow efficient oligomer synthesis to occur under prebiotic conditions that produce informational molecules capable of catalytic activity? Subsequently, how did these functional sequences replicate their information efficiently even in the face of high intrinsic mutation rates which is a hallmark of non-enzymatic replication mechanisms?

We are specifically interested in delineating the catalytic role of amphipihiles on nonenzymatic polymerization reactions since amphiphilic boundary structures are believed to have been crucial in setting the stage for emergence and evolution of encapsulated life. We use simple fatty acids and fatty alcohols as model systems because their physical and chemical properties make them an excellent candidate for components of protocells. These studies will also enable discerning the mechanistic details of how individual components of a putative protocell interact which we hope will contribute towards what seems might be a reality soon—to evolve synthetic life in the lab using a bottom-up approach.

SELECTED PUBLICATIONS


Girish Ratnaparkhi received his PhD in Molecular Biophysics at the Indian Institute of Science (IISc), Bangalore, India. He had postdoctoral stints at the National Centre for Biological Sciences (NCBS), Bangalore, India as also in the Chemistry and Biochemistry Department at the University of California at Los Angeles, USA. He joined IISER Pune in 2008.

UNIVERSAL MECHANISMS IN ANIMAL DEVELOPMENT

Animals as different as humans, worms, and flies use remarkably similar molecular mechanisms to control their development. Discoveries of developmental paradigms in one organism have provided insights into development processes of other organisms.

My group utilizes Drosophila melanogaster and Hydra magnipapillata as model organisms to study common molecular principles underlying animal development and disease.

In Drosophila, we are studying the role of the small ubiquitin like modifier SUMO, a post-translational modifier, in regulating gene expression in the innate immune system using a proteomics based approach. In Hydra, we are interested in roles for SUMOylation in stress, immunity, and regeneration.

Lineage-specific gene family expansion (LSE) appears to be an important source of structural and regulatory diversity in eukaryotes during evolution. We are studying LSE in the Drosophila MADF-BESS family of proteins with a focus on understanding roles for this interesting family in transcriptional regulation.

Amyotrophic lateral sclerosis (ALS) is a progressive, lethal neurodegenerative disease characterized by loss of motor neurons leading to gradual paralysis and death of the patient. VAP-B is one locus identified in humans to be associated with familial ALS. We are conducting a genome wide reverse genetics screen in Drosophila to identify pathways and molecules that interact with Drosophila VAP and contribute to disease pathogenesis.

SELECTED PUBLICATIONS


Richa Rikhy did a BSc in Life Sciences and Biochemistry from St Xavier’s College, Mumbai University followed by a Masters in Biochemistry at Maharaja Sayajirao University, Baroda and a PhD with K.S Krishnan at the Tata Institute of Fundamental Research, Mumbai, India. She continued her postdoctoral fellowship with Jennifer Lippincott Schwartz at the National Institutes of Health, Bethesda, USA and has joined as a faculty with IISER Pune in August 2010.

CELL AND DEVELOPMENTAL BIOLOGY

Higher metazoan animals are composed of different cell types specialized to perform diverse functions such as nutrient uptake, secretion, sensory perception, contraction and reproduction. They have diverse cell shapes to achieve their function. The first morphologically distinct cell type to form during embryo development is an epithelial cell. It has an apical plasma membrane and a basolateral plasma membrane separated by junctional barriers. This epithelial layer is modified by developmental cues to form germ layers, which determine various tissues. The follicular epithelial cell layer during *Drosophila* oogenesis and the transparent *Drosophila* embryo development are good model systems to understand mechanisms regulating polarized plasma membrane architecture formation and modification. We are interested in elucidating the cellular mechanisms responsible for polarized epithelial plasma membrane architecture formation and determination. Currently we are working on two different areas of research interest, one of them involves deciphering how the polarized plasma membrane domains are formed during the syncytial *Drosophila* embryo development and the other is how mitochondrial dynamics and metabolism control these events of epithelial cell formation and differentiation.

SELECTED PUBLICATIONS


Kundan Sengupta received PhD in Molecular Biology from Tata Institute of Fundamental Research, Mumbai, India. His postdoctoral research was in Cancer Biology from the National Cancer Institute (NCI), National Institutes of Health (NIH), Bethesda, MD, USA and he worked as a research fellow in Cancer Biology at the Laboratory of Pathology, Division of Clinical Research, NCI, NIH, USA. He joined IISER Pune in July 2010.

CHROMOSOME BIOLOGY IN DISEASE AND DEVELOPMENT

Recent advances in fluorescent labeling technologies combined with high resolution imaging have revealed remarkable details of nuclear structure and function. Gene rich chromosomes (human chromosome 19) are localized towards the center, while gene poor chromosomes (Chromosome 18) are closer to the nuclear periphery in human cells. Such an arrangement is strikingly conserved in evolution, strongly suggesting a functional significance. The mechanisms of non-random chromosome positioning are unclear.

The current focus of my laboratory is to address (1) Molecular mechanisms of chromosome positioning (2) Nuclear organization of gene loci and its relationship with gene expression in cancer cells. We are using molecular cytogenetics, fluorescence in situ hybridization (FISH), Spectral karyotyping (SKY) and laser scanning confocal imaging in close conjunction with gene expression studies using microarrays to obtain critical mechanistic insights on nuclear structure-function relationships both in normal and cancer cells.

SELECTED PUBLICATIONS


L S Shashidhara obtained his BSc and MSc (Genetics and Plant Breeding) in 1987 at the University of Agricultural Sciences, Dharwad, India; and PhD (Molecular Genetics) in 1991 from the University of Cambridge, UK. After postdoctoral work at the University of Cambridge, UK and at the National Centre for Biological Sciences, Bangalore, India, Shashidhara joined the Centre for Cellular and Molecular Biology (CCMB), Hyderabad, India as a scientist in 1995 and moved to IISER Pune in August 2007.

GENETICS AND EVOLUTIONARY DEVELOPMENTAL BIOLOGY

Research in our laboratory aims to understand developmental mechanisms that determine physical position, size and shape of various cells/tissues/organs in our body. Our experimental model system is the development of flight appendages in the fruitfly Drosophila melanogaster. At the molecular level, insect-wing developmental pathway is conserved and is similar to limb development in vertebrates including human.

While most insects have four wings (all directly contribute to the flight), flies such as Drosophila have only one pair of wings. In these insects, only the forewings perform the flight function and the hind-wings are modified as small club-shaped balancing organs called haltere.

Specification of haltere by the transcription factor Ultrabithorax (Ubx: a member of Hox family of genes) in Drosophila is the first example for the genetic control of the specification of body plan in any animal (Ed Lewis was awarded the Nobel Prize in 1995 for this seminal work).

Several observations from our lab suggest that Ubx modulates activities of certain key signaling pathways such as Wg/Wnt, TGF-β and Egfr/Ras pathways to suppress wing development and specify haltere development. Our work has opened up many avenues to study genetic mechanisms and to identify novel components that help in fine-tuning these pathways, which are implicated in many cancers and other diseases. Our current work involves comparative genomic analyses to identify those genetic elements that are subjected to evolutionary changes causing differences in wing number, shape and size amongst various insect groups such as Apis, butterflies, silkworm, Tribolium, mosquito, and Drosophila.

SELECTED PUBLICATIONS


Nishikant Subhedar, PhD, FNASc, obtained PhD at Nagpur University, India and did his postdoctoral work at University of Florida and University of Kentucky, USA. He served as a Professor of Pharmacology at the Department of Pharmaceutical Sciences, Nagpur University, India for several years before joining IISER Pune in 2008.

GLUCOSE SENSING MECHANISMS IN THE ZEBRAFISH BRAIN

Our studies show that the neurons of the entopeduncular nucleus in the brain of teleosts play a crucial role in processing energy metabolism-related information. The neurons and their fibers contain cocaine- and amphetamine-regulated transcript (CART) and neuropeptide Y (NPY); the agents are known to process hunger and satiation in the brain of vertebrates. The two systems seem to work antagonistically. CART system is up-regulated with improved energy supply, and NPY with energy depletion. Output from these systems seems to regulate feeding behavior and rate of metabolism. Currently we are testing the possibility that the neurons of entopeduncular nucleus may also serve a role in glucose sensing and in feeding behavior. Studies on the role of the entopeduncular nucleus in the integrating the information on energy status and reproductive maturity have interesting ramifications.

We are also engaged in studying the central actions of CART in a rodent model. Our data suggest that while CART in hypothalamic-amygdala circuitry may be involved in anxiety and fear, hypothalamic-nucleus accumbens shell circuitry may process reward and reinforcement. CART also serves to promote learning and formation of spatial memory, and play an important role in drug addiction.

SELECTED PUBLICATIONS


My research interests involve plant genetics, cytogenetics and improvement of crop plants through conventional and molecular breeding tools. Over the last century genetic principles have been used extensively to improve crop plants in a desired and planned direction leading to “green revolution”. I was a part of the group at Agharkar Research Institute (ARI), Pune which had several popular wheat varieties to its credit. The explosion of molecular biological tools in recent years has helped plant breeders to bring in more precision into the breeding programs by practicing “molecular breeding”. I was responsible for setting up a plant molecular biology unit at ARI which focused on development of molecular marker strategy for crop improvement. DNA marker technology was successfully incorporated into breeding programs at ARI in wheat, soybean and grapes, and for authentication of medicinal plants. A strong group of plant biotechnology, including transgenic and marker platform, will be essential to help plant breeders accelerate product development and bring in more precision. Although this work is application-oriented, there is a lot of scope for basic work, like developing novel marker systems, understanding the genome organization, identifying gene rich regions, development and screening of tilling populations, ecotilling etc. which can form the basis for practical utility.

**SELECTED PUBLICATIONS**


Milind Watve obtained PhD from Indian Institute of Science (IISc), Bangalore, India and chose a teaching career soon after. He has taught in Abasaheb Garware College in Pune for several years before joining IISER Pune in 2009.

**EVOLUTIONARY BIOLOGY IN BEHAVIOR, METABOLISM AND HEALTH**

I specialize in not specializing. I used research more as a tool in education and tried to motivate undergraduates to identify novel problems and use a variety of tools to handle them including modeling, simulations, observations, surveys, meta-analysis, field experiments as well as lab experiments. Since students come with a variety of interests and aptitudes, while catering to them I got into a diversity of research areas including bacterial cell division, predatory bacteria, behavior of plasmids, behavior of mitochondria, diseases of wild animals, behavior and infectious diseases, pollination biology, social behavior, animal cognition, sex, human behavior and health. Nevertheless, there is a common theme that runs through all the work. The connecting link is evolutionary biology. I like to give maximum freedom of ideas and experimental designs to students and don’t mind if a student’s interest goes out of my comfort zone.

Areas of current interest: (i) Evolutionary origins and basic biology behind type 2 diabetes and other age related conditions: We have completely reinterpreted metabolic syndrome which has important implications for clinical practice and drug discovery. A behavioral intervention protocol for the reversal of type 2 diabetes is undergoing clinical trials. (ii) Bacterial life in calorie restricted environments: Theoretical and empirical work on oligophilic growth, aging and asymmetric cell division in bacteria. (iii) Ecology and evolution of secondary metabolites of Actinomycetes: Recently we discovered some novel ecological roles that Actinomycetes and their secondary metabolites play; having important implications for drug discovery. (iv) man-wildlife conflict- crop raiding by wild herbivores.

**SELECTED PUBLICATIONS**


Cleaved MMP substrate fluoresces red in and outside cells expressing CAAX-GFP in a 3D collagen matrix (Image: Trupti Thite, Adhesion Lab)
EDUCATIONAL PHILOSOPHY AND INQUIRY-BASED PEDAGOGY

After forays through Physics and English literature, my real academic life began in theoretical linguistics. My work on foundations of linguistic theory and the nature of linguistic inquiry began about twenty years back, and from there, broadened into the nature of scientific inquiry, and then to the nature of academic knowledge and inquiry against the backdrop of human beliefs in general.

My current preoccupation is located within the epistemology of scientific inquiry, comparative epistemology of academic disciplines, critical thinking and understanding, and education. An example of work resulting from these interests is available in the open source web course on Academic Knowledge and Inquiry (http://wiki.nus.edu.sg/display/aki/).

SELECTED PUBLICATIONS


Satishchandra Ogale's research focus over the last thirty years or so has been in the following areas of physical and materials chemistry: thin films and nanomaterials (optical/magnetic/electronic), magnetic oxides and spintronics, superconductivity, ion beam and laser processing of materials. He did his PhD from Pune University (1980) and was a faculty member at the university until 2006. He was also a Senior Research Scientist at University of Maryland, College Park (1996-2006). Dr Ogale was a Ramanujan National Fellow (2006-2011), and has been named NCL Scientist of the Year in 2010 and IBM-IUSSTF Fellow in Nanotechnology in 2011. (Photo from www.ncl.res.in)

S A Katre received Masters degree in Mathematics from University of Pune and PhD from Panjab University, Chandigarh, India. He began his academic career from SP College of Pune and moved to University of Pune in 1988 as a faculty member and has been there since. Prof Katre's work is in the area of Algebra and Number Theory, in particular, cyclotomy, number of points on curves over finite fields, Waring’s problem for matrices, coding theory, and group theory. His pedagogical interests include contributing to mathematics olympiads, open source mathematical software, and e-learning in mathematics. Prof Katre had served as the editor of pedagogical journal Bona Mathematica and has organized the NBHM sponsored ATM Schools in Mathematics during 2004-2012.

Sourav Pal has contributed to diverse areas of theoretical chemistry including that of the response theory formulation for closed and open shell atomic and molecular systems, chemical reactivity and density functional theory response. He obtained his integrated masters degree in Chemistry from Indian Institute of Technology (IIT) Kanpur in 1977. He received his PhD degree from Calcutta University and joined NCL in 1982. He was a post-doctoral fellow at the University of Florida, Gainesville, USA (1986-87) and has been Alexander von Humboldt Fellow at the University of Heidelberg, Germany (1987). He has received numerous awards and honors including the Shanti Swarup Bhatnagar Prize in Chemical Sciences in 2000; JC Bose National Fellowship of DST in 2008; and Chemical Research Society of India Silver Medal in 2009. (Photo from www.ncl.res.in)
Adjunct Faculty Members

**CHITTARANJAN S YAJNIK**
Diabetes Unit, K E M Hospital & Research Centre, Pune

Chittaranjan Yajnik is a Consultant Physician, Diabetologist and the Director of Diabetes Unit at the King Edward Memorial Hospital, Pune. He heads the Pankunwar Firodia Daycare Centre and the Kamalnayan Bajaj Diabetology Research Centre. He received his MD (Medicine) from B.J. Medical College, Pune (1980) and was awarded an honorary FRCP from Royal College of Physicians, London (2004) and an honorary visiting professorship at the Peninsula Medical School, Exeter (2008). He was appointed on the advisory panel of the Wellcome Trust’s Population and Public Health Council (2009). Over the last three decades or so, Dr Yagnik’s work has investigated the high susceptibility of Indians to diabetes and continues to contribute toward finding novel solutions to combat the condition.

(photograph from www.name_list.net)

**SUJATHA RAMDORAI**
Canada Research Chair, Department of Mathematics
University of British Columbia, Canada

Sujatha Ramdorai obtained her PhD in TIFR/Bombay University in 1992 and was with TIFR till January 2012. She currently holds a Canada Research Chair at the Department of Mathematics, University of British Columbia. Her research interests include Iwasawa theory and the theory of motives. Prof Ramdorai is a recipient of the Shanti Swarup Bhatnagar Award and the ICTP Ramanujan Award. She was a Member of the National Knowledge Commission and is a Member of the Scientific Advisory Council to the Prime Minister, and also the National Innovation Council. She is also interested in broader educational issues and in policy matters related to Higher Education and Research.

**S Ramakrishnan**
Senior Professor
Department of Condensed Matter and Materials Science
Tata Institute of Fundamental Research, Mumbai
ramky@tifr.res.in

S Ramakrishnan received a Master’s degree in Physics at IIT Madras and a PhD from TIFR through the University of Bombay. The central theme of his research is the experimental study of strongly correlated electron systems, with an emphasis on investigating competing ground states in systems that exhibit multiple phase transitions at low temperatures. His research output includes several outstanding contributions to the study of unconventional superconductivity, magnetism, heavy fermions and charge density waves. Prof Ramakrishnan is a former Dean of the Natural Sciences Faculty at TIFR and a Fellow of the Indian Academy of Sciences, Bangalore. He is a recipient of the Friedrich Wilhelm Bessel Research Award bestowed by the Alexander von Humboldt Foundation.
Sunanda Banerjee received a Bachelor’s degree with Honours at Presidency College, Kolkata, and a PhD in High Energy Physics at the University of London. He is an experimental high-energy physicist who has had a close research involvement with most of the major particle accelerators over the last few decades. He worked in the e+e- collider experiment L3 at LEP, CERN where he played a major role in testing the Standard Model both in the electroweak sector as well as for strong interactions. He has been a member of the CMS experiment at CERN since 1994 and has worked on the radiation damage of crystals and the design and construction of the hadron calorimeter, in addition to software and simulations. Prof Banerjee has supervised several PhD students and is a Fellow of the Indian Academy of Science, Bangalore, and the Indian National Science Academy, New Delhi.
<table>
<thead>
<tr>
<th>Name</th>
<th>Page</th>
<th>Name</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambika, G</td>
<td>1</td>
<td>Dharmadhikari C V</td>
<td>11</td>
</tr>
<tr>
<td>Anand, V G</td>
<td>47</td>
<td>Galande, Sanjeeev</td>
<td>89</td>
</tr>
<tr>
<td>Ananth, Sudarshan</td>
<td>2</td>
<td>Ganesh, Krishna N</td>
<td>56</td>
</tr>
<tr>
<td>Assisi, Collins</td>
<td>81</td>
<td>Gangal, Anil D</td>
<td>12</td>
</tr>
<tr>
<td>Athale, Chaitanya</td>
<td>82</td>
<td>Ghose, Aurnab</td>
<td>90</td>
</tr>
<tr>
<td>Athreya, Ramana</td>
<td>3</td>
<td>Ghosh, Prasenjit</td>
<td>57</td>
</tr>
<tr>
<td>Bagchi, Arjun</td>
<td>4</td>
<td>Ghosh, Sujit K</td>
<td>58</td>
</tr>
<tr>
<td>Bajpai, Ashna</td>
<td>5</td>
<td>Goel, Pranay</td>
<td>35</td>
</tr>
<tr>
<td>Balasubramanian, Nagaraj</td>
<td>83</td>
<td>Gopi, Hosahudya N</td>
<td>59</td>
</tr>
<tr>
<td>Balasubramanyam, Baskar</td>
<td>29</td>
<td>Goswami, Anindya</td>
<td>36</td>
</tr>
<tr>
<td>Ballav, Nirmalya</td>
<td>48</td>
<td>Habib, Farhat</td>
<td>91</td>
</tr>
<tr>
<td>Banerjee, Anjan</td>
<td>84</td>
<td>Hazra, Anirban</td>
<td>60</td>
</tr>
<tr>
<td>Banerjee, Sunanda</td>
<td>112</td>
<td>Hazra, Partha</td>
<td>61</td>
</tr>
<tr>
<td>Barua, Deepak</td>
<td>85</td>
<td>Hotha, Srinivas</td>
<td>62</td>
</tr>
<tr>
<td>Basu, Rabeya</td>
<td>30</td>
<td>Jayakannan, M</td>
<td>63</td>
</tr>
<tr>
<td>Basu, Sudipta</td>
<td>49</td>
<td>Jeganmohan, M</td>
<td>64</td>
</tr>
<tr>
<td>Bhagwat, Chandrasheel</td>
<td>31</td>
<td>Kabir, Mukul</td>
<td>13</td>
</tr>
<tr>
<td>Bhat, Ramakrishna G</td>
<td>50</td>
<td>Kalia, Jeet</td>
<td>65</td>
</tr>
<tr>
<td>Bhattacharyay, Arijit</td>
<td>6</td>
<td>Karmodiya, Krishanpal</td>
<td>92</td>
</tr>
<tr>
<td>Boomi Shankar, R</td>
<td>51</td>
<td>Katre, S A</td>
<td>110</td>
</tr>
<tr>
<td>Borah, Diganta</td>
<td>32</td>
<td>Kayarat, Saikrishnan</td>
<td>93</td>
</tr>
<tr>
<td>Chakrapani, Harinath</td>
<td>52</td>
<td>Khan, Shabana</td>
<td>66</td>
</tr>
<tr>
<td>Chatterji, Aparatim</td>
<td>7</td>
<td>Khare, Avinash</td>
<td>14</td>
</tr>
<tr>
<td>Chaturvedi, Akanksha</td>
<td>86</td>
<td>Kikkeri, Raghavendra</td>
<td>67</td>
</tr>
<tr>
<td>Chaturvedi, Harsh</td>
<td>8</td>
<td>Kulkarni, Sulabha</td>
<td>15</td>
</tr>
<tr>
<td>Chaudhury, Srabanti</td>
<td>53</td>
<td>Lahiri, Mayurika</td>
<td>94</td>
</tr>
<tr>
<td>Chorwadwala, Anisa</td>
<td>33</td>
<td>Madhava Rao, B S</td>
<td>68</td>
</tr>
<tr>
<td>Chugh, Jeetender</td>
<td>54</td>
<td>Madhusudhan, M S</td>
<td>95</td>
</tr>
<tr>
<td>Dahanukar, Neelsh</td>
<td>87</td>
<td>Mahalanobis, Ayan</td>
<td>37</td>
</tr>
<tr>
<td>Das, Alok</td>
<td>55</td>
<td>Mahesh, T S</td>
<td>16</td>
</tr>
<tr>
<td>Datta, Shouvik</td>
<td>9</td>
<td>Maity, Soumen</td>
<td>38</td>
</tr>
<tr>
<td>Deshpande, Aparna</td>
<td>10</td>
<td>Mallick, Vivek</td>
<td>39</td>
</tr>
<tr>
<td>Deshpande, Jayant</td>
<td>34</td>
<td>Mandal, Pankaj</td>
<td>69</td>
</tr>
<tr>
<td>Dey, Sutirth</td>
<td>88</td>
<td>Mishra, Rama</td>
<td>40</td>
</tr>
</tbody>
</table>
Mohanan K P 109 Ratnaparkhi, Girish 101
Mukherjee, Arnab 70 Rikhy, Richa 102
Mukhi, Sunil 17 Santhanam, M S 23
Nadkarni, Suhita 96 Sengupta, Kundan 103
Nag, Angshuman 71 Shashidhara, L S 104
Nair, Sunil 18 Singh, Anupam Kumar 42
Natu, Arvind Anant 72 Singh, Surjeet 44
Nityananda, Rajaram 19 Sinha, Kaneenika 43
Ogale, Satishchandra B 110 Spallone, Steven 44
Pal, Sourav 110 Srivatsan, S G 75
Pananghat, Gayathri 97 Subhedar, Nishikant 105
Patil, Shivprasad 20 Subramanian, Prasad 25
Pavan Kumar G V 21 Suryaprakasa Rao V 106
Pucadyil, Thomas 98 Talukdar, Pinaki 76
Puranik, Mrinalini 73 Vaidhyathanath, R 74
Raghuram, A 41 Vardarajan, Suneeta 26
Rajamani, Sudha 100 Venkatnathan, Arun 77
Rajan, Raghav 99 Verma, Seema 78
Ramadorai, Sujatha 111 Wavve, Milind 107
Ramakrishnan, S 111 Yajnik, Chittaranjan S 111
Rapol, Umakant D 22