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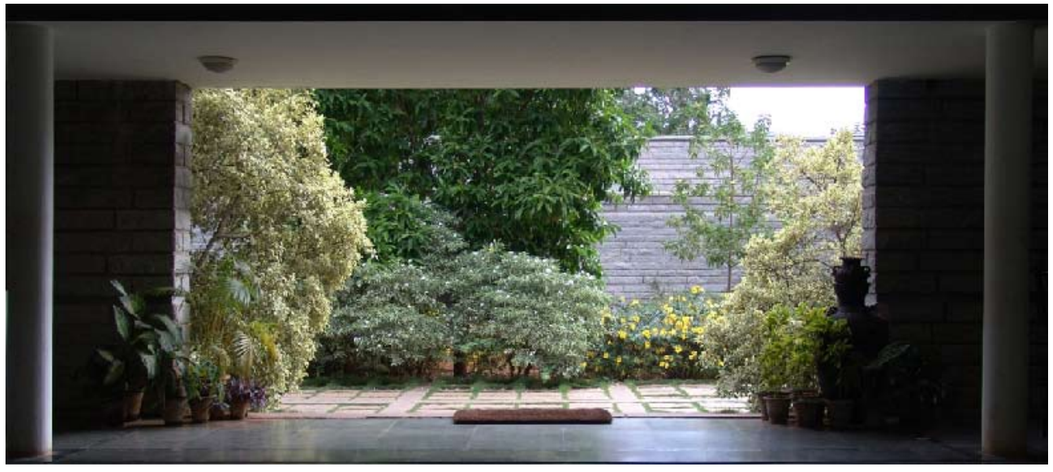

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Introduction

Not so long ago, Jakkur was a small village on the outskirts of Bangalore, where the sheep grazing in the verdant fields paused in their ruminations only to cast incurious glances at the gliders and helicopters taking off from the famous Jakkur Flying Club. Today, however, Bangalore has spread outwards to embrace Jakkur in its high-tech grasp, and high-flyers of a different kind flock to Jakkur, enticed here by the lively scientific atmosphere of the Jawaharlal Nehru Centre for Advanced Scientific Research.

We are a relatively young but already well-known multidisciplinary research institute. Our mandate is to pursue and promote world-class scientific research and training at the frontiers of science and engineering. The Centre was established in 1989 by the Department of Science and Technology of the Government of India, to mark the birth centenary of Pandit Jawaharlal Nehru. However, the bulk of our growth has been in the past decade.

Our small size (26 faculty members, spread over several disciplines) is an advantage: not segregated in far-flung labs, our chemists, physicists, biologists and engineers rub shoulders throughout the day, whether it be in seminars, the library, the dining hall or the bus to-and-from work; this fosters a spirit of interdisciplinary collaboration which is one of the hallmarks of JNCASR. Amongst the many such on-campus collaborations that have sprung up over the years: a fluid dynamicist has joined forces with a statistical mechanician to look at flow in nanochannels, and with an experimental physicist to study the freezing of laser-induced metal droplets when they impinge on a substrate; another experimental physicist and a biologist are jointly developing a portable system that uses Raman markers to detect CD4 (used in HIV diagnostics); a theoretical molecular-dynamics study of the arrangement of water molecules around a protein has emerged from coffee-table discussions between a biochemist and physicist; and a many-body theorist is modelling the devices developed in the molecular electronics lab… there are many other such examples.

In addition to our young and dynamic faculty, other strengths of JNCASR include the presence of bright and energetic graduate students (we have an excellent faculty-to-student ratio of about 1:4), and state-of-the art experimental, computational and infrastructural facilities. Visitors to our campus are also invariably impressed by our physical environment: the architecturally innovative buildings blend inobtrusively into several acres of lush landscape, with only the buckyball dome rising above the treetops; while kingfishers and herons flit among the bamboo groves surrounding our local pond.

Researchers at the Centre are divided into six units: Chemistry and Physics of Materials, Engineering Mechanics, Evolutionary and Organismal Biology, Molecular Biology and Genetics, Theoretical Sciences, Educational Technology and Geodynamics. We also have two off-campus units at the Indian Institute of Science: the Chemical Biology and Condensed Matter Theory Units. Though it is of course difficult to quantify scientific performance, by all numerical indications (numbers of publications, citations, grants, patents filed, etc.), science at the Centre is flourishing. In the last few years, the Centre's faculty members have published their research in some of the most prestigious scientific journals, including Nature, Nature Medicine, Science, Evolution, the Journal of the American Chemical Society, Angewandte Chemie, the Journal of Fluid Mechanics, and Physical Review Letters. The work of the Centre's faculty is also being recognized by various awards: of course, the list of honours and prizes received by CNR Rao, our Honorary President and Linus Pauling Research Professor, runs into many pages; however, we were all still very excited when he was recently awarded the Dan David Prize for Science in the Future Dimension, in 2005. Our younger faculty members too, are making their mark: for example, this year, Tapas K Kundu was awarded the Shanti Swarup Bhatnagar Prize for biological sciences, Anuranjan Anand received the Outstanding Research Award from the Department of Atomic Energy, and Srikanth Sastry, GU Kulkarni and Balasubramanian Sundaram received the BM Birla Science Prize.

In addition to carrying out innovative scientific research, the Centre has a commitment towards fostering scientific education. We are now a "Deemed University", and over a hundred graduate students are currently working towards Master's and PhD degrees at the Centre. Apart from training our own students through a wide spectrum of courses, we are also actively supporting a range of educational outreach activities: every year, our highly competitive Summer Research Fellowship programme hosts some of the very brightest undergraduates in the country; the Educational Technology Unit produces a range of teaching aids and educational material; we organize and teach short term courses at universities across India; and promising young chemists and biologists are trained intensively as part of our programmes of Project Oriented Chemical Education (POCE) and Project Oriented Biological Education (POBE).

Before Bangalore became IT-City, it was already renowned as Science-City, and our faculty and students benefit from interacting with scientists at the many research institutions in the greater Bangalore area. The intellectual atmosphere at JNCASR is further livened by a regular stream of visitors from all over the world, who contribute to spirited scientific discussions at seminars, conferences and summer schools. We believe we possess all the necessary ingredients to excel in scientific research and education, and look forward to growing further in the coming years.

Research Areas

Chemistry and Physics of Materials Unit
Education Technology Unit
Engineering Mechanics Unit
Evolutionary and Organismal Biology Unit
Geodynamics Unit
Molecular Biology and Genetics Unit
Theoretical Sciences Unit
CSIR Centre of Excellence in Chemistry
Chemical Biology Unit
Condensed Matter Theory Unit

Chemistry and Physics of Materials Unit

Chairman
CNR Rao

Faculty
S Balasubramanian
N Chandrabhas
M Eswaramoorthy
GU Kulkarni
KS Narayan
A Sundaresan

Distinguished Fellows
AK Cheetham
Gerard Ferey
Bernard Raveau

Materials research is one of the frontier areas of science and technology today. Accordingly, materials constitute major aspect of research investigations in both chemistry and physics. In recent years, biology has also become an essential aspect of this area. This unit is involved in the study of various facets of this interdisciplinary subject, the primary goal being the design, structure, properties and phenomena associated with advanced materials, both inorganic and organic. In the last few years, the Unit has acquired and developed sophisticated experimental facilities. The Unit employs state-of-the art methodology to synthesize and study interesting properties and phenomena in novel materials.

Material synthesis forms a strong forte of this unit. This unit has produced novel synthetic methods to produce organic and inorganic materials including the nanowires and nanotubes. Materials at nanometer scale exhibit novel electronic, optical and magnetic properties which are different from their bulk materials. These properties lead to potential technological applications. Therefore, the nanotechnology is strongly dependent on the synthesis of nanomaterials. A variety of chemical methods have been used to prepare nanoparticles of various metals, semiconductors and magnetic materials. Dip-pen lithography using AFM setup has been applied to synthesize patterned nanoobjects on surfaces as well as making nanocircuitry. Besides this technique, pulsed laser deposition, RF magnetron sputtering methods have been employed to produce metals and metal oxides thin films, nanostructures and superlattices. Materials in different forms are also being made by template aided strategies, which are otherwise difficult to make in the conventional methods. For example, supramolecular preorganization of organic molecules were used to synthesize functionalised clays with spherical and tubular morphologies which would find application in controlled drug release, ions sequestration and anisotropic composites. The materials synthesized are characterized by the state-of-the art characterization techniques (see research facility page).

Studies of electronic, optical, photophysical and device aspects of organic, polymeric, nanoparticle, and biomolecule based materials are being pursued. This includes the study of the rich photophysics and electrical transport mechanisms in these systems as well as probing new phenomena and device development such as Field Effect Transistors (FET), Light Emitting Diodes (LED) for flexible displays, solar cells and image sensors. Optical probes such as infrared, Raman and Brillouin scattering at ambient and extreme conditions, for example, at high pressure have been used to understand the structure, bonding and various interactions in various materials including those having technological importance. Recent research interest is on the surface enhanced Raman spectroscopy (SERS) by tagging the gold and silver nanoparticles to proteins, polypeptides in order to use it as a diagnostic tool in biology.

Theoretical study of materials using computer simulation methods is a part of this unit. This group focuses on an interdisciplinary area bridging physics and chemistry. The simulation methods are derived from classical, quantum, and statistical mechanics. This group work closely with experimentalists, and attempt to mimic actual experimental conditions in the simulations, for a direct comparison and thereby able to provide microscopic detail to explain macroscopic phenomena.

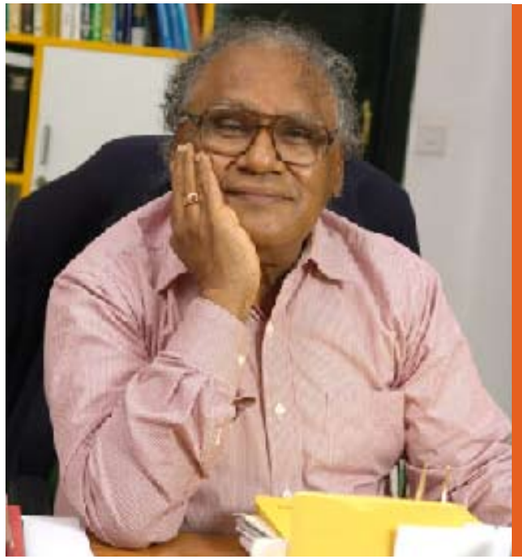
Research Facilities

- **S**ingle Crystal X-ray diffractometer with CCD facility (Bruker)
- ESCA facility with UVPS, and LEED
- Pulsed laser reactive ablation apparatus attached with mass spectrometer
- Scanning Tunneling and Atomic Force Microscopes (STM/AFM) operating in air
- Variable Temperature STM
- Catalyst characterization with Gas chromatograph
- Quadrupole Mass Spectrometer and Residual Gas Analyzer
- Carbon arc-discharge Unit
- Large number of furnaces for making samples in various atmospheres in the range 300°C to 1700° C
- A closed cycle cryocooled 15 T superconducting magnet with a room temperature bore and an optical window
- Floating zone melting crystal growth apparatus
- High Resolution Transmission Electron Microscope (HRTEM) (300 kV, JEOL 3010)
- Scanning Electron Microscope (SEM) with EDAX (Leica440I)
- Magnetometer (VSM) and Faraday balance
- Surface area measuring apparatus
- Powder X-ray diffractometers (Siefert and Mini Rigaku)
- Four Probe conductivity setup (15 K-325 K)

Figure 1: High Resolution Transmission Electron Microscope (HRTEM)

Figure 2 (left and right): Scanning Electron Microscope (SEM)

- Fourier Transform Infra-red Spectrometer to operate in the 200-7500 cm^{-1} range along with DRIFTS, environmental cells (77 K to 523 K) (Bruker) for controlled studies
- Thermal characterization up to 1250 K (Mettler)
- UV-VIS spectrometer (Perkin-Elmer)
- Fluorescence spectrometer (Perkin-Elmer)
- Mössbauer Spectrometer
- Brillouin Spectrometer
- Micro and Indigenously built Raman Spectrometers
- Crystal polishing instrument
- Diamond anvil cell for high pressure research
- Optical stereo microscope with 200X magnification
- Low temperature compressed Helium cryostat
- Glove Box (< 2 ppm O_2 and H_2O environment) integrated with spin coating unit and accessories for device fabrication
- Fabrication facilities for Light emitting diode (LED), photovoltaic (PV) diodes and solar cells, field effect transistor (FET)
- Beowulf clusters for computational research
- Device LED, PV, FET measurement facilities
- Soft-lithography and Photolithography Implementation facilities
- Time (> 10 ns) and spatially (~ 50 nm) resolved photocurrent measurements
- Photolumiscence emission and excitation spectroscopy
- Physical Property Measuring System (PPMS, Quantum Design, USA) Evercool with 9T magnet (options: AC/DC susceptibility, AC/DC transport and heat capacity)
- RF magnetron sputtering for making thin films and superlattices
- Chemisorption-Physisorption Analyzer-Quantachrome Autosorb®-1-C
- Zetasizer Nano ZS particle size analyzer-Malvern instruments
- Precision Workstation (Radiant Technologies Inc) for dielectric measurements
- Near field current contrast optical microscopy under development



CNR Rao

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Chemistry of Materials

The subject of Chemistry of Materials, in its present form, is relatively of recent origin and has absorbed all the elements of solid state chemistry, which, by and large, dealt with inorganic solids. Today, chemistry of materials deals with inorganic, organic, biological and hybrid materials, of all varieties and complexities. While synthesis and characterization of materials form a significant part of the subject, properties and phenomena as well as their relationships consitute an equally important component.

I have been involved in materials chemistry research for nearly half a century and my interests have included novel synthetic strategies, development of new tools of characterization, phase transformations, transition metal oxide systems, open-framework materials and nanomaterials. Transition metal oxides, which represent the most exciting family of materials with the widest range of properties, have been of great interest to me. Of special interest are the phenomena of metal-insulator transitions, high-temperature superconductivity, colossal magnetoresistance, and biferroicity. In the last few years, we have carried out extensive studies to understand charge ordering and electronic phase separation in rare earth manganates and cobaltates. We have also discovered new biferroic materials such as $BiMnO_3$ and $YCrO_3$. In the area of nanomaterials, zero-dimensional nanocrystals, one-dimensional nanowires and nanotubes as well as two-dimensional nanowalls and nanofilms have been explored. Thus, nanocrystals of materials such as CdS, transition metal oxides, III and V nitrides such as GaN have been synthesized by employing novel chemical strategies and characterized by various means. Magnetic properties of nanoparticles of CoO, MnO and NiO have been investigated. Metalli ReO_3 nanoparticles have been prepared for the first time and characterized by their plasmon resonance. Nanowires of various metal oxides, chalcogenides, nitrides and carbides have been prepared by carbothermal means and also by soft chemistry. Typical of the inorganic nanowires studied include Ga_2O_3, SiO_2, Si, SiC, GaN, InN, CdS and ZnS. Several properties (e.g. gas sensing) of the nanowires and their composites have been examined.

Besides finding new methods of preparing different types of carbon nanotubes (including junction nanotubes), nanotubes of various inorganic materials have been synthesized for the first time by employing novel strategies. Properties of some of these materials are being investigated (e.g. supercapacitance). Organically templated open-frame inorganic materials are an important class of hybrid materials. Major contributions from here have been on open-framework metal phosphates and carboxylates. The use of oxyanions such as sulfate, selenate and selenite to design open-framework structures has been successfully explored. The mechanism of formation of these complex architectures has been another important aspect of study.

CNR Rao is the Linus Pauling Research Professor, founder and honorary president of JNCASR.

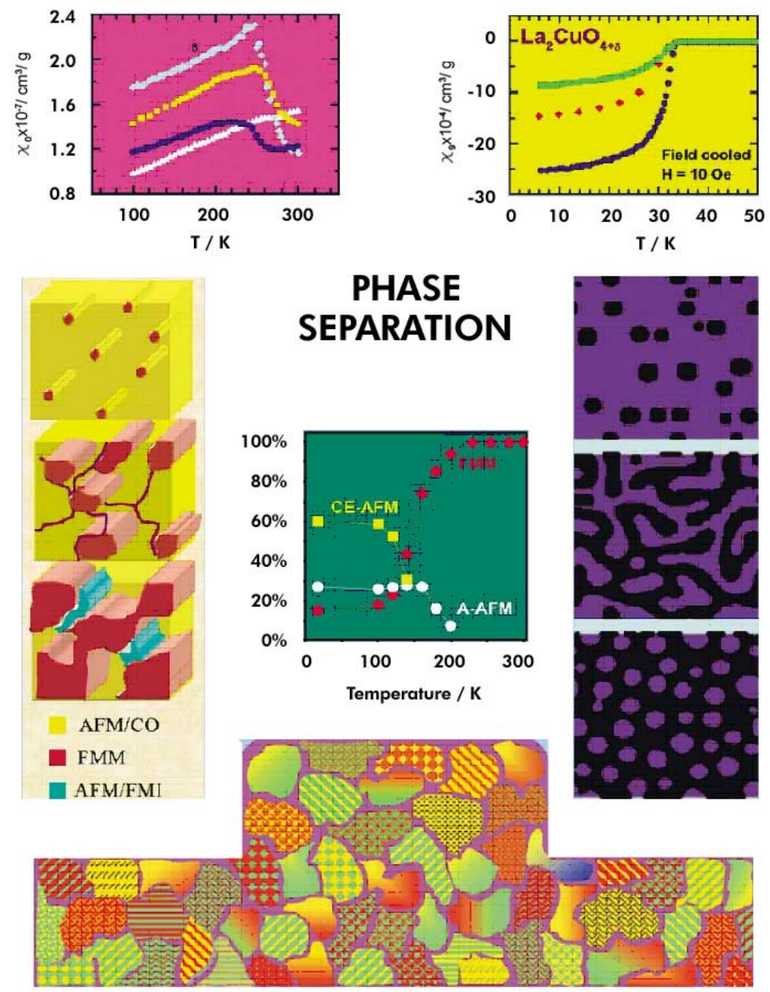

Figure 1: Phase separation in Metal Oxides

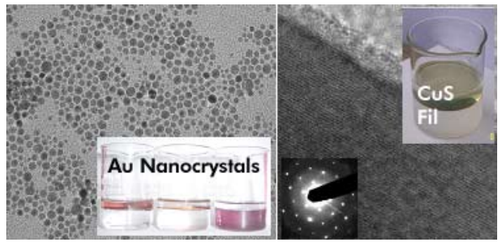

Figure 2: Organic water interface for large scale syntheis of nano crystals and single crystalline films

PhD Students

From JNCASR: Venkata Prasad Bhat, SRC Vivek Chand, F Leonard Deepak, A Gomathi, KP Kalyanikutty, Asish Kumar Kundu, V Rakesh, Chandra Sekhar Rout, Jyoti Ranjan Sahu, A Thirumurugan

From IISc: JN Behera, Kanishka Biswas, Meenakhsi Dan, Moumita Ghosh, Kripa Sindhu Sardar, Motin Seikh, Claudy Rayan Serrao

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Molecular Modelling of Materials

Our research is focused on molecular interactions and its role in the organization of molecules in condensed systems. We study crystalline, amorphous solids, liquids, supercritical fluids, interfaces, biological and complex systems using molecular dynamics (MD) methods. Realistic modelling of materials can enable one to obtain insight into microscopic processes that underlie experimental observations, and computational techniques such as MD provide us with such details which complement experiments. Molecular interactions can be treated in an empirical fashion using classical laws of electrodynamics, or can be treated in a more sophisticated manner using quantum density functional theory. The time evolution of the degrees of freedom (say, atomic) of substances can then be studied using classical dynamics such as Lagrange's or Hamilton's equations of motion and a trajectory of the system in phase space can be generated. Both static averages and dynamical quantities can be obtained which are related to experimental observables. We employ two flavours of the MD technique, one called classical molecular dynamics, and another, *ab initio* molecular dynamics (AIMD). Using these methods, we have been able to provide a rare insight into the structure and dynamics of molecular substances and have been able to interpret various experimental observations on the phase transitions exhibited by molecular crystals, the hydration layer in aqueous micellar and protein solutions, Green solvents such as supercritical carbon dioxide, and room temperature ionic liquids. All these calculations are highly compute intensive and hence parallel computers (PC clusters) are employed.

Balasubramanian Sundaram has obtained his PhD (1994) in Chemical Sciences from the Indian Institute of Science. He was a post-doctoral fellow in Chemistry at University of Pennsylvania before joining JNCASR in 1998. He is also the Coordinator for the Centre for Computational Materials Science at JNCASR.

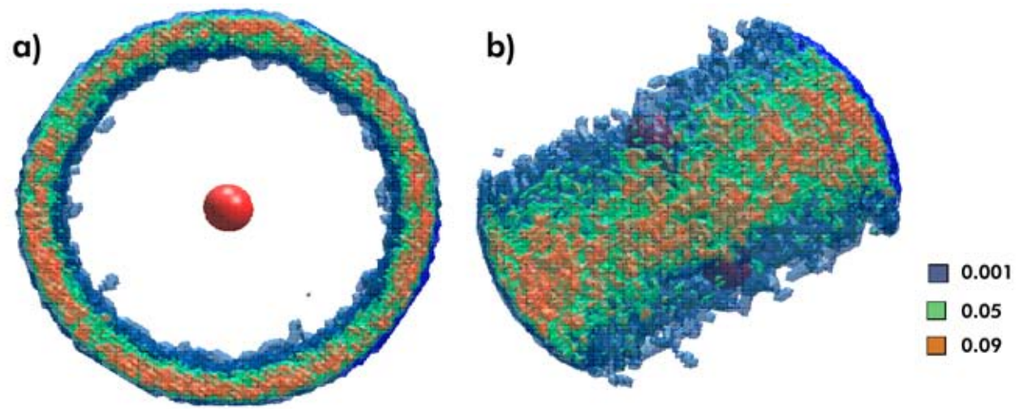


Figure 1: *Ab initio* MD simulations reveal the geometry of the first coordination shell of a carbon dioxide (CO_2) molecule in supercritical CO_2. Blue, cyan, and orange represent the increasing probability of finding an oxygen atom belonging to a neighbouring molecule in the first coordination shell of CO_2. Panel (a) shows the top view and Panel (b) shows the side view

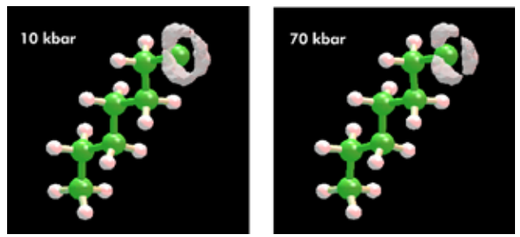


Figure 2: The kinetic freezing of methyl rotation in a system of crystalline *n*-heptane studied using atomistic molecular dynamics simulations. Shown here are the atomic probability density maps of methyl hydrogen around the carbon atom shown at two pressures

Sponsored Projects

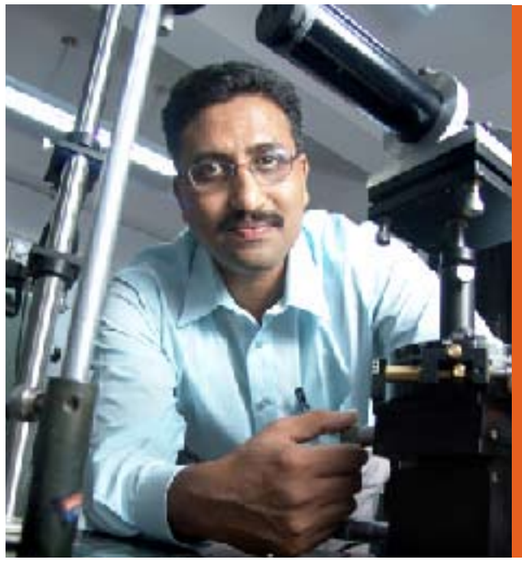
1) *Computer simulation studies of room temperature ionic liquids,* DST, 2005–2008.
2) *Simulation studies of structure, dynamics, and solute-solvent interactions in supercritical carbon dioxide,* CSIR, 2005–2008
3) *Computer simulations of aqueous protein solutions: A study on the role of biological water,* DBT, 2003–2006.
4) *Molecular modelling of discoid amphiphilic aggregates,* CSIR, 1999–2002.

Key Publications

1) Bhargava BL, Balasubramanian S. Dynamics in a room temperature ionic liquid: A computer simulation study, *Journal of Chemical Physics,* 123, 144505, 2005.
2) Krishnan M, Balasubramanian S. Phase behaviour of ultrathin crystalline n-Heptane films on graphite: An atomistic simulation study, *Physical Chemistry Chemical Physics,* 7, 2044-2052, 2005.
3) Pal S, Bagchi B, Balasubramanian S. Hydration layer of a cationic micelle, C10TAB: Structure, rigidity, slow reorientation, hydrogen bond lifetime and salvation dynamics, *Journal of Physical Chemistry B,* 109, 12879-12890, 2005.
4) Krishnan M, Balasubramanian S. n-Heptane under pressure: Structure and dynamics from molecular simulations, *Journal of Physical Chemistry B,* 109, 1936-1946, 2005.
5) Saharay M, Balasubramanian S. Enhanced molecular multipole moments and solvent structure in supercritical carbon dioxide, *ChemPhysChem,* 5, 1442-1445, 2004.
6) Saharay M, Balasubramanian S. Ab initio molecular dynamics study of supercritical carbon dioxide, *Journal of Chemical Physics,* 120, 9694-9702, 2004.
7) Krishnan M, Balasubramanian S. Order-disorder transitions and melting in a helical polymer crystal: Molecular dynamics calculations of model poly(ethylene oxide), *Chemical Physics Letters,* 385, 351-356, 2004.
8) Krishnan M, Balasubramanian S. Vibrational dynamics of solid poly(ethylene oxide), *Physical Review B,* 68, 064304-1 to 064304-10, 2003.
9) Krishnan M, Balasubramanian Clarke S. An atomistic simulation study of a solid monolayer and trilayer of n-hexane on graphiteand, *Journal of Chemical Physics,* 118, 5082-5086, 2003.

PhD Students

BL Bhargava, Moumita Saharay, Soumya Saswati Sarangi



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Raman Spectroscopy, Brillouin Scattering and High-Pressure Research

My group is interested in study of materials using optical spectroscopy under ambient and extreme conditions. Our group's activities can be divided into three categories: (a) Raman spectroscopy, (b) Brillouin scattering and (c) High pressure research using light and x-ray as probes. We are interested in use of non-contactual probes to study materials in ambient and especially in extreme conditions, like high pressures. Vibrational spectroscopy has been an important component of study of materials and of late with the recent advancements in lasers Raman spectroscopy has been seen as an effective probe in studying materials properties, such as, properties related to say low-demensionality, structure, bonding, interactions, etc. Brillouin spectroscopy gives an edge over ultrasound and neutron diffraction in understanding the mechanical properties such as bulk modulus, young's modulus etc. The biggest advantage being that the sample requirements are not stringent.

My group looks at the materials to answer the following questions: (a) what aspects of chemical bonding and microscopic couplings relate to the specific properties of a material, (b) what are the significant interactions and implications of electrons and phonons (c) phase transitions in materials under extreme conditions.

Most of the materials we study exhibit some novel phenomena and are of technological importance. These include nano-materials such as nanotubes, fullerenes, nanowires, magnetic materials, biosystems, etc. We are currently persueing research in surface enhanced Raman spectroscopy (SERS) by tagging the gold and silver nanoparticles to proteins, polypeptides in order to use it as a diagnostic tool in biology. We are in the process of developing Raman markers that would help in this regard.

Chandrabhas Narayana has obtained his PhD (1995) in Physics from Indian Institute of Science, Bangalore. He was a post-doctoral fellow in Material Science and Engineering at Cornell University before joining JNCASR in 1998.

Elastic Properties and Optical Constants of Opaque Materials
Brillouin scattering is complementary tool for ultrasonic studies and has a large advantage over ultrasonic studies too. Brillouin scattering is a non-destructive tool and can look at any sample, be it thin films, polycrystalline, big or small crystals, under high pressures and varying temperature conditions. Recently we have been studying nanotubes (like double walled carbon nanotubes, boron nitride nanotubes), manganites, low-dimensional conductors, oxides and semiconductors.

Brillouin scattering studies of manganites at ambient and varying temperature condition: Manganites have attracted lot of attention due to their colossal magneto-resistance shown by them and their potential application in the reading and recording industries. They are derived from the rare-earth perovskite of the type $ReMnO_3$. We were able to observe the magnons (surface and bulk) along with acoustic excitations in these manganites and looked at their behavior as they go through the various phase transitions. We are extending the research on these materials as a function of pressure looking at it using Raman and X-ray scattering as well.

Brillouin scattering studies on nanotubes and related systems at ambient and high pressures: Carbon nanotubes have been lately been investigated for their chemical, physical as well as strengthening properties. Carbon and Boron Nitrides have great similarities in them, such as, both of them form the graphite and diamond structures. BN is the second hardest material next to carbon. Both of these form nanotubes. The difference is that BN nanotubes do not show property dependence on chirality unlike carbon. We have been looking at the mechanical properties of these and trying to understand them as a function of pressure. We have been able to see the acoustic phonons for the first time from the double walled nanotubes and have been able to determine the elastic properties of these nanotubes. Recent x-ray scattering studies under pressure on BN carried out at Cornell High Energy Synchrotron Source (CHESS) by us on hexagonal BN multi-wall nanotubes showed that they transform to the distorted diamond like structure (wurtzite) at pressure in excess of 12 GPa at ambient temperature. We are interested in understanding the strength properties of these materials in their different forms and are going to study them using Brillouin scattering studies.

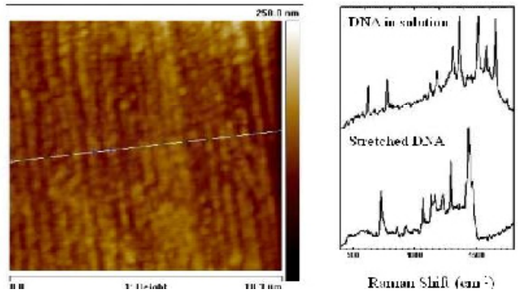

Figure 1: Stretched-λ-DNA templated metal nanostructures based plasmonic biosensors described with SERS detection scheme

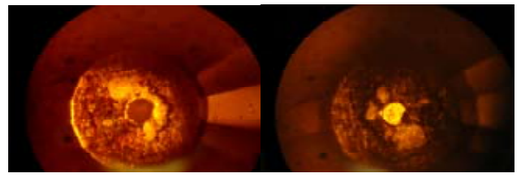

Figure 2: High pressure studies on BN nanotubes (a) at ambient conditions and (b) at 17 GPa. Note the phase transition in BN from graphite structure to distorted diamond like structure is associated with a color change

High Pressure Raman Spectroscopy

High pressure Raman scattering on mid chain hydrocarbons, oxides, low dimensional system: Mid chain hydrocarbons have been interesting to both experimentalist and theoreticians alike. There has been an interest in these to study their behavior under high pressures especially their solid-solid transformation. We have been able to see a solid-solid transformation in n-heptane and are looking into the other mid chain hydrocarbons to understand the behavior of the high pressure. We have been using Raman spectroscopy to study the various oxides under pressure such as $PbWO_4$, $BaWO_4$. We have carried out studies on carbon fibers, carbon nanotubes and its derivatives, organic polymers as a function pressure. These forms of carbon and carbon derivatives show a varied electrical, magnetic as well as chemical properties, which have potential applications, and our interest is in understanding their physics by applying pressure to change their inter-atomic spacing.

SERS in Biology

Surface Enhanced Raman Spectroscopy on proteins, DNA, polypeptides: Recently our laboratory in collaborations with our Biology colleagues have been looking at interaction of various chemical species with proteins, or simply trying to locate the protein and its concentration around the cell. We had looked at the interaction of a non-specific HAT activator with p300 in the concentrations in which the bio-chemical experiments are carried out and we could compliment the bio-chemical findings. We have used SERS in detecting the effect of nano-particle array on stretched lambda DNA that has biosensor applications. We are in the process of developing important Raman labels to be used in SERS in tracking specific proteins on the cell membranes, one of the potential applications of this is to detect the CD4 counts in HIV infected cells.

PhD Students

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From IISc: MD Motin Seikh

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Nanomaterials and Catalysis

Nature, the doyen of science constructs complex functional materials with hierarchical architectures. Horns or bones, shells or skulls, it selectively picks up the bricks, the requisite building blocks, from organic or inorganic components and organizes them in a programmed manner. Over the period of evolution, it learnt the art of intertwining organics and inorganics in an impeccable way to make light, but tough materials and pass on this trick from generation to generation. Many times, it elegantly uses the vesicles made up of lipid bilayers as the reaction containers to make biominerals with defined shapes which defy the thermodynamic rules. Taking a leaf out of Nature's book, we are attempting to make materials in different forms by template aided strategies, which are otherwise difficult to make in the conventional methods.

Eswaramoorthy Muthusamy has obtained his PhD (1996) in Chemistry from Anna University. He was a post- doctoral fellow at JNCASR, India, STA and AIST fellow, Japan and Research Assistant at Bristol University, UK before joining JNCASR in 2004

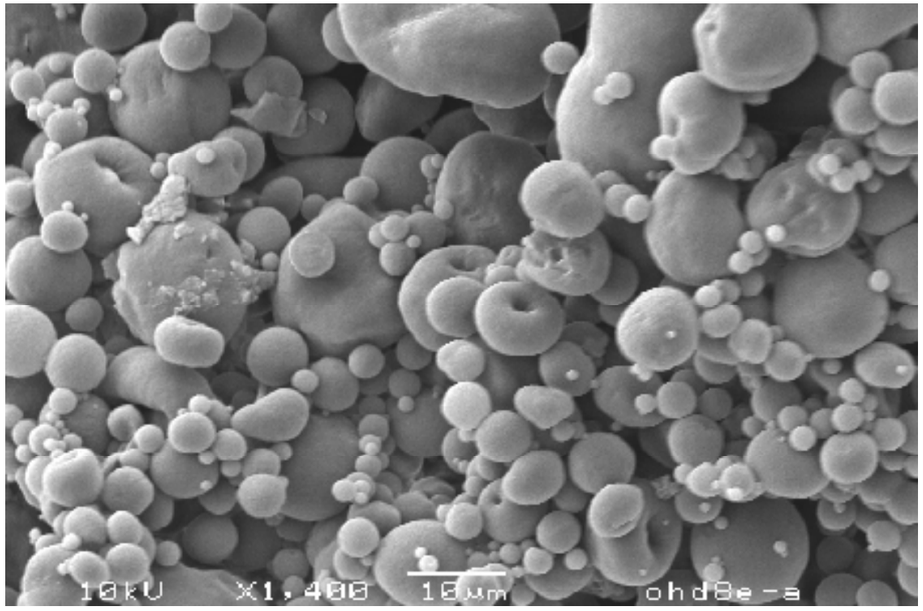


Figure 1: Organoclay with apple-like morphology synthesized by emulsion based method

For example, supramolecular preorganization of organic molecules were used to synthesize functionalised clays with spherical and tubular morphologies which would find application in controlled drug release, ions sequestration and anisotropic composites
Another area which is of interest to us is the bio-inorganic nanohybrids, materials which are expected to have size-dependant properties of nanoparticles infused with the molecular recognition features of the biomolecules, like proteins and DNAs.

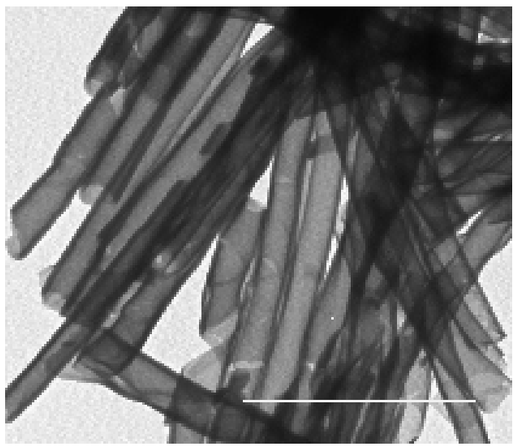


Figure 2: Aminoclay with tubular/helical structures synthesized using phospolipid template

Catalysis using porous materials also caught our attention both in terms of shape-selective and green chemistry point of view. Nothing (pores) is equally important as something (walls) in a catalytic material which controls the molecular level transport. Porous nanoparticles, nanotubes and materials with different morphologies synthesized here would be used to test some catalytic reactions like NOx removal, methane conversion and selective oxidation of hydrocarbons.

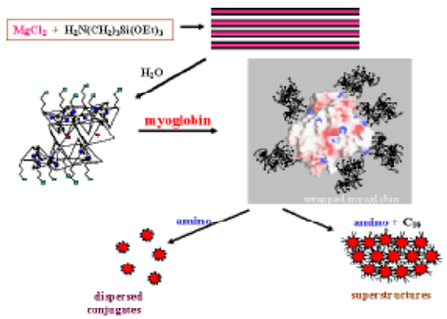
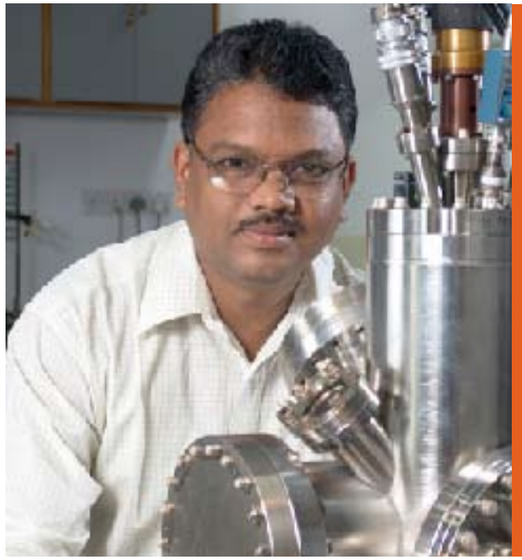


Figure 3: Armoured protein. Clay-Biomolecule nanoconjugates, a reaction scheme

PhD Students

Dinesh Jegadeesan, K Sai Krishna



GU Kulkarni

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Experimental Nanoscience, Electronic Charge Density from Molecular Crystals

The main theme of research in my group is studying matter at the Nanoscale. When the size of a material is reduced to a length scale typical of the interactions therein, quantum confinement of electrons sets in leading to unusual properties that depend on the size of the system itself. This explains the growing interest in both academic and industrial circles to synthesize new nanomaterials with tailor made properties. Our research interests are focused on (a) Synthesis and characterization of metal nanocrystals and their meso-scalar assemblies, nanocrystalline metal films, inorganic-organic hybrid bilayers (b) Size dependent properties of individual nanocrystals, collective properties in a meso-assembly, (c) Scanning probe methods for nanolithography and nanodevices, (d) Exotic nanostructures from pulsed laser deposition and (e) Molecular properties from electronic charge density method.

Metal nanocrystals, Au, Ag, Pt, Pd etc. have been prepared employing soft-chemical routes and thiol derivatized to form extended 2D ordered lattices. Such mesostructures have been obtained with magic nuclearity Pd_{561} and Pd_{1415} clusters as well. In addition, Pd-Ni core-shell arrays have been made and characterized using magnetic measurements. The novelty of this work is that the obtained nanocrystals are essentially monodispersed and have the ability to self-assemble into an extended mesolattice. Structural properties of the mesostructures have been studied using particles of different sizes and ligands of different lengths. In a 'single-step' procedure, organic-water liquid-liquid interface has been exploited to synthesize ultrathin (~100 nm) nanocrystalline films of metals, Au, Ag, Pt, Pd, Cu as well as their alloys. These free-standing films may be extracted on flat substrates.

GU Kulkarni has obtained his PhD (1992) in Solid State Chemistry from the Indian Institute of Science. He was a post-doctoral fellow in Chemistry at Cardiff University before joining JNCASR in 1995.

The particle size in the nanocrystalline film has been varied systematically by changing experimental parameters such as reaction temperature and concentration. The film at the interface readily forms hydrosol or organosol upon adding appropriate capping agents.

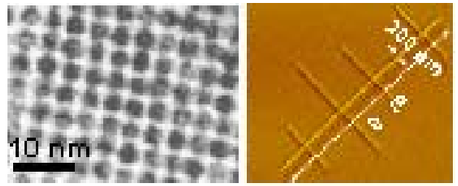

Figure 1: A mesoscopic assembly of Pd-Ni core shell nanocrystals
Figure 2: Dip pen nanolithography patterns filled with magnetic nanocrystals

Oriented nanocrystalline Au(111) films have been prepared on silicon substrates by the galvanic displacement method. By adding additives during the reaction, the structural properties of the film can be varied. This method has also been used to create segregated Au nanoislands, nanowires etc. Pd alkanethiolates that are soluble in organic media have been prepared and characterized using a host of structural tools. These thiolates exhibit lamellar structure with the bilayer thickness corresponding to nearly twice the hydrocarbon chain length. The tendency of alkane thiols to self-assemble has been put to 'acid-test' in the formation of hybrid bilayers containing thiols of two different chain lengths. It is also demonstrated that a hybrid bilayer can act as an 'ion-trap'. The work is extended to magnetic Ni thiolates as well.

Size dependent properties, electrical, optical and magnetic, of the nanosystems have been studied. Nanocrystalline Au films containing smaller particles (~ 8 nm) behave like activated conductors while those with above 20 nm particles resemble closely the bulk metal. The dependence of the single electron charging energy on the size of the nanocrystal has been studied independently using scanning tunneling microscopy (STM). The electronic coupling prevalent in the mesolattice results in a red shift of the surface plasmon band of the constituent nanocrystals. The band shifts gradually towards lower wavelengths as the particles are pulled out of the film to form a colloidal sol.

The magnetic moment associated with the Pd-Ni core-shell nanocrystals was found to scale with the amount of Ni loaded on the particle. The magnetic properties of the Pd-Ni arrays have been studied in view of their potential application as high density media. Similarly, iron oxide nanoparticles cast in the form of a film on silicon substrate exhibit high magnetic anisotropy, an important property sought after in applications. The Ni thiolates have been subjected to low temperature magnetic measurements in order to understand their chain length dependence. Interestingly, they are found to exhibit a dimensional crossover below 4K.

Of the various nanolithography methods, dip-pen lithography using AFM setup is receiving considerable attention in the recent years. In our laboratory, well characterized metal sols and other colloidal dispersions have been used as inks for dip-pen raised patterns. Using this method, nanoscale rectangles filled with the metal nanocrystals have been drawn on mica substrates at different aspect ratios, the narrowest line being 20 nm wide. Besides metal sols, dispersions such as Eu doped LaPO4 nanoparticles with interesting fluorescing properties have been tried out as inks. Colloidal iron oxide has been used to produce magnetic patterns. The internal structure of the patterns has been studied using nanospectroscopy techniques on a synchrotron beamline. The method is being used for patterned synthesis for nanoobjects on surfaces as well as for making nanocircuitry.

Conducting-atomic force microscopy (C-AFM) has become a popular tool lately, for the electrical characterization of nanodimensional materials. We have studied some practical issues involved while employing gold-coated AFM probes. Mechanical wear and electrical breakdown characteristics of the gold coating have been studied by way of monitoring the effect of the applied force on the resistance of the nanocontact. The CAFM method has been employed in our group to study electrical properties of a number of nanosystems- the diode action in metal particle-organic layers and charge storage in alkanethiolate bilayers. Tunneling spectroscopy using STM has also been used to study electrical properties of conducting molecules, carbon nanotubes, Se and Te nanowires.

Pulsed laser deposition has been employed to produce metal and metal oxide nanostructures on substrates. Metal droplets from laser ablation impinging on flat substrates are shown to form ring-like structures. Such nanostructures result from a surface tension driven hydraulic jump of the spreading liquid. The method is very general and can produce femto-litre cups of any metal. The cups may have wide applications ranging from nanoscale synthetic chemistry to single cell biology. The PLD method is also being used to produce ZnO pyramids and other oxide nanostructures whose properties as nanosensors have been measured.

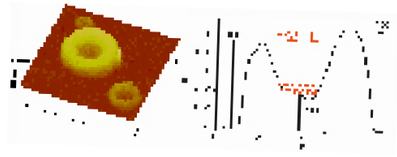

Figure 3: AFM image of femtolitre Ag cups

Experimental charge density: of molecules in crystals are derived using low temperature, high resolution X-ray diffraction. The method employs multipolar refinement on diffraction data to yield valuable information on the bonding aspects, conjugation as well as intermolecular interactions. With this method, one can obtain molecular properties such as in-situ electrical dopole moment. In our group, many molecular systems have been investigated using the charge density approach. These include- polymorphic forms, organic NLO crystals, hydrogen bonded systems, aromatic ring systems and conjugated conducting molecules.

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Organic Electronics and Optoelectronics Device-Physics and Photophysics, Solution Processing and Patterning, Soft Matter and Hard Properties, Biophotonics

My group has been actively involved in studying electronic, optical and optoelectronic phenomena and exploring device structures in synthetic polymeric/organic/nano and biomolecular based systems over the last decade. Our current research activities include (i) photophysical studies of conjugated polymers (ii) device fabrication such as field effect transistors; light emitting diodes; photovoltaics/detectors consisting of active organic media (iii) Photo-induced charge transport processes in membrane-protein/smart electrode systems. Polymers/organics are now attractive materials for active components in opto-electronic devices, flat-panel displays, solar cells and sensors besides being model systems for studying correlated phenomena in low-dimensional systems. We stress on implementation of ideas which are original and insightful with direct potential utility in technological applications. Some of our noteworthy contributions to this research community and inventions are: *(a) Polymer –Photo Field Effect Transistors (b) Tunable Resonant Microcavity Photodiode based on organic semiconductors (c) Synergestic Processes at bacteriorhodopsin-conducting polymer interface (d) flexible polymer based light-position sensor spanning sub-micron to few millimeter range.*

KS Narayan has obtained his PhD (1991) in Condensed Matter Physics from The Ohio State University. He was a scientist at the Polymer Branch, Wright Patterson Air Force Base before joining JNCASR in 1994.

Figure 1 and 2: Lab Facilities

We have been actively involved in studying electronic, optical, and magnetic phenomena and exploring device structures in synthetic polymeric/organic/ nanoparticle and biomolecular based systems. The lab's primary interest and activities focuses around understanding the electronic and optical processes in synthetic conjugated polymeric systems. The understanding of these properties has a direct bearing to the various phenomena in these systems from the perspective of interesting devices. In terms of the technologcal impact, the device development in this field addresses a wide spectrum ranging from "cheap plastic sensors and electronics" to high end applications involving lasers, waveguides and single molecule transistors.

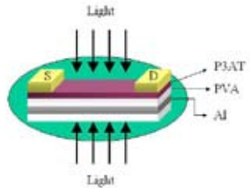

Figure 3: OLEDs and detectors on flexible substrate

Our research essentially covers the study of the basic physics and materials science of these systems as well as probing new phenomena and device development and the research activities covers the following areas: (i) Photophysical studies of conjugated polymers (PPV and Polythiophene based systems) (ii) Study of Photoinduced charge generation and relaxation process in a field effect transistor geometry (iii) Development of a quasi-near field current contrast microscopy technique to examine various interfaces (metal-semiconductor), mixed phases (polymer blends) and extract length scales governing electronic properties (iv) Device fabrication such as field effect transistors; light emitting diodes; photovoltaic cells; light detectors consisting of active organic media.

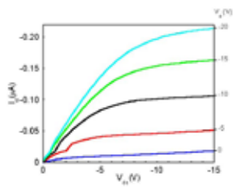

Figure 4: Polymer PhotoFET

The device inventions from our laboratory are now widely cited in the organic-electronics community and in particular: Optical control of polymer field effect transistors (Applied Physics Letters 79, 1891, 2001, and write-ups featured in MRS Bulletin and Nature India), a polymer based resonant microcavity ultrafast photodetectors, (Vol. 80, 1213, Appl. Phys. Lett 2002), flexible position sensor spanning 5 mm to 5 mm (Appl. Phys. Lett. 2004 and News article featured in Laser Focus World Feb. 2005).

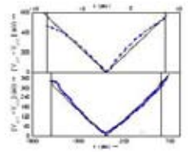

Figure 5: Response of a position sensitive detector of 10-um diameter gaussian beam spot over (a) 25um gap (b) 1.2mm gap

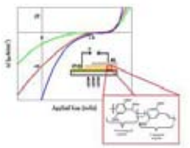

Figure 6: Bulk Heterostructure Solar Cell

Other allied research areas include investigation of membrane protein photoelectric signals immobilized and oriented on conducting polymer substrate/electrode. It was realized in our laboratory that spectral tuning of photoelectric signals in a conducting polymer-bacteriorhodopsin device could be achieved using a voltage control . (Appl. Phys. Lett. 83, 3614, 2003) and (Biosensor and Bioelectronics Journal 2004).

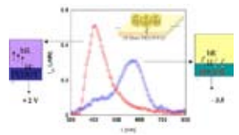

Figure 7: Voltage controlled spectral tuning of photoelectrical signals, observed in oriented bacteriohodopsin film deposited on a conducting polymer layer

Other major activities are studies on Single Wall Nanotube FET in different environmental and optical conditions, electric field controlled patterning of elastomeric surfaces, and micro-printing conducting inks.

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Synthesis and Study of Novel Functional Oxides: Superconductivity, Magnetism and Ferroelectricity

Transition metal oxides are very interesting because they exhibit a wide range of properties such as high temperature superconductivity, colossal magnetoresistance, ferroelectricity and magnetism. In these materials, the relatively narrow band width of d electrons close to the Fermi level leading to a high density of states and electron-electron interactions or correlations which play an important role in magnetic and transport properties. We are interested in synthesizing new materials with various transition metals and characterize their structural and physical properties and explore the structure property relationship so that a material with desired properties may be designed. Our main interest is the preparation of oxides exhibiting metal-insulator transition, superconductivity, magnetism and ferroelectricity. The materials exhibiting a simultaneous ferromagnetism and ferroelectricity and coupling between them are of particular interest.

Another area of our research interest is thin films of functional materials, particularly the multilayers or superlattice of various transition metal oxides. These superlattices exhibit fascinating properties including superconductivity, mangetoresistance and multiferroics although the individual layers itself do not exhibit such properties. Presently, our focus has been on the fabrication of superlattices of $(Cu,C)Ba_2CuO_{4+y}$ and $CaCuO_2$ layers that is equivalent to $(Cu,C)Ba_2Ca_{n-1}Cu_nO_{2n+2+y}$ system having highest T_c without containing a toxic element.

A Sundaresan has obtained his PhD (1994) in Chemistry from IIT Bombay. He was a post-doctoral fellow at Laboratoire Crystallography, Caen, Invited Researcher, LEPES, CNRS, Grenoble, France and Research, JST-CREST, AIST Tsukuba, Japan before joining JNCASR in 2004.

Thin Films: Atomic Engineering Of High T_c Cuprate Superconductors

All high T_c copper oxides have CuO_2 layers in common. In these materials, T_c increases with number (n) of CuO_2 layers in a unit cell and reaches a maximum around n=3. Beyond which the T_c decreases, which may be due to inhomogeneity in the distribution of charge carriers in different CuO_2 layers. Our work is focused on the preparation of such materials ($n \geq 3$) with homogeneous carrier distribution by layer-by-layer deposition of infinite layer copper oxides by RF magnetron sputtering. This is expected to increase the T_c beyond the present value of 132 K.

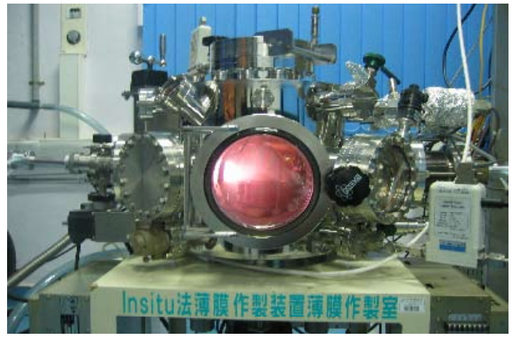


Figure 1: Computer controlled multi-target RF magnetron sputtering system for the fabrication of multilayers and superlattices

Multiferroics: Ferroelectric and Ferromagnetic

Multiferroic has been named for materials in which two or all ferroic properties, ferroelectric, ferromagnetic, antiferromagnetic and ferroelastic coexist in the same material to produce new phenomena that are more than just the sum of the individual properties. Multiferroics exhibiting both ferromagnetic and ferroelectric properties are interesting because their coupling lead to electric field switchable magnetization or vice versa. The ability to couple to either the electric or the magnetic polarization allows an additional degree of freedom in device design. Other applications include multiple state memory elements, in which data is stored both in the electric and magnetic polarizations, or a novel memory media, which might allow the writing of a ferroelectric data bit and the reading of the magnetic field generated by association. Magnetism and ferroelectricity are involved with local spins and off-center structural distortions, respectively.

Most common pervoskite oxide (ABO_3) ferroelectric materials have a formal charge corresponding to the d^0 electron configuration on the B cation. The transition metal d electrons, which are essential for magnetism, reduce the tendency for off-center ferroelectric distortion. So the choice of single phase materials exhibiting coexistence of strong ferromagnetism and ferroelectricity is limited. Consequently, an additional electronic or structural driving force must be present for ferromagnetism and ferroelectricity to occur simultaneously. Some pervoskite materials are known to have ferroelectric and magnetic (mostly of the antiferromagnetic type) ordering. A classical way to obtain a magnetic ferroelectric is to locate Bi^{3+} or Pb^{2+} ions and a magnetic transition metal ion on A and B sites of a ABO_3 pervoskite structure. $BiMnO_3$ is the only ferromagnetic (T_{CM} = 110K) ferroelectric (T_{CE} = 760K) among Bi, Pd-3d transition metal pervoskites. $BiFeO_3$ is an antiferromagnetic (T_N = 643K) ferroelectric (T_C = 1103K).

Our focus is the preparation and study of new materials containing bismuth and magnetic transition metal oxides. For example, we have prepared several oxides which have γ-Bi_2O_3 structure rather than perovskite structure. However, they exhibit multiferroic properties. For example, the X-ray diffraction pattern of $Bi_{26-x}(Co,Fe)_xO_{40}$ system after final Rietveld refinement is shown in Fig. 2. Small amount of impurity phases, Fe_2O_3 and Co_3O_4 were observed and included in the structural refinement.

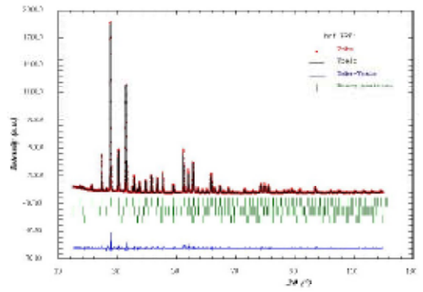


Figure 2: Observed, calculated and difference powder x-ray diffraction pattern of $Bi_{26-x}(Co,Fe)_xO_{40-\delta}$ system after final Rietveld refinement. Vertical tick marks are the symmetry allowed reflections for the main and two impurity phases

Key Publications

1) Eto T, Sundaresan A, Honda F, Oomi G. Valence instability of cerium under pressure in Kondo like perovskite $La_{0.1}Ce_{0.4}Sr_{0.5}MnO_3$, *Phys. Rev. B,* 72, 060402(R), 2005.

2) Sundaresan A, Asada H, Kito H, Iyo A, Tanaka Y, Kusunoki M, Oshima S. Effect of surface needles on microwave surface resistance of Tl(Ba,Sr)2Ca2Cu3Oy superconductor thin films on LSAT substrate. *Supercond. Sci. Technol,* 17, 350, 2004.

3) Vengadesh Kumara Mangalam R, and Sundaresan A. Structural, magnetic and magnetotransport properties of $La_{0.7-x}Ce_xBa_{0.3}MnO_3$ (x=0.0–0.4), *J. Chem. Sci.,* 118, 99 (2006).

PhD Students

R Vengadesh Kumaramangalam, Shipra

Education Technology Unit

Members
V.Krishnan
Indumati Rao
Jatinder Kaur
Sanjay Rao

Education technology unit was established in 1996. The focus of the unit is to develop learning and teaching materials, develop and produce multimedia CD-ROM packages in various science subjects in different languages for use by teachers and students to improve science education in schools/colleges. In addition the unit is involved in science popularization programs, teacher training workshops in science education and in the development of small scale kits to conduct simple, interesting science experiments with a view to modernize science teaching at various levels of education.

The end-users of the multimedia CD-ROM packages were identified as students in high schools and colleges. It was decided that the package would not be strictly based on any particular school curriculum. It would be supplementary material with the main objective of creating interest in various disciplines, with emphasis on experimental science. The CD-ROM's and books developed and produced at ETU are:
Understanding Chemistry by Prof. CNR Rao (Also available in Kannada and Hindi)
Learning Science by Prof. CNR Rao and Mrs. Indumati Rao
Vignyana Kaliyona (4 CD-ROM's and books in Kannada)
Bhugola Parichaya (A CD-ROM in Kannada on geography)
Our Earth in the Sky (A CD-ROM on astronomy)

The unit has produced CD-ROM packages and books in English and other vernacular Indian languages for the Directorate of State Research and Training (DSERT), Government of Karnataka, Department of Science and Technology (DST), Government of India. Thousand copies each of the four volumes of `Vignayana Kaliyona' as both CD-ROM's and books were completed and handed over to DSERT for distribution in schools all over Karnataka.

The unit has bought out four parts of **Learning Science** books in English. The four volumes were formatted with the graphics, layout designed and the print-ready copies completed at ETU. The first part consists of three main topics—**Universe, Solar System and Earth,** the second part titled **The world of physics and energy**: **Learning physical principles** has two main topics. The third part consists of three topics—**The world of chemistry**: **Of molecules and materials, Air around us and All about water.** The fourth in the series deals with **Biology and life**.

In the area of science popularization, `*Celebration of Chemistry'* and `*Learning Science'* programs were conducted at different places in the country. The unit has the distinction of Prof. CNR Rao offering lectures addressed to large number of young students in different cities to promote and instill curiosity in science subjects. The unit has made presentations at various international fora using excerpts from the multimedia CD-ROM's Learning Science and Understanding Chemistry.

The unit has conducted several workshops for teachers and students to provide hands-on training of performing experiments using the small scale chemistry kit developed by the unit.

The unit will be actively involved in the science popularization programs and the teacher training programs as these programs have proved to be very popular amongst teachers and students. As part of the global curriculum, the unit has plans to develop Mathematics, Geography and other subjects as multimedia packages. It is proposed to put some of the topics in the modules of The world of physics: Learning physical principles and The world of chemistry: Of molecules and materials from the CD-ROM Learning Science on the web. It is also planned to create a Geography web site.

Engineering Mechanics Unit

Chairman
Roddam Narasimha

Senior Associate
SM Deshpande

Faculty
Meheboob Alam
Rama Govindarajan
KR Sreenivas
Ganesh Subramanian

Distinguished Fellows
M Gaster
A Roshko
KR Sreenivasan

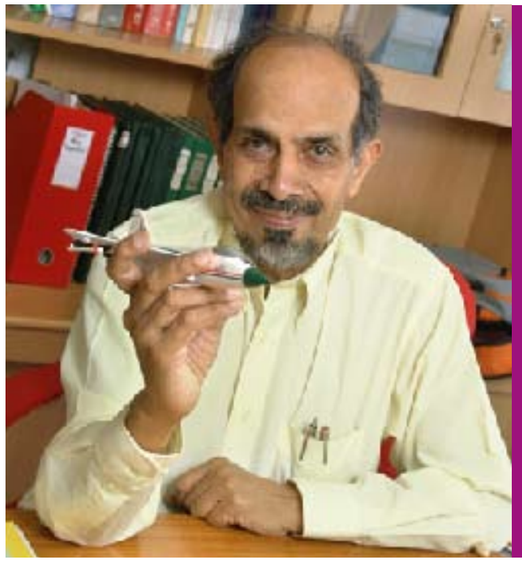
The Engineering Mechanics Unit pursues research on a variety of topics where fluid and solid mechanics and heat transfer play a critical role in providing insight into various phenomena. This insight is essential for enhancing predictive skills and also for solving fundamental problems in both theoretical and applied mechanics. From this point of view, work done in the Unit ranges from areas of direct interest in a variety of technological applications to phenomena encountered in nature.

The Unit's technologically oriented studies primarily focus on aerospace and chemical applications. For example, studies on flow stability and transitions between laminar and turbulent states in a wide variety of situations have direct relevance to aerospace and chemical technologies. New insights into the action of polymers on turbulent flows—as well as the nature of transition on swept wings—have been obtained from such work. Another area of special interest is computational fluid dynamics, chiefly in problems connected with aerospace technology. Research on the dynamics of granular media explores fundamental scientific problems and also have direct applications in chemical and other technologies.

Biological problems and natural phenomena—from insect flight to the fluid dynamics of clouds—are being investigated employing both theoretical and experimental methods. Using wavelets as a tool, faculty members in the Unit have analysed the temporal structure of monsoon rainfall, revealing a possible link to solar activity at vastly higher levels of statistical significance than had been previously possible. Another area of research, chiefly of geophysical interest, is double diffusive convection, which is being investigated through experiments as well as numerical simulations. Research on insect flight—which involves both experiments in a wind tunnel using particle image velocimetry techniques and also computer simulations with discrete vortices—is shedding light on the underlying mechanisms of flight. This work is also relevant to the design of micro air vehicles, which is now an area of considerable technological interest. Additionally, since clouds exhibit unusual characteristics in entrainment of ambient air, current research in the Unit explores this interesting phenomenon.

The Unit's faculty members are engaged in extensive collaborations with scientists located elsewhere in India and abroad. Examples of recent collaborations within India have been with the National Aerospace Laboratories (NAL) and IISc Bangalore; international collaborations include those with Queen Mary and Westfield College (UK), QinetiQ (UK), Boeing Research Centre (USA), the Weizmann Institute (Israel) and the University of Stuttgart (Germany). In a collaborative project with scientists at the NAL, it has been shown that a Navier-Stokes code properly optimized for a parallel computer (the *Flosolver* built at NAL) has led to super linear speed-up of 11 on 8 processors.

The EMU's on-site facilities support the faculty members' broad experimental and theoretical research interests. Experimental facilities include a low-speed wind tunnel, which has a transparent test section of 2 metre length and 0.6 metre x 0.6 metre cross-section. This tunnel can be operated with uniform velocities from 1m/s up to 10 m/s. An Nd-Yag laser (10 Hz, 120 mJ/pulse) is part of a Particle Image Velocimeter that yields instantaneous velocities over a plane. Computing facilities of the Unit include a computer centre with several PCs, an eight-node Flo-solver Mk6 system, and a six-node Xeon processor cluster.



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Aerospace and Atmospheric Fluid Mechanics

My major interests have been in fluid dynamical problems associated with aerospace technology and atmospheric sciences. A connecting link between the two is that turbulent fluid flow plays an important role in both fields.

In aerospace problems, both fully turbulent flow and the transition to and from that state are at one and the same time of both practical and fundamental scientific interest. Turbulence has remained 'the chief outstanding difficulty of the subject' for about a hundred years now! Transition from laminar to turbulent flow, as well as the less widely studied reverse transition from turbulent to laminar, have been a major area of my research. The ubiquity of these problems was dramatically revealed recently when we showed (in collaborative work with NAL scientists, sponsored by Boeing) that the swept wings characteristic of modern transport aircraft can sometimes experience several transition cycles within the immediate neighbourhood of the leading edge.

In the atmosphere turbulent flow in the tropics has a strongly convective character, and the laws governing it at low winds are of great interest in monsoon predictions. There is the intriguing question of the possible connections between monsoon rainfall and solar processes. There is also the basic question of the mix of order and disorder in turbulent flows—in technology as in nature, and of the possibility of teasing out the order from chaos using wavelet techniques.Fluid flows remain fascinating because of their diversity, and of their fundamental scientific interest as well as their technological applications. We intend to pursue both in my group.

R Narasimha received his PhD in Aeronautics and Physics from the California Institute of Technology in 1961. He is currently Chairman of the Engineering Mechanics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.

Wavelet Analysis of Monsoon Rainfall
Continuing previous research on the use of wavelets in the analysis of the temporal structure of Indian monsoon rainfall, we have now made detailed studies with wavelet maps. One earlier discovery was that the maps show a distinct quasi-cyclic behaviour around the 11-12 year period band, immediately suggesting an association with sun spots. As the subject has been controversial, it was decided to investigate the matter in detail. We found it convenient to compare the two intervals 1878-1913 and 1913-1964—each of which comprises three complete solar cycles—where the former has the lowest and the latter the highest amplitudes in the period since 1870. (This is the range over which reliable data are available for rainfall—see Figure 1). In all the five homogeneous rainfall zones of the country, we have found that rainfall is higher when solar activity is higher. If we examine the 8-16 year band, the difference between the two intervals is significant at confidence levels exceeding 99.99%. This provides the strongest known evidence for the association between Indian monsoon rainfall and solar activity. Further studies on the problem have now been made using wavelet cross spectra, providing further support for the above conclusion.
[R Narasimha, Subarna Bhattacharyya]

Convective Boundary Layers
Our work on the fluxes in convective boundary layers has continued, and an analysis of data acquired at Jodhpur through the field experiment MONTBLEX-90 has been completed. The trends revealed by the Jodhpur data are confirmed by a reanalysis of the experiments carried out during the BLX-83 project in the United States. This reanalysis shows that the US data are consistent with the new scaling arguments that we have proposed.
[R Narasimha, Kusuma Rao, HV Raju, ISRO]

Near-Surface Temperature
We have devised a simple theoretical model to describe and explain the dynamics of the evolution of the 'Ramdas' layer (a notable feature of temperature distributions on bare soil on a calm clear night.) The model provides closed-form solutions that qualitatively reproduce all major features of the observed phenomena.
[R Narasimha; AS Vasudeva Murthy, TIFR]

Non-Parallel Flows
Earlier work on the stability of nonparallel flows had shown that it is possible to derive an ordinary differential equation governing shear flow instability at the lowest order in the Reynolds number—including the effect of flow nonparallelism. However, it is in principle not possible to determine the dependence of the disturbance amplitude along the flow solely from such an ordinary differential

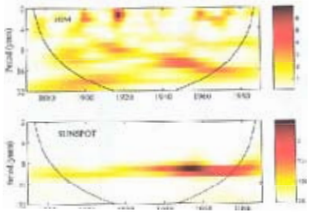

Figure 1: Wavelet maps of the Homogeneous Indian Monsoon rainfall index (top) and sunspot number (bottom). The latter shows strong periodicity around a 12-year period, and high activity after 1940. This is reflected in the rainfall map as well—but along with strong activity at other periods and times.

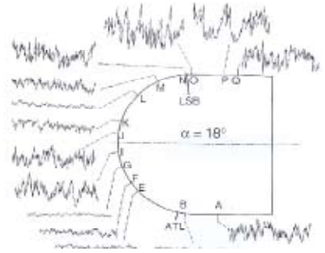

Figure 2: The leading edge of a swept wing, of the kind that is common on a modern passenger/transport aircraft. Under conditions characteristic of landing and take-off, experiments carried out on a Boeing-sponsored project (in collaboration with NAL scientists Dr. PR Viswanath and Dr. R Mukund) suggest the occurrence of several 'transition cycles' (as we call them); that is, flow goes from laminar to turbulent and back—as many as six such transitions are seen in the above diagram. The traces here represent wall shear stress.

equation. We have now shown that the evolution of the disturbance amplitude along the flow can be accurately computed without *solving* the primitive partial differential equation but making use of our knowledge of the partial differential *operator.* Comparison with direct Navier-Stokes solutions shows excellent agreement with the present results. We have now formulated an extension of this approach to the problem of computing amplitude growth to the case of three-dimensional flows, in particular the swept wings that are so important in all high speed aircraft design.
[R Govindarajan, R Narasimha]

Transition 'Cycles'
In a project sponsored by Boeing Commercial Airplane Co. and carried out in collaboration with Dr PR Viswanath and Dr R Mukund at the National Aerospace Laboratories, analysis of data obtained on a swept wing has revealed some surprising features in the flow. It has been found that, at fairly high angles of attack, the flow near the leading edge can go from laminar to turbulent and back to laminar several times. We have called this phenomenon 'transition cycles'. We have found that, in one case, three complete cycles (involving six transitions) can be detected. Signs of the tendency towards such 'transition cycles' have been found even at lower angles of attack (Figure 2). [R Narasimha; PR Viswanath, R Mukund, NAL]

History Of Science
We are also continuing certain studies related to the history of science in India and on technology issues in security. An essay on Ludwig Prandtl, on the occasion of the centenary of the publication of his boundary layer theory, has appeared in *Nature*.

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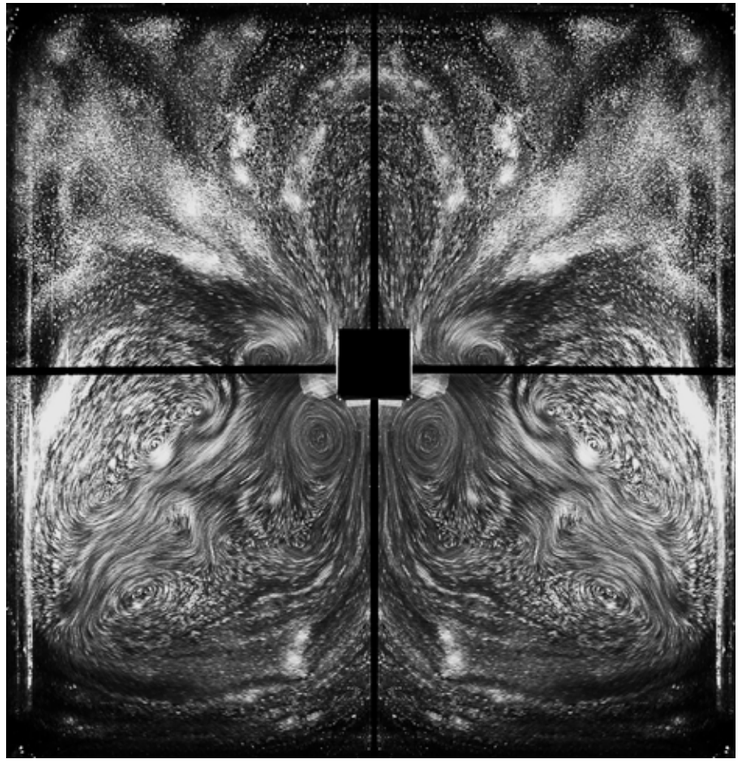
Computational Fluid Dynamics

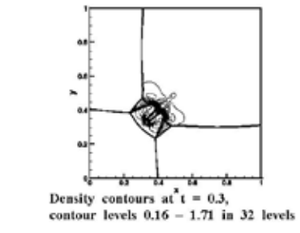
Our research primarily focuses on aerodynamics, aero-elasticity, computational fluid dynamics, and strongly rotating flows.

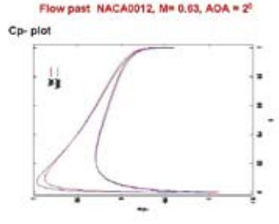
We are especially interested in the development of novel numerical methods in computational fluid dynamics (CFD). For example, we have studied kinetic methods and kinetic flux vector splitting (KFVS), as well as least squares KFVS, KFVS on moving grids (KFMG), and grid-free methods. We are also currently researching a modified Courant-Isaacson–Rees (MCIR) method, rotationally invariant LSKUM, and the use of entropy variables in LSKUM. Development of methods of point generation, adaptation based on D^2–distance, and connectivity generation are also of interest to our group.

We have also studied applications of various methods to problems in aerospace engineering, such as: flow past multi element airfoils used in compressors and turbines, rotating viscous flow, unsteady aerodynamics, and aerodynamic shape optimization through evolutionary and classical methods. Computational work has been carried out on the flow around various flight vehicles, the flow through multi passage multistage compressors and turbines, and on viscous flow within a grid-free framework. Studies on computational aeroelasticity are continuing in addition to our predictive studies on transonic flutter and research on fast methods for flutter prediction.

SM Deshpande received his PhD from IISc and was the ISRO sponsored Prof Satish Dhawan Chair from 2000–2003. He has received numerous awards—such as the Biren Roy Trust Award of the Aeronautical Society of India—for his contributions.







Key Publications

1) Krishnamurthy R, Sarma BS, Deshpande SM. Kinetic scheme for compuational aeroelastic analysis of 2-D airfoils in transonic flows. In *Proceedings of 34th AIAA Fluid Dynamics,* Portland, Oregon, USA, AIAA 2004–2236, 2004.

2) Deshpande SM, Kinetic meshless method in computational fluid dynamics. In *Proceedings of Symposium on Advances in Fluid Mechanics,* JNCASR, 13–33, 2003.

3) Krishnamurthy R, Sarma BS, Deshpande SM. 3-D KFMG based Euler solver for unsteady flows around oscillating geometries. 2nd *ICCFD Journal,* Sydney, 2002.

4) Deshpande SM, Anandanarayanan, Praveen C, Ramesh V. Theory and applications of 3-D LSKUM bases on entropy variables. *International Journal for Numerical Methods in Fluids,* 40, 47–62, 2002.

5) Deshpande SM, A second order accurate kinetic theory based method for Inviscid compressible flows. *NASA Technical Paper,* 2613, 1986.

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Complex Fluids: From 'Microscopic' to 'Hierarchical' Modelling

Microstructures play a prominent role in the dynamics of complex fluids that are rheologically complex; this is in contrast to simple fluids whose rheology is of order-one. Common examples of complex fluids include: polymers (e.g. DNA), suspensions (e.g. milk, mayonnaise, paints, and slurries), and granular materials (e.g. sand and coal). Granular materials are important in numerous chemical processing and pharmaceutical industries, as well as in geophysical contexts—such as avalanches, volcanic eruptions, and sand dunes. The importance of understanding the behaviour of these granular materials can be ascertained from one simple fact: the granular processing accounts for as much as $60 billion, which equals approximately 40% of the worldwide investment in the chemical industry.

In my group, we carry out microscopic/particle-level simulations, formulate rheological models and analyse continuum models of complex fluids using the tools of nonlinear dynamics and numerical methods, with a goal to come out with better mathematical models.

Meheboob Alam received a PhD (1998) from the Indian Institute of Science (Bangalore), and is the recipient of the Alexander von Humboldt Fellowship of Germany. He joined JNCASR in 2003.

Non-Newtonian rheology of granular matter

We have started a concerted effort to probe the non-Newtonian rheology of granular matter using particle-level simulations and kinetic theory. We have recently outlined a rheological model for binary mixtures that takes into account the non-equipartition of granular energy (as found in reference 3), in addition to a model for normal stress differences. Currently, we are probing the dense-phase rheology of granular matter, focusing on the normal stress behavior, the force-chain formation, and the fluid-solid transition (shown in Figure 1).

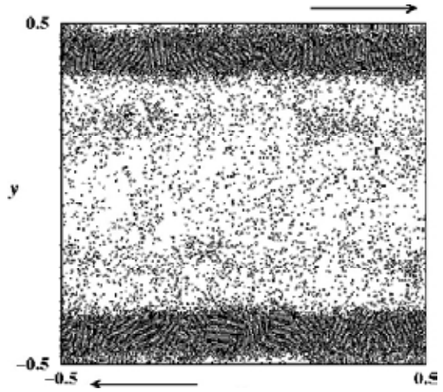

Figure 1: Phase separation and the coexistence of fluid and solid phases in a sheared granular material. For details, see Ref. 1

Instabilities, patterns and granulence in complex fluids

Instability-induced patterns and turbulence have been extensively studied in classical fluid mechanics. In rapid granular flows and suspensions, many interesting patterns in the form of roll-waves, Kelvin-Helmholtz instability, fingering instability and vortices have recently been reported. We are trying to understand the underlying mechanism of pattern formation and granulence in complex fluids.

The focus of our work is to use accurate (non-Newtonian) rheological models and molecular dynamics simulations to predict the onset of instabilities. Moreover, this research will also unveil the related nonlinear patterns in dry granular flows and suspensions in various simple geometries (e.g. channels and pipes). One goal is to devise control strategies to manipulate microstructure formation in complex fluids according to process requirements.

In collaboration with the PhD student Mr M Malik and Prof J Dey of IISc, we are trying to understand the non-modal temporal and spatial stability characteristics of compressible fluids. My long-term goal is to understand the elusive connection of patterns in rapid granular flows with those in compressible fluids.

Segregation and mixing of granular matter

In most practical applications, it is required to maintain a homogeneous mixture of particles during processing, with segregation being the 'unwanted' phenomenon. For example, to make tablets, one has to homogeneously mix the active and inactive agents that are in powder form.

One project deals with the well-known size-segregation phenomenon in vibrated granular mixtures where the larger particles rise to the top of the container. This is known as the Brazil-nut phenomenon and is shown in Figure 2. The reverse-Brazil-nut phenomenon (where the larger particles sink to the bottom) can also occur under certain conditions. We have recently proposed a `unified' model in reference 2 that captures many features of the segregation process, including reverse buoyancy and nonmonotonic ascension dynamics of Brazil nuts.

In another project, we are trying to explain particle-segregation via the stability analyses of continuum equations of polydisperse mixtures.

Fluid mechanics at micro-scales

For fluid flows at micro- and nano-scales, it is well-known that the no-slip boundary condition does not hold and that the surface forces play a prominent role. Another important issue is the lack of scale separation that invalidates the standard continuum models. Our current work on this topic is to understand these issues by using theory and multiscale simulations.

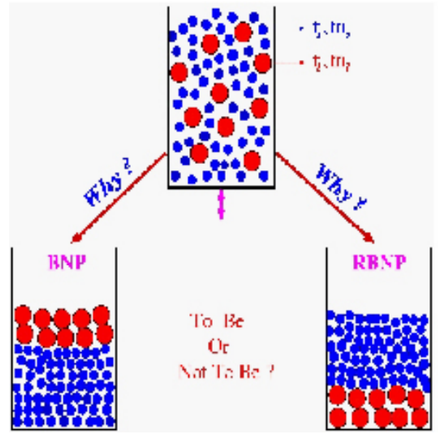

Figure 2: Segregation of granular mixtures under vertical vibration

Key Publications

1) Alam M et al. Ordering, universal unfolding and the role of gravity in granular Couette flow. *Journal of Fluid Mechanics,* 523, 277–306, 2005.

2) Trujilo L, Alam M, Herrmann H. Segregation in a fluidized binary granular mixture. *Europhysics Letters,* 64, 190–196, 2003.

3) Alam M, Luding S. Rheology of bidisperse granular mixtures via ED simulations. *Journal of Fluid Mechanics,* 476, 69–103, 2003.

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Flow Instabilities and Transition to Turbulence

One of the main areas of interest of this group is the transition from order to chaos, with high emphasis on the laminar-turbulent transition. We also study turbulent flows under some specific contexts, as described below.

Flow is either turbulent, laminar, or in a transitional state between the two. The fluid's flow state decides many things, such as how much energy is dissipated and how much mixing takes place. If you are an aircraft engineer designing a wing, you would want the air flow close to the wing surface to remain laminar as much as possible in order to save money on fuel. If you are a chemical engineer designing a reactor, you might want better mixing of various ingredients—and therefore desire a turbulent flow.

For Newtonian fluids in relatively simple geometries, laminar flow is well-studied both experimentally and theoretically. Although turbulent flow is highly researched, it is less understood as compared to laminar flow. We know a lot about the statistical characteristics of homogeneous isotropic turbulence, but not so much about the turbulence in shear flows that occurs all around us. What we understand the least is what makes a certain laminar flow become turbulent, and also what is the route for completing the transition. This process is usually very specific to a particular flow. For example, the route to turbulence over an aircraft wing is very different from that in the flow of water through a pipe.

Rama Govindarajan received a PhD (1995) in Aerospace Engineering from the Indian Institute of Science, Bangalore. She did post- doctoral research at the California Institute of Technology, and was at the National Aerospace Labs before joining JNCASR in 1998.

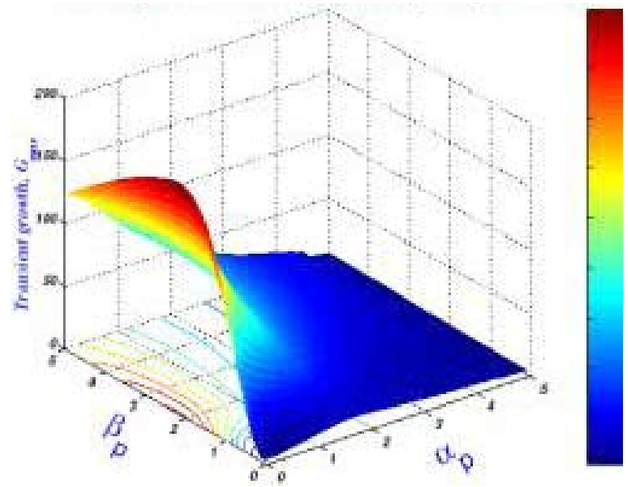

Figure 1: Growth of disturbance energy of viscosity-stratified channel flow

Viscosity-stratified flows
A stratification of viscosity has always been considered to be a good way of controlling transition to turbulence. In his PhD thesis, Sameen studied the physics of variations in viscosity and temperature on various routes to turbulence in a channel flow. He showed that the effect depended on the route and also on the type of stratification. In some cases, there is a large stabilization; in other cases, there is a large destabilization. In his work with Vijay, he showed that there is hardly any effect in other cases. This tells us to be cautious when using viscosity-stratification for flow control. A connection to drag reduction in dilute polymeric flows was made in collaboration with Itamar Procaccia and colleagues at the Weizmann Institute in Israel.

Transition in boundary layers
When a solid body moves through a fluid, a thin boundary layer of fluid close to its surface moves with it. This is due to viscosity and the no-slip boundary condition. The nature of the flow within the fluid determines drag, surface heating, and other important quantities. The early part of the process of transition to turbulence is now well understood: there are regular patterns of disturbance highs and lows in a laminar boundary layer unstable to secondary modes. In the late stages, however, there are turbulent "spots" which grow as they convect downstream to make the flow fully turbulent asymptotically. Previously, no connection had been made between the early and late stages. For his PhD thesis, however, Vinod has been able to show a direct relationship between the pattern of secondary instability and the space-time distribution of the birth of turbulent spots. Vinod is also studying the flow past a cylindrical body; he has found that the process of instability of the laminar flow here is very different from that over a flat-plate boundary layer.

Instability of spatially developing flows
This is another instance of a big effect due to a small change. The laminar flow through a pipe always is known to be stable to linear (small) perturbations. In his PhD work, Kirti shows that if the pipe is divergent as in a funnel, the flow is now unstable to linear disturbances. The transition process may become qualitatively different now. With Abhijeet Reddy, he is studying the unsteady flow through arteries.

Turbulent flows
In his Masters work, Pinaki is studying free shear layers in collaboration with R Narasimha, and trying to arrive at the dominant structures in turbulence from a stability perspective. Kaushik is studying density-stratified flows for his Masters' thesis to find out what happens to the dimensionality of turbulence.

Vortical flows
Srevatsan Muralidharan (who was a summer student in this group) has proved that a system of two co-rotating vortex pairs of opposite sign is chaotic for any finite separation between the pairs. With KR Sreenivas, we have shown that viscosity has the effect of reducing the entrainment of external fluid into a vortical system.

Small scale flows
Antina did some preliminary work on this for her MS thesis in collaboration with Srikanth Sastry. We wish to pursue research in this area further.

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Post-docs
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Fluid Mechanics and Heat Transfer

In our group we carry out research in the general area of heat transfer and fluid mechanics. Some of the specific research problems our group is currently working on are role of radiative heat transfer in the dynamics of nocturnal atmospheric boundary layers. This problem has relevance in the retrieval of ground-surface temperatures from satellite, and in climate modeling. The physics related to this problem may also have relevance in coronal temperature distribution in stars. Second research project is on the study of double diffusive finger-convection (DDF), which plays an important role in determining salt and heat flux transported in oceans, in metallurgy controlling microstructure formation in alloys, crystal growth, and in geology DDF may have a role in determining some of the basaltic rock structures. Third research problem is on the study of dynamics of free-shear flows with an aim to understand the physical mechanism that results in variation of entrainment coefficient in free-shear flows. The fourth research project is on the study of insect flight dynamics. Our research in this area is aimed towards developing engineering guidelines needed for an optimum design of small mechanical objects, which can use unsteady aerodynamics for their means of propulsion and lift generation. We employ flow visualization, velocity and temperature measurements in our research. Some of the facilities used for these purpose include high power, double pulsed Nd-Yag laser, low speed wind tunnel, mechanical models mimicking insect flight, Particle Image Velocimetry (PIV), hot-wire and thermocouple probes.

KR Sreenivas received his PhD from the Indian Institute of Science, Bangalore and was at University of Delaware, Newark, Delaware as a postdoctoral research fellow for two years.

Lifted Temperature Minimum (Ramdas Layer):

Mukund Vasudevan (Doctoral research student) and Punit Tiwari (MS Research student)

Measured vertical temperature profiles in the field (left) and time variation of radiative heat-source term in the heat equation derived from the vertical temperature profile. When the wind speed is below 0.5 m/s, it will represent only radation contribution.Lifted temperature minimum is an atmospheric phenomenon discovered in the 1930's by L.A. Ramdas in Pune, India. On calm and clear nights, the minimum in vertical temperature profile does not occur at the ground (as was generally believed) but is located a few decimeters above. The measured temperature profile is extremely stable even though the estimated Rayleigh number for the unstable Ramdas layer is about 10^5, much above the critical value for the onset of convection. In our research work we study various parameters those affect this phenomenon, role of radiative heat transfer in the nocturnal atmospheric boundary layer by doing field observation and laboratory experiments.

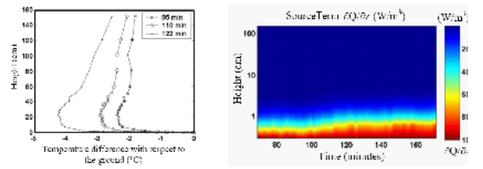


Figure 1: Measured vertical temperature profiles in the field (left) and time variation of radiative heat source term in the heat equation derived from the vertical temperature profile. When thw wind speed is below 0.5 m/s, it will represent only radiation contribution.

Double Diffusive Convection

OP Singh (Doctoral research student) and G Ganesh (Summer Research Fellow)

In double-diffusive convective (DDC) system two components having different molecular diffusivities (e.g. heat & salt) have opposite contributions to the vertical density distribution of the medium. We will have two types of DDC systems based on whether faster diffusing component has stabilizing effect (finger-type) or the slower diffusing component has stabilizing effect (diffusive-type). Research on this topic is relevant to oceanography, metallurgy, mantle-convection and other engineering applications. On set of convection in a double-diffusive system is due to the unequal diffusivities of two components. We use experiments and numerical simulations to study the effect of governing parameters like thermal and salinity Rayleigh numbers, Prandtl number and density stability ratio on the convection pattern and on the transport processes.

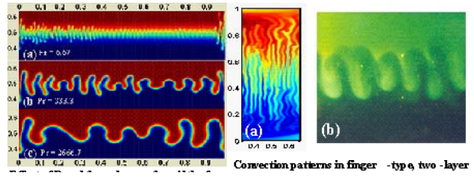


Figure 2: Effect of Prandtl number on the width of convection cells in the double diffusive finger system. Convection patterns in finger-type, two layer double-diffusive system (a) salinity field numerical simulation (b) fluorescent dye flow visualisation observed in an experiment.

Unsteady Aerodynamics of Insect Flight:

JV Shreyas (MS Research student)

With many years of research, principles of steady aerodynamics (2-D aerofoils and finite wings) applicable to a fixed wing aircraft are quite well understood. In contrast, the engineering principles needed for an optimum design of small mechanical objects, which can use unsteady aerodynamics for their means of propulsion and lift, have not yet been established. Emphasis of our research is to have a systematic and comprehensive study of the principles of unsteady aerodynamics that pertains to the fluid dynamical problem of flapping flight. The research will help in understanding the rationale for its use in nature and to obtain design-guidelines to exploit unsteady aerodynamics for making small flying devices. We study the flow filed using mechanical models mimicking insect flight.

Experimental and Numerical Study of Entrainment Process in Turbulent Free Shear Flows:

MS Manikandan (MS research student)

Turbulent free-shear flows spread in a direction normal to their primary-flow direction by incorporating irrotational ambient fluid into the turbulent jet-flow; this process is known as entrainment. In our research program, using both experimental and computational techniques we address the issue of variation in the rate of entrainment due to changes in ambient viscosity, axial pressure gradient and axial acceleration. Some of the important results on this problem are, (a) we have developed a model to explain the observed variation in entrainment coefficient (α) which highlight the stability of shear layer as the prime factor in controlling entrainment process, (b) we have demonstrated, using experiments and numerical simulation, how large scale eddy structures are responsible for entrainment, (c) how increasing shear layer stability can suppress the formation of large eddy structures and hence reduce entrainment and finally (d) need for looking at concentration width rather than velocity width while quantifying entrainment.

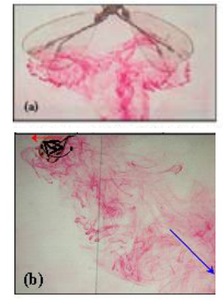


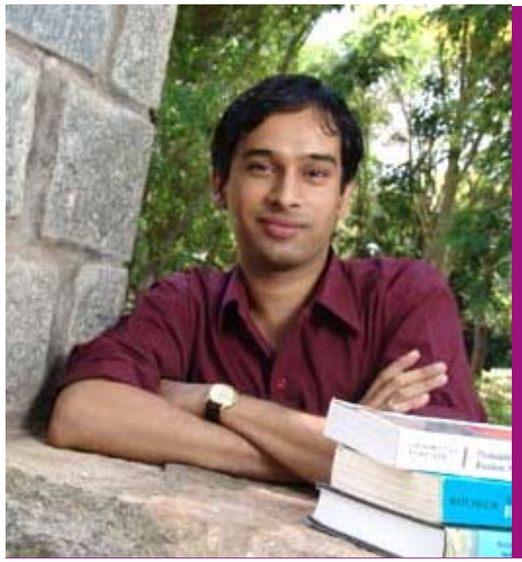
Figure 3: Flow visualisation pictures obtained usinf mechanical mimicking insect flight (a) Flow field during fling (opening of wings) (b) Flow field observed after many cycles of assymetry flapping.

MS (Engg) Students

MS Manikandan, A Rajapandian, JV Shreyas, Punit Tiwari

PhD Students

Mukund Vasudevan, Om Prakash Singh, S Subudhi



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Dynamics, Rheology and Stability of Complex Fluids

Our research endeavors relate to transport processes in complex fluids, e.g., suspensions, bubbly liquids, emulsions, and granular gases. Disperse phase interactions in such fluids lead to unique flow properties, and in many instances, are responsible for instabilities leading to pattern formation. We examine theoretically the microstructural dynamics in order to understand the macroscopic behavior. This ranges from investigating the response of a single disperse phase element such as a particle or a drop in an external flow to simulating the collective dynamics of large interacting systems.

One of our research goals is to clarify the role of inertial forces at the microstructural level—both the inertia of the disperse phase elements (particles in granular gases or aerosols) and, in particular, that of the continuous phase (processing of cellulose fibre suspensions in the paper industry). Much insight has been gained into the behavior of suspensions and emulsions in the inertialess limit. Our understanding of the flow behavior in presence of micro-scale inertia remains rudimentary, however. In the absence of inertia, the linearity of the governing equations and related symmetry considerations often lead to degenerate scenarios. New physics accompanying the inclusion of even a small amount of inertia leads to results that differ profoundly from the inertialess case.

Another continuing interest is the study of particle motion in non-Newtonian fluids. Many intriguing phenomena involving particle interactions in visco-elastic media have been identified and studied experimentally, but most of these remain unexplained. It is our aim to try and rigorously account for some of the experimental observations from a theoretical standpoint.

Ganesh Subramanian has a PhD (2002) in Chemical Engineering from the California Institute of Technology, USA. He was a post-doc at Cornell University, USA, before joining JNCASR in November 2005.

Inertial Pair-particle Trajectories: Application To Aerosol/hydrosol Coagulation And Suspension Rheology

Aerosol/colloid stability is vital to the shelf-life of paints, insecticides and pharmaceuticals. Stability is influenced by several factors including Brownian motion, gravity, colloidal forces, and hydrodynamic forces due to the ambient laminar or turbulent flow field. For sufficiently large particles, thermal effects are negligible, and the initial coagulation rate may be obtained via a trajectory analysis involving the relative motion of a pair of particles under hydrodynamic and colloidal forces. Previous analyses have, however, neglected the effect of particle inertia on pair-trajectories. The latter is expected to be important in gas-solid systems. We have shown that pair-particle trajectories in simple shear flow are dramatically altered for even a tiny amount of inertia. These modifications lead to a non-trivial microstructure and a non-Newtonian rheology. Simple shear is, however, a degenerate flow wherein extension and vorticity exactly balance; it is our aim to extend the analysis to a generic linear flow. One again expects inertial effects to be significant since inertialess pair-trajectories in planar linear flows with vorticity form structurally unstable configurations. The results will also relevant to turbulent coagulation of sub-Kolmogorov particles.

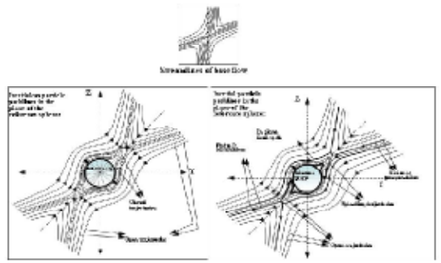


Figure 1: The figures show the anticipated modifications of inertial pair-particle trajectories in a hyperbolic linear flow

Orientation Dynamics Of Anisotropic Particles In Shearing Flows

The rheology of suspensions of anisotropic particles depends on the orientation distribution of the particulate phase. It is desirable to predict the orientation dynamics as a function of particle size, aspect ratio, concentration and flow parameters. In the dilute limit when inter-particle interactions may be neglected, the problem reduces to analyzing an isolated orientable particle in a shearing flow.

Without inertia, a non-Brownian axisymmetric particle in simple shear flow rotates in closed Jeffery orbits, leading to the peculiar scenario where fibre orientation for all times is determined by initial conditions. We have recently shown that inertia causes a slender fibre to eventually tumble in the flow-gradient plane, while causing a slightly prolate spheroid to spin about the vorticity axis. We intend to examine the orientation dynamics of an arbitrary spheroid, and thereby determine the critical aspect ratio at which the exchange of stability between the flow-gradient plane and the vorticity axis occurs.

Slender body theory may be used to study the effect of inertia on fibre motion beyond the perturbative limit. The analysis for small inertia shows that dominant changes in fibre trajectories occur close to the flow-aligned state. This enables a quasi-steady analytical investigation for a fibre nearly aligned with the flow axis. The work should serve as a bridge between the inertialess periodic motion of fibres and the boundary-layer flow past an aligned slender body for dominant inertia.

We aim to study inertial fibre motion in non-linear flows. For instance, an inertialess fibre in Poiseuille flow rotates in Jeffery orbits with no lateral drift despite the asymmetry of the flow about its centre. Inertia must lead to a transverse drift. An analysis of this transverse motion should help in the design of electrostatic precipitators, where the deposition rate depends on the nature of particle motion in boundary layers. Orientation dynamics of tri-axial ellipsoids in shearing flows is also of interest. Trajectories of a torque-free ellipsoid in free space are well documented in textbooks. In the other extreme, an inertialess ellipsoid in simple shear, one observes the onset of chaos for sufficiently slender axis ratios. The chaotic orientation behavior enables one to change the (strange) attractor domain by appropriate tuning of flow parameters, thereby obtaining a range of material properties. Our aim is to the study the effect of inertia in the latter problem, and its effect on the chaos that exists in the inertialess limit.

Inertial Dynamics Of Sedimenting Particle Clusters

Inertialess particle clusters sedimenting in a quiescent fluid have been studied in detail, their behavior being akin to drops with the same effective density. However, neglect of inertial forces imposes a severe restriction on the cluster size. Using a scaling analysis, we have delineated the regimes of cluster evolution as a function of the cluster volume fraction and the Reynolds number (*Re*).

A numerical study of cluster evolution would help verify the postulated regimes. The intended kinematic simulation will use a simplified representation of inertial interactions based on the single-particle velocity field. This should yield valuable insights into what is otherwise an intractable problem owing to the non-linearity of the governing equations. Applications include gravity currents, pollutants dispersion, and explosive ejecta.

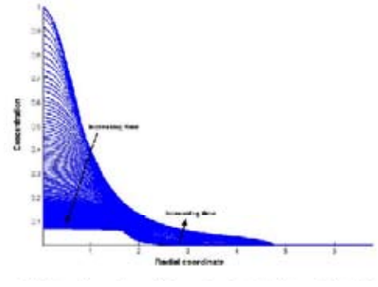


Figure 2: The figures show the particle number density field in a self-similarly expanding planar cluster as a function of time

We are also pursuing the following projects:

1) Particle-pair motion in visco-elastic fluids–sedimentation and shear
2) Finite *Re* velocity field around a sphere in a linear flow—rheological implications

Evolutionary and Organismal Biology Unit

Faculty
MK Chandrashekaran
Amitabh Joshi
Vijay Kumar Sharma

Distinguished Fellow
Gerhard Neuweiler

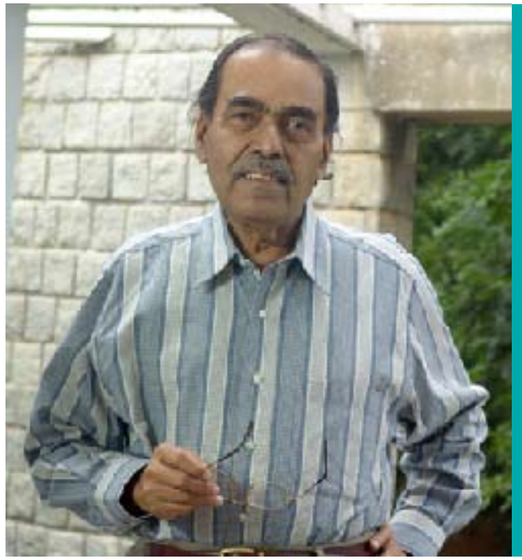
Biological systems are organized in an hierarchical manner structurally, and can be studied at levels ranging from molecules to ecosystems. Decades of narrowly focussed studies at one or the other level of structural complexity have greatly enhanced the body of information we possess about biological systems, leading to a state exemplified by T S Eliot's lament: "where is the knowledge we have lost in information?" Consequently, biology today is entering an integrative phase in which we are attempting to synthesize vast amounts of information into a holistic understanding of how living systems function and evolve.

Although biological systems are hierarchical in terms of structure, functionality in biological systems is typically integrated across scales of structural complexity. Functionality in biological systems, moreover, needs to be interpreted and understood in a meaningful natural context. In the vast majority of cases, the principal structural level of complexity which is also a functionally integrated entity is the multicellular organism, and it is also the organism that is most often the primary unit upon which natural selection acts to shape the functionality of organisms over generations. Biological questions regarding the fundamental processes of life—such as metabolism, physiology, behaviour and evolution—are, consequently, best posed in the context of an organism embedded in its ecology. Indeed, biological understanding today is increasingly an effort to understand the functioning of organisms in the context of their ecology i.e. their habitat, their way of life, and the other organisms of their own and different species with which they interact.

In Organismal Biology, the organism is the entity around which (a) questions regarding functionality in biological systems are framed, and (b) information gleaned from studies at various structural levels of biological complexity is welded together in an attempt to answer such questions. In a sense, the term ''Organismal Biology" is overkill: by and large, only organisms have a biology. Molecules do not have a biology any more than mathematical models do. Nevertheless, understanding the structure and dynamics of molecules, and of mathematical models, can be very useful in understanding the biology of organisms. Indeed, in its quest to understand functionality in living systems, Organismal Biology uses tools, techniques and information from a variety of disciplines, including molecular genetics, evolutionary genetics, biochemistry, physiology, neurobiology, behaviour, ecology, computation, physics, statistics and mathematics.

Our Unit is the principal centre in the country for research and training in the following broad areas: (a) **Chronobiology**: Studies of biological rhythms, especially biological clocks, (b) **Evolutionary Genetics**: Studies of how selection and genetics interact to shape life-histories and evolutionary trajectories, and (c) **Population Ecology**: Studies to understand how life-histories and factors such as migration interact to produce patterns of dynamical behaviour in populations and metapopulations.

We do mostly empirical research, using a combination of experimental tools from evolutionary quantitative genetics, molecular genetics, neurobiology, developmental biology, animal behaviour, and population biology. We also conduct theoretical research, largely through computer simulations of mathematical models of biological processes. Our Unit is well equipped for studies using a range of experimental and computational tools, with two labs for routine handling of large numbers of *Drosophila* populations, two wet labs for experiments in physiology, biochemistry, molecular biology, and immunocytochemistry, and three separate sets of Chronocubicles, for maintaining *Drosophila,* ants and mice under controlled light conditions, and monitoring various rhythms in these organisms. With over 1000 channels, our activity recording system for insects and small mammals is the largest such facility in the world.



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Chronobiology and Animal Behaviour

I have spent most of my professional life studying the behavioural expression of biological rhythms in fruitflies, bats, mice and humans. As a PhD scholar, I studied tidal rhythms in crabs, and this led to a life-long interest in biological rhythms and clocks. Over two stints at the University of Tübingen, and one stint at UC Berkeley, I worked largely on various aspects of light relations of the eclosion clock in fruiflies. In 1975, I moved to Madurai Kamaraj University and eventually established the first department of Animal Behaviour and Physiology in India, which I headed for many years. During this time, my students and I were involved in research on circadian rhythms in bats and mice, as well as research on the foraging behaviour of bats. Among other things, we experimentally demonstrated social synchronization of circadian flight activity rhythm in the bat *Hipposideros speoris,* as well as maternal entrainment of the rhythms of pups in the field mouse *Mus booduga*.

At Madurai, in 1986, I also established an Human Isolation Facility – one of a handful of its kind in the world – in order to empirically study circadian rhythms in humans. These studies yielded evidence for internal desynchronization of sleep-wake and temperature rhythms, the lack of correlation between the menstrual cycle and sleep-wake rhythm, and a positive correlation between sleep and preceding wakefulness.

After joining JNC in 1996, I established the Evolutionary & Organismal Biology Unit with Amitabh Joshi and Vijay Kumar Sharma. At JNC, I have been involved in continuing studies of circadian rhythms in fruitflies and mice, as also some newer work on circadian consequences of social organization in ants.

MK Chandrashekaran did his PhD (Zoology) at Madras University in 1964, was DAAD scholar and Humboldt Fellow at Tübingen, and Miller Invitation Fellow at UC Berkeley, before joining Madurai Kamaraj University, from where he moved to JNC in 1996.

Amitabh Joshi

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Evolutionary Genetics and Population Ecology

My work on evolutionary genetics is centred around selection experiments with *Drosophila*. Through selection, we have created populations with rapid pre-adult development. Comparison of these populations with those adapted to high larval crowding showed that faster development and competitive ability are negatively correlated, and comprehensively changed our understanding of the relationship between these traits in *Drosophila*. We are now using these populations to understand the genetic control of developmental timing and the developmental underpinnings of variation in life-history related traits. We are also using species of *Drosophila* other than *D. melanogaster* to investigate how the genetic architecture and genotype-by-environment interaction patterns underlying adaptive evolution may differ among congeners. I am also interested in evolutionary aspects of circadian organization and the possible role of biological clocks in timing life-history events.

In population dynamics, I am interested in how life-history, environment and migration affect the dynamics of metapopulations, and how such dynamic behaviour evolves. We were the first to show that population stability can evolve as a by-product of life-history evolution, and also the first to experimentally test hypotheses about the effects of migration on metapopulation dynamics. We have also developed integerized population growth models and individual based models, that we use as a foil for testing the utility of classical difference equation based models of population growth.

More recently, I have been intrigued by the possibility that our conceptual framework for describing evolutionary dynamics might have serious shortcomings, and that new conceptual approaches may be needed to overcome them, leading to a growing interest in many philosophical issues in evolution.

Amitabh Joshi did his PhD in Genetics at Washington State University, and was a post-doc at UC Irvine before joining JNC in 1996.

N Sharmila Bharathi
I joined the lab in 2001, and am studying whether patterns of life-history related tradeoffs are conserved across different species of *Drosophila*, as part of a more general investigation of how conserved the genetic architecture of fitness related traits is in congeners. The two species I use are *D. ananassae* (Melanogaster group) and *D. nasuta nasuta* (Immigrans group), and I am presently focussing on adaptations to larval crowding in these species, and how the genetic architecture of these adaptations compares with what is known from earlier studies in *D. melanogaster.* I have also developed mass scale assay techniques for immunocompetence in *Drosophila* and am using those techniques to investigate the possible role of immunocompetence in mediating or affecting tradeoffs among life-history related traits. I have also studied competitive ability and life-history variation in several local *Drosophila* spp. and examined how this variation is correlated with sexual dimorphism for size and development time.

Sutirth Dey
I joined the lab in 2002, and I do theoretical and empirical studies on the effects of life-history, environment, and the interplay between the two, in shaping the dynamics of laboratory populations of *D. melanogaster*. I develop classical as well as individual-based mathematical models of population growth and study their dynamic behaviour through computer simulations. I then test the predictions arising from these studies by running experiments on small laboratory populations and metapopulations of *D. melanogaster*. In particular, I have been studying the evolution of different aspects of population stability (e.g. constancy, persistence) as a by-product of life-history evolution, the effects of different patterns of migration and demographic and environmental heterogeneity on metapopulation stability and the mechanisms by which these effects are brought about (e.g. damping, incoherence). I am also experimentally investigating the impact of seemingly small changes in ecology/husbandry on the dynamic behaviour of populations.

Shampa Ghosh
I joined the lab in 2003, and am working on populations of *D. melanogaster* selected for faster development and early reproduction for more than 260 generations. I have recently characterized the life-history of these populations extensively, revealing reductions in the duration of all life stages. I am presently studying various aspects of these populations, including resistance to various abiotic, biotic and genetic stresses, reproductive behaviour, and whether extreme directional selection for development time has led to developmental instability or incipient reproductive isolation vis-à-vis ancestral control populations. I am also interested in studying the degree to which direct and correlated responses to selection in these populations are canalized along various environmental axes.

N Archana
I joined the lab in 2004, and am working on the evolution of larval growth rates and the underlying physiological and molecular mechanisms of adaptation to larval crowding in two species of *Drosophila* (*D. nasuta nasuta* and *D. ananassae*). I am particularly interested in examining the possible role of genes involved in lipid and glycogen metabolism pathways in mediating the evolution of larval growth rates.

KM Satish
I joined the lab in 2004, and am working on the developmental and molecular correlates of life-history evolution in *D. melanogaster* flies which have been selected for faster development and early reproduction for more than 260 generations. My major aim is to probe the underlying developmental and molecular genetic mechanisms underlying variation in life-history related traits in order to get a better understanding of life-history evolution, an area classically studied through quantitative genetics interpretation of variation at the gross phenotypic level.

Key Publications

1) Mueller LD, Joshi A. *Stability in Model Populations*. Monographs in Population Biology 31, Princeton University Press, Princeton, NJ, USA, 2000.

2) Sheeba V, Sharma VK, Shubha K, Chandrashekaran MK, Joshi A. Effect of different light regimes on adult lifespan in *Drosophila melanogaster* is partly mediated through reproductive output. *Journal of Biological Rhythms*, 15, 380–392, 2000.

3) Joshi A. Interspecific Competition. In *Encyclopaedia of Life Sciences*, Nature Publishing Group, MacMillan, London, UK (www.els.net), 2001.

4) Prasad NG, Shakarad M, Anitha D, Rajamani M, Joshi A. Correlated responses to selection for faster development and early reproduction in *Drosophila*: The evolution of larval traits. *Evolution*, 55, 1363–1372, 2001.

5) Prasad NG, Dey S, Shakarad M, Joshi A. Evolution of population stability as a by-product of life-history evolution. *Proceedings of the Royal Society of London: Biological Sciences (Supplement: Biology Letters)*, 270, S84–S86, 2003.

6) Sharmila Bharathi N, Prasad NG, Shakarad M, Joshi A. Correlates of sexual dimorphism for dry weight and development time in five species of *Drosophila*. *Journal of Zoology (London)* 264, 87–95, 2004.

7) Shakarad M, Prasad NG, Gokhale K, Gadagkar V, Rajamani M, Joshi A. Faster development does not lead to correlated evolution of greater pre-adult competitive ability in *Drosophila melanogaster. Biology Letters*, 1, 91–94, 2005.

8) Dey S, Dabholkar S, Joshi A. Effect of migration on metapopulation stability is qualitatively unaffected by demographic and spatial heterogeneity. *Journal of Theoretical Biology* 238, 78–84, 2006. doi:10.1016/j.jtbi.2005.05.013, 2005.

PhD Students
N Archana, N Sharmila Bharathi, Sutirth Dey, Shampa Ghosh, KM Satish

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Circadian Rhythms in Fruit Flies, Ants and Mice

In my laboratory we take an integrated approach to understanding circadian timing mechanisms, using behavioural, evolutionary, sociobiological, physiological, and genetic studies, augmented by molecular manipulations of genes that modify circadian phenotype. Most of our work stems from laboratory selection paradigms using fruit flies *Drosophila melanogaster.* We carry out behavioural and molecular neurogenetic studies on the selected populations to understand the molecular neurogenetics of circadian rhythms. We also plan to search for new rhythm variants using various screening methods and investigate the underlying molecular genetics. In recent years we have been able to create populations of *Drosophila* with early ("morning") and late ("evening") adult emergence peaks. We have also shown that circadian clocks evolve as a correlated response to selection on timing of eclosion. We have been able to get some leads on the molecular basis of the early and late phenotype. In another set of selection lines wherein light/dark cycles alone were used as selection force, we were able to show that dark reared flies become relatively more photophobic than light or light/dark reared flies. We have also been able to demonstrate the role of circadian clocks in timing life history traits such as development and life span.

In ants, we are interested in understanding the circadian consequence of social organization. The colony of the ant species *Camponotus compressus* comprises of two sexually active castes, the queens and the males, and three worker castes, namely the major, media and the minor workers. In a series of preliminary studies we have shown that circadian clocks of these ants are labile and dependent upon the tasks assigned to them in the colony. We are planning to conduct extensive studies on this ant species to understand the molecular and physiological basis of circadian plasticity in social insects. In addition, we have also undertaken projects on oscillatory, ecological and clinical relevance of circadian clocks.

Vijay Kumar Sharma did his PhD in Biophysics at North Eastern Hill University, Shillong, and was a guest researcher at NTNU, Norway before joining JNC as a Fellow in 1998.

Dhanashree A Paranjpe
I started in 2000 and I am investigating the extent to which light/dark cycles are effective in shaping circadian clocks and the associated fitness consequences using fruit flies *D. melanogaster.* The results of my studies have shown that circadian clocks play a crucial role in determining life history traits and that rearing flies in different light/dark environment modifies photic-responses of circadian clocks. I have demonstrated that pre-adult development of *D. melanogaster* can be made faster or slower by speeding up and slowing down circadian clocks. My studies have shown that light/dark conditions cause reduction in lifespan and such reductions in males are mediated via increased activity and in females via enhanced reproductive output. I have also been able to show that rearing in constant darkness makes flies more photo-phobic and that this behaviour is under the control of circadian clocks.

Shailesh Kumar
I joined the lab in 2002 and I am working on the effect of selection on timing of adult emergence on circadian clocks and associated traits in *D. melanogaster.* My studies have revealed that selection on timing of adult emergence yields populations that have waveforms of adult emergence and activity skewed towards dawn or dusk. I have also been able to shown that the flies constituting the selected stocks have different circadian clocks and underlying clock mechanisms.

Gitanjali Howlader
I joined the lab in 2003 and I am currently working on the neurogenetics of egg-laying rhythm in *D. melanogaster.* To identify pertinent portions of the adult CNS, we used (i) targeted genetic manipulation of specific tissues, (ii) mutants specifically defective in the metabolism of a centrally acting neurotransmitter, PIGMENT DISPERSING FACTOR (PDF), (iii) *disconnected (disco)* mutants in which the neural connections and the dorsal lateral group of clock cells are abolished, and (iv) by ablating clock neurons by expressing *reaper (rpr),* or *diphtheria toxin (dti)* genes. Our most recent studies suggest that the dorsal group of clock cells called Dorsal Neurons (DNs) is the site for circadian pacemaker for egg-laying rhythm. Further, our studies on clock mutants suggest that the mechanisms underlying egg-laying rhythm do not involve some of the known core-clock genes such as *per* and *tim,* and it persists even in the absence of PDF. Currently studies are underway to identify the molecular components of this important physiological phenomenon using loss and gain-of-function mutants and other genetic manipulations.

Ambika Mohan
I joined in 2004 and I am currently working on two projects: (i) Effect of circadian dysfunction on adult lifespan (ii) Effect of selection for gating of adult emergence on the precision of circadian clocks. Preliminary studies have shown that circadian dysfunction is deleterious, as it leads to early death and that consolidation of activity/rest cycle by maintaining the arrhythmic flies in periodic light/dark cycle rescues loss of lifespan.

Koustubh Vaze
I joined the lab in 2005 and I am currently working on the fly lines that have been selected for early and late emergence. The early and late selection lines have altered a circadian clock, which suggests that the underlying mechanisms of these flies have been altered. I am interested in understanding the molecular neurogenetics basis of the early and late phenotype.

Key Publications

1) Sharma VK, Chidambaram R, Chandrashekaran, MK. Probing the circadian pacemaker of a mouse using two light pulses. *Journal of Biological Rhythms* 15, 67–73, 2000.

2) Sheeba V, Chandrashekaran MK, Joshi A, Sharma VK. 2001. A case for multiple oscillators controlling different rhythms in *Drosophila melanogaster. Journal of Insect Physiology*, 47, 1217–1225, 2001.

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4) Sharma VK, Lone SR, Goel A, Deepa M, Chandrashekaran MK. Circadian consequences of a social organization in the ant species *Camponotus compressus*. *Naturwissenschaften,* 91, 386–390, 2004

5) Paranjpe DA, Anitha D, Chandrashekaran MK, Joshi A, Sharma VK. Possible role of eclosion rhythm in mediating the effect of light-dark environments on pre-adult development in *Drosophila melanogaster. BMC Developmental Biology,* 5, 5, 2005.

6) Paranjpe DA, Sharma VK. Evolution of temporal order in living organisms. *Journal of Circadian Rhythms.* 3, 7, 2005

7) Howlader G, Paranjpe DA, Sharma VK. Non-ventral lateral neuron based non-PDF mediated clocks control circadian egg-laying rhythm in *Drosophila melanogaster. Journal of Biological Rhythms,* (in press) 2005.

PhD Students
Gitanjali Howlader, Shailesh Kumar, Ambika Lalit Mohan, Dhanashree Ashok Paranjpe, Koustubh Vaze, Sudeshna Das.

Geodynamics Unit

Chairman
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Neotectonics and Environmental Geology

Identification of belts where sudden and swiftly occurring geological phenomena often destabilize the natural configuration of life and threaten the balance of ecosystems, is the principal objective and the main thrust of activities of this one-man Unit. Regions vulnerable to landslides and occurrence of earthquakes repeatedly in the central sector of the Himalayan arc (Kumaun in Uttaranchal), the Biligirirangan Range in southeastern Karnataka, and the Sahyadri Range in western Karnataka and central Kerala are taken up for studies. Various signs of physical changes taking place in the natural systems in the study areas are interpreted through analysis of patterns in topographical maps and satellite imagery, intensive as well as extensive field work, interpretation of uncommon behaviours of rivers and streams in response to continuing tectonic movements, and visual observations of common hazard indicators.

The field-based studies carried out in the last decade demonstrated that geomorphological rejuvenation of landforms, changes in courses of rivers, their anomalous knee bends, and their blockages manifesting itself in the formation of lakes and subsequent development of flat ground of black-clay deposits, modification of landform due to acceleration of gully erosion, development of mountain/hill barriers along active faults in southeastern Karnataka and adjoining Tamil Nadu, the southern Sahyadri and its foothill-belt in central Kerala and in the Sor Valley in eastern Kumaun in Uttaranchal Himalaya, are related to continuing movements on ancient faults. It is realized that the reactivation in the present time of older faults is contributing towards relaxation of strain in the earth's crust in these earthquake-prone belts. Another area of study is the delineation of a regional terrane-defining boundary fault in the High Himalaya, gaining insight into the mechanism of recent movements on it, and obtaining information on the changes taking place. Another area of activity is the writing of books in simple language for students and researchers in geology, as well as laymen.

Key Publications

1) Valdiya KS. *Dynamic Himalaya,* Universities Press, Hyderabad, 1988.
2) Valdiya KS. *Himalaya: Emergence and Evolution,* Universities Press, Hyderabad, 2001.
3) Valdiya KS. *Saraswati: The River that Disappeared,* Universities Press, Hyderabad, 2001.
4) Valdiya KS. *Geology, Environment and Society,* Universities Press, Hyderabad, 2004.
5) Valdiya KS. *Understanding Earthquakes and Landslides: Preparing for Hazards,* DST, New Delhi, 2004.

KS Valdiya is an INSA Golden Jubilee Research Professor

Molecular Biology and Genetics Unit

Chairman
MRS Rao

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Hemalatha Balaram
Maneesha Inamdar
Tapas Kumar Kundu
Udaykumar Ranga
Kaustuv Sanyal
Namita Surolia

Distinguished Fellows
Akira Ishihama
Azim Surani

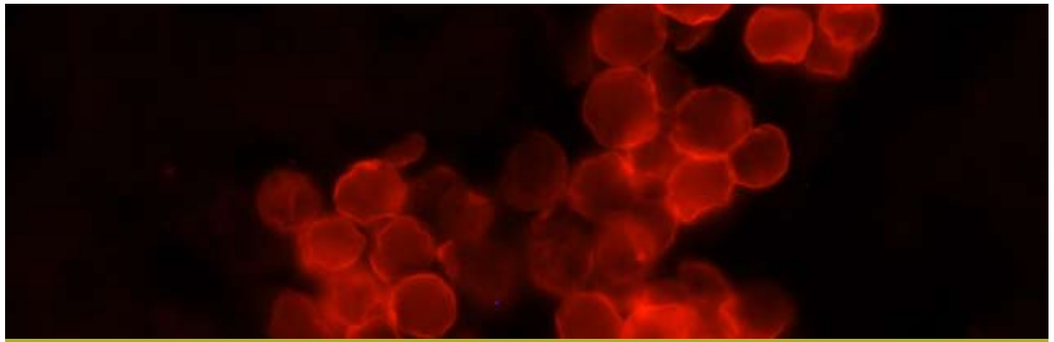
Research in the Molecular Biology and Genetics Unit is in diverse areas of biology bound by the common thread of biomedical applications. The current research areas fall into the categories of Infectious Diseases, Chromatin Organization and Transcription Regulation, Developmental Biology and Genetics. Students have the opportunity to use approaches involving molecular biology and biochemistry, genetics, modern cell and developmental biology and the most recent genomics approaches. Individual laboratories are well equipped for such studies. In addition, a central instrumentation facility contains several state of the art equipments. A sophisticated animal facility is available for biological experiments.

The pathogenic agents for AIDS and Malaria, two infectious diseases of great significance to India, are being investigated at JNCASR. Udaykumar Ranga's laboratory is focused on characterizing Indian strains of HIV. Different therapeutic strategies, such as design of DNA vaccines and screening of natural products for anti-viral therapy, are also being evaluated. Two parasitology laboratories are studying different aspects of *Plasmodium falciparum*. Namita Surolia's group was the first to demonstrate the anti-malarial effect of the common anti-bacterial agent triclosan. Current research is on developing natural and synthetic inhibitors of Type II fatty acid biosynthesis. Hemalatha Balaram is manipulating metabolic pathway enzymes of *Plasmodium,* such as HGPRT and ADSS in the purine salvage pathway. Her group has recently solved the crystal structure of ADSS.

The basic mechanisms of chromatin organization and transcription regulation are being studied in the context of mammalian spermiogenesis and cancer. MRS Rao studies chromatin remodeling during mammalian spermiogenesis, chromatin packaging during sperm maturation, DNA repair and susceptibility to cancer and gene expression profiling in development and differentiation. Tapas Kumar Kundu is studying functional mechanisms of human nucleophosmin in cancer, and has identified small molecular modulators of histone modifying enzymes. His group has elucidated the role of PC4 in chromatin organization and in the activation of p53. Kaustuv Sanyal is studying chromosome segregation in *Candida albicans*.

Anuranjan Anand's group has recently identified a genetic locus associated with epilepsy. Using human genetics approaches his group is involved in a large scale collaborative effort to scan epilepsy-affected families for novel genes associated with epilepsy. His laboratory is also identifying genes and mutations causing deafness and has shown that mutations in Cx26 are a major cause of profound deafness in the Indian population. Maneesha Inamdar is studying mechanisms of blood vessel formation and hematopoiesis, two fundamental processes involved in normal development as well as pathological states such as tumor angiogenesis. Using Embryonic Stem cells, mouse transgenics and *Drosophila* genetics, her group has found new genes required for cardiovascular development.

Figure 1: Embryonic blood cells



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Chromatin Biology and Genomics

The fundamental unit of chromatin is the "Nucleosome" which is organized into a 10 nm filament, wherein approximately 200 bp of DNA is packaged with the help of histones, H1, H2A, H2B, H3 and H4. Various transaction processes like Replication, Transcription and Recombination have to encounter this DNA-Protein complex and naked DNA in the nucleus. It is becoming increasingly clear that this structure is not static but very dynamic, and undergoes both local and global remodeling to facilitate different processes. Mammalian spermatogenesis is a unique differentiating model system wherein there is extensive global remodeling occurring to generate the highly compacted spermatozoa.

The spermatogenesis process is also associated with genetic recombination between the homologous chromosomes at the pachytene interval. Our laboratory has made significant contributions in understanding the role played by the various histone variants in modulating chromatin structure. We have also delineated the molecular anatomy of one of the transition proteins, TP2, which is a novel zinc finger containing protein. This protein also gets covalently modified by phosphorylation, acetylation and methylation. We have shown earlier that the phosphorylation is brought about by protein kinase A, and plays an important role in DNA and chromatin condensation. We are now beginning to understand the role of acetylation and methylation, and are also further exploring the molecular function of this protein *in vivo*.

MRS Rao obtained his PhD at the Indian Institute of Science. He was then a postdoc and Assistant Professor at the Baylor College of Medicine, before returning to IISc, where he was a Professor and Chairman of the Department of Biochemistry. He is the President of JNCASR.

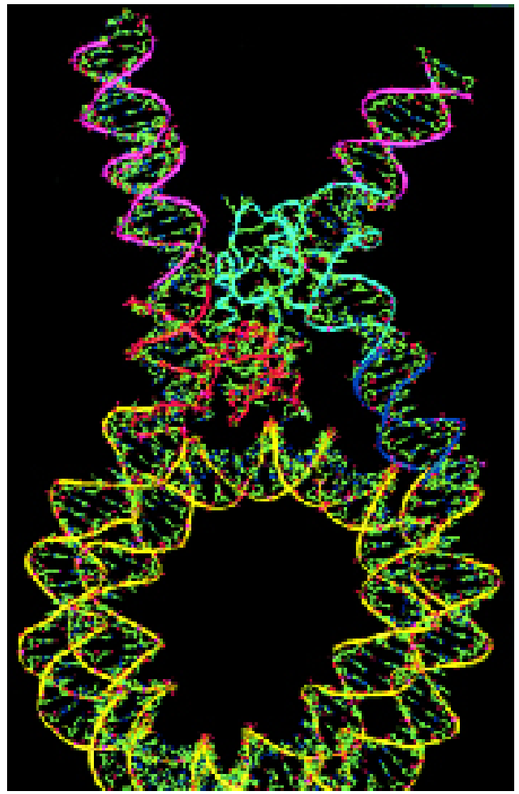

Figure 1: Model of chromatosome particle

Histone H1 is the linker histone in the nucleus, which is necessary for the organization of chromatin into higher order structures. We have shown that the testis specific linker histone H1t organizes the chromatin into loosely organized chromatin to facilitate recombination using a genetic assay in *S. cerevisaie*. Although the crystal structure of the nucleosome core particle has been determined, the structure of H1 containing chromatosome particles is not yet available. Using molecular modeling techniques, we have proposed a model for the chromatosome particle.

We have analyzed the differential gene expression in somatic diploid, spermatogenic diploid, tetraploid and haploid germ cells, making use of a microarray technique. This study has identified several genes, which are uniquely expressed in a particular stage of development of the germ cells. Nucleolin, that is closely associated with ribosomal biogenesis, is one of the genes that is differentially expressed during spermatogenesis. We are thus interested in studying the regulation of ribosome biogenesis and the expression pattern of ribosomal genes during spermatogenesis.

Genetic recombination between the homologous chromosomes is the hallmark of meiotic prophase of germ cell development. Earlier we had identified DNA repair sites in the pachytene spermatocytes using a novel approach. More recently we have mapped one of the repair loci in the mouse genome to chromosome 8, and shown it to be a hotspot of recombination, using genetic approach at nucleotide resolution. Interestingly, this hotspot locus also encodes a noncoding RNA polymerase II transcript whose function is yet to be determined. Extending this study, we have also mapped the corresponding human locus in chromosome 3, and shown that it also is a recombination hotspot, by using population genetic approach. By using Bioinformatic approach, we have identified a new conserved sequence motif associated with all the reported human meiotic recombination hotspots.

Key Publications

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Towards Understanding the Molecular Genetic and Cellular Mechanisms of Human Diseases

The research focus of my laboratory is molecular genetics and cell biology of neurological and sensorineural human disorders. Two main areas of our current research activities are (i) deafness and (ii) epilepsy disorders. A number of projects aimed at understanding the fundamental biological mechanisms of particular types of epilepsies and deafness are presently underway. We are examining functional roles of novel genes that the laboratory has recently identified to be related to causation of epilepsy and deafness, in the context of these disorders and mammalian brain and cochlear development. Our research work encompasses different scientific areas, and ranges from molecular, cellular, gene-regulation studies in mice and humans, creation of gene knockouts and conditional mutations in mice to family- and population-based genetic studies in humans. This knowledge is useful, as it should pave the foundation for development of enhanced therapeutics, intervention and early-detection strategies for the disorders. Much of our work is at the dynamic interface between basic sciences and medical sciences, and is carried out in collaboration with medical institutions. For the epilepsy genetics, we collaborate with neurologists from the National Institute of Mental Health and Neurosciences, Bangalore, Sree Chitra Institute of Medical Sciences and Technology, Thiruvanathapuram and other specialty hospitals. Ali Yavar Jung National Institute of Hearing Handicapped, Mumbai, ALM Post Graduate Institute of Basic Medical Sciences, Chennai, Maulana Azad Medical College, New Delhi and a few additional medical centres are our collaborators in the area of deafness genetics.

Anuranjan Anand did his PhD (1994) at the Department of Microbiology and Cell Biology, Indian Institute of Science, Bangalore and postdoctoral training at the Department of Biological Sciences, Stanford University before joining JNCASR in 1997.

Novel human epilepsy genes and brain-specific biological roles

Epilepsy is a neurological disorder in which brain function is affected as a result of abnormal, excessive and synchronous activity of neuronal cells. Genetic factors are exclusively involved in etiology of certain forms of human epilepsies. Epilepsy genetics is emerging as one of the most useful paradigms to understand biological basis of complex genetic disorders. Finding genes causing epilepsy and examining their functions is one of the best ways to understand the diversity of molecular, cellular and developmental mechanisms underlying epilepsies. Recent advances in human genetics and cell biology are accelerating research in the area, with the hope that a number of novel genes related to epilepsy will be identified. Mouse genetics is providing a major boost to studies in epilepsy.

We have recently identified three novel epilepsy-causing genetic loci, *Seizure-1* (Figure 1), *Seizure-2* and *Seizure-3*. Mutational studies of genes at the *Seizure-1* and *Seizure-2* genomic regions have lead to the identification of rare single nucleotide polymorphisms in particular genes suggesting the potential role of these genes in the causation of epilepsy. *Seizure-1* encodes a protein belonging to a family of G-protein coupled receptors (Figure1). *Seizure-2* belongs to a conserved family of transcription regulators known to play role in neuronal cell fate specification and developmental regulation of gene expression.

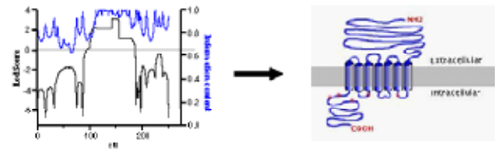

Figure 1: From genetic linkage and significant LOD score (>3.0 at ?=0) at human chromosomal location 3q21, to finding a potential epilepsy-causing gene, Seizure-1 that encodes a protein belonging to the G-Protein Coupled Receptor (GPCR) family

These findings are interesting as they represent a departure from our current thinking of epilepsies as channelopathies, and are permitting us to explore novel molecular and cellular mechanisms of the mammalian brain that when disrupted, can predispose to epilepsies and perhaps additional neurological disorders. There is indeed a growing body of evidence for a shared genetic susceptibility of epilepsies with other brain disorders. We are conducting experiments to examine the role of *Seizure-1* and *Seizure-2* in the context of the disease and brain development. We are studying the expression of these genes in human and mouse brains, examining effects of pathogenic mutations at the genes using cell biological assays, analyzing effects of their misregulation on global gene expression in cell lines and are initiating experiments to generate mouse models for their detailed functional evaluation. A detailed molecular characterization of *Seizure-3* is being conducted to identify pathogenic mutations in the crucial genomic interval.

Defining the auditory genetic code: Studies on genes and molecules causing non-syndromic deafness

Hearing impairment is the most frequent sensory defect in humans. About 80% of hereditary deafness is non-syndromic and occurs due to defects in the genes' functioning almost exclusively in the cochlea, auditory signal transduction apparatus in mammals. Mutational complexities of the deafness-causing genes are rather poorly explored. One line of research in our lab focuses on the analysis of over a dozen known deafness genes for isolating pathogenic mutations, and analyzing their effects in relation to the biological roles of the genes. A second line of research is aimed at the characterization of novel genetic loci responsible for severe-to-profound, non-syndromic, prelingual, sensorineural hearing loss.

Recent work from our laboratory has shown that about 25% of hereditary deafness in Indian populations is caused by mutations at a single gene, *Connexin26 (Cx26)*. *Cx26* encodes gap junction molecules postulated to be involved in recycling of potassium ions and additional small molecules essential for the initiation of action potentials in sensory cells in the cochlea. The high prevalence of *Cx26* mutations is apparently due to an 8000-year old founder effect in Indian populations. Functional analysis of a number of missense and nonsense mutations at *Cx-26,* using cellular localization studies and cell-based, dye-transfer assays shows defective membrane localization of the gap junctions or defective dye- transfer or both (Figure 2). Additional deafness genes being studied at the mutational and functional level are *Connexin-30 (Cx-30), Transmembrane channel like gene 1(TMC1), Transmembrane inner ear (TMIE), Transmembrane serine protease (TMPRSS3), Ushers syndrome 1C (USHIC), Myosin 15 (MYO15), Cadherin-like 23 (CDH23), Claudin 14 (CLDN14), Myosin 6 (MYO6), POU-domain, class 3, transcription factor 4 (POU3F4) and Pendred syndrome (PDS)*.

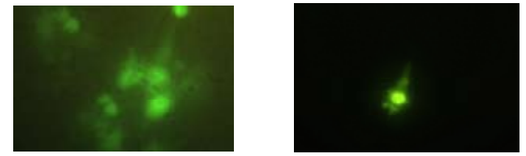

Figure 2: Lack of lucifer yellow dye-transfer in a Cx-26 mutation: Cluster of CX-26, R75W-GFP-expressing cells (left) and no transfer of the dye between cells expressing defective gap junctions (right).

Towards the identification of novel deafness-causing genes, we are using the strategy of genome-wide molecular mapping in multi-generational families with multiple affected members. These studies have identified novel genetic loci at the human chromosomes 18 and X, and these loci are being presently characterized at a functional level.

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Protein Engineering and Molecular Parasitology

Plasmodium falciparum, the causative agent of malaria, is one of the world's most pathogenic microbes. The annual morbidity of malaria is close to 500 million, and the mortality, predominantly among young children, between 1 and 2 million. *Plasmodium falciparum,* being an intra-erythrocytic parasite, has evolved a unique set of biochemical pathways to adapt to the specific milieu that it resides in. Metabolic pathways that are indispensable for parasite survival are an obvious choice as targets for the development of new antimalarials. The purine salvage pathway is one such potential target as it provides the sole source of purine nucleotides to the parasite. Studies in the laboratory have lead to the extensive characterization of the purine salvage enzymes, hypoxanthine guanine phosphoribosyltransferase and adenylosuccinate synthetase. Tools of molecular biology, protein chemistry and biophysics are used to address different issues of protein structure-function analysis.

Hema Balaram has a PhD in biophysics from the Indian Institute of Science, Bangalore and did post-doctoral research at the University of California, San Francisco, USA. She was also a Scientist at Astra Research Centre India, Bangalore.

Hypoxanthine guanine phosphoribosyltransferase (HGPRT)
HGPRTs catalyse the conversion of 6-oxopurine bases to their respective nucleotides, the phosphoribosyl group being derived from phosphoribosylpyrophosphate. Recombinant *Plasmodium falciparum* HGPRT (PfHGPRT) has negligible activity on purification and can be activated by incubation with its product IMP. Studies carried out on PfHGPRT reveal that the enzyme is destabilized in the presence of IMP. These stability studies suggest that the active, product bound form of the enzyme is less stable than the ligand-free unactivated enzyme. The property of ligand-mediated activation is not seen with recombinant human HGPRT, which is highly active in the unliganded state. The reversibility between highly active and weakly active states suggests a novel mechanism for the regulation of enzyme activity in *P. falciparum*. (*FEBS J.* 2005, 272:1900–11).

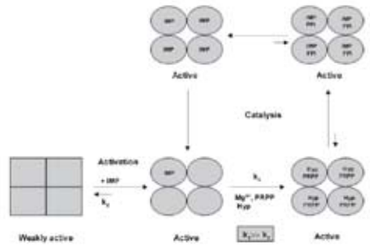


Figure 1: Schematic representation of the process of activation and catalysis by PfHGPRT.

Substrate specificity in HGPRTs
Human HGPRT lacks the ability to phosphoribosylate xanthine, a property exhibited by HGPRTs from many parasitic protozoa. Using random mutagenesis we have obtained a mutant, F36L, of human HGPRT that phosphoribosylates xanthine. Examination of the structure indicates that F36 does not make direct contact with the purine, but long-range modulation via loop IV, a segment contacting purine at C2 position, could influence substrate specificity. Mutation of the corresponding residue, L44 in PfHGPRT, also results in alteration of K_m and k_{cat} for xanthine, substantiating its role in affecting purine base affinity. (*Arch Biochem Biophys.*2004, 427:116–22)

Figure 2: L44 in the structure of PfHGPRT. Yellow: Loop IV, Green : active site.

Adenylosuccinate synthetase (AdSS)
ADSS catalyses the Mg^{2+} dependent formation of adenylosuccinate from IMP and aspartate, the reaction being driven by the hydrolysis of GTP to GDP. All characterized AdSS thus far exhibit a random kinetic mechanism. Studies in the lab have provided kinetic evidence that unlike all other AdSS, *P. falciparum* AdSS (PfAdSS) has ordered substrate binding. The crystal structure of PfAdSS has been solved to 2Å resolution (in collaboration with Prof MRN Murthy, IISc, Bangalore). The structure provides the basis for the unique kinetic mechanism of PfAdSS. (*J Mol Biol.* 2004, 335:1251–64.

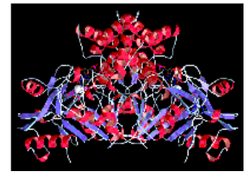


Figure 3: PfAdSS dimer

Regulation of PfAdSS by a glycolytic intermediate
The glycolytic intermediate fructose 1,6 bisphosphate (F16BP) is a known modulator of AdSS activity. It is an inhibitor of mouse AdSS. However, PfAdSS differs from the mammalian in that fructose-1,6-bisphosphate, a potent inhibitor of the mammalian enzyme, is an activator of PfAdSS. Molecular docking has been used to find a probable site for F16BP binding. (*Mol Biochem Parasitol.* 2004, 138:1–8).

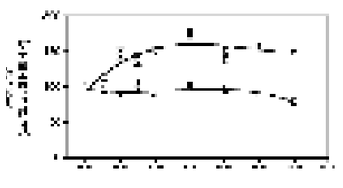
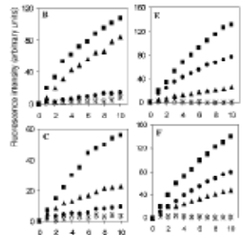


Figure 4 (left): Activation of PfAdSS by F16BP.
Figure 5 (right): Docking of F16BP on PfAdSS

Stage specific profiling of *Plasmodium falciparum* proteases using an internally quenched multispecificity protease substrate
We have designed and used an internally quenched fluorescence peptide substrate for profiling the stage specific expression of proteases in the intraerythrocytic *P. falciparum*. Efficient energy transfer between the donor and acceptor groups flanking the peptide sequence was achieved by incorporation of a central DPro-Gly segment, which serves as a conformation nucleating site, inducing hairpin formation. Graph shows levels of protease activity at acidic and neutral pH in different stages of the intraerythrocytic parasite. (*Biochem Biophys Res Commun.* 2003, 309: 974–9).



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Molecular, Genetic and Developmental Analysis of the Cardiovascular System

My laboratory is interested in studying the development of circulatory systems, with a focus on mouse cardiovascular development. Blood vessels are the earliest organs to form and carry the vital fluid of life and yet their development is poorly understood. The cardiovascular system is complex and several of the molecules involved in its development, their cellular functions and interactions remain to be identified. Several human disorders are caused by defects in cardiovascular development. Hence studies on the regulation of blood vessel formation have potential implications on devising pro- and anti- angiogenic therapies for combating ischemic diseases or cancer, respectively. However, the limited knowledge of gene expression changes that occur in normal vascular development and in tumour angiogenesis has hindered the development of specific treatments and therapies. Transport of oxygen, nutrient and waste products is a fundamental requirement of all multicellular organisms. Hence, it is not surprising that several components as well as mechanisms of developing and regulating a circulatory system are often conserved. Hence when and how the circulatory system arises and functions can be asked in the simplest as well as most complex model organisms. Well-studied examples are the insect and mammalian circulatory systems, where several parallels can be drawn during cardiogenesis and hematopoiesis. We have taken a comparative approach using embryonic stem cell models, mouse developmental biology and transgenics, and *Drosophila* genetics, to decipher the roles of novel genes expressed early in the cardiovascular and hematopoietic systems. Our aim is to understand function and regulation of these genes in mammals and flies using a comparative approach.

Maneesha Inamdar has a PhD (1995) in Molecular Biology from the Tata Institute of Fundamental Research, Mumbai. She was a postdoctoral fellow in Biology at the University of North Carolina, Chapel Hill before joining JNCASR in 1999.

Embryonic stem cell-derived model of cardiovascular development

The appearance of precursors of blood vessels and their support tissues and their subsequent differentiation into a functioning vasculature is poorly understood. While genetically tractable models like the zebra fish are proving to be useful, molecular mechanisms involved in blood vessel formation have been studied mainly in the mouse and chick till recent times. The mouse embryo remains the most accessible model for studying the mammalian vasculature. However, analysis of early mammalian vascularization is hindered, as development occurs *in utero*. This problem is overcome to some extent by embryonic stem cells (ESCs) and *in vitro* differentiation models. ESCs are derived from the pluripotent cells of the inner cell mass of blastula-stage embryos, which give rise to the embryo proper and to several extraembryonic tissues. Under appropriate conditions in suspension culture ESCs can differentiate to form functional cardiovascular structures. ESCs can be used to study the molecules and processes by which early stem cells become committed to specific programs of cell differentiation. They tolerate a variety of genetic manipulations *in vitro* and efficiently form chimeras when re-injected into blastocysts. This property has been used extensively to introduce reporter gene constructs into ESCs and analyze their expression in chimeric embryos. We use mouse embryos and also murine embryonic stem cell-derived embryoid bodies as models for our analysis.

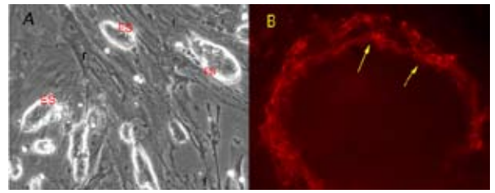

Figure 1: (A) Embryonic stem (ES) cells grown on a feeder layer of mouse embryonic fibroblasts (f). (B) Embryoid body stained to show vascular endothelial cells forming blood vessels (arrows).

The OCIA domain family: A novel family of proteins expressed in the cardiovascular system.

Using a functional genomics approach in ES cells and comparative analysis of gene expression patterns, we have identified a novel gene family that is expressed in cardiovascular development. This family comprises two novel genes that we have identified, namely, *asrij* and *padosan*. Both genes express in ES cells and the developing vascular system. Their expression patterns are largely overlapping. Proteins encoded by both genes localize to endocytic vesicles. The Asrij and Padosan proteins have a novel conserved hydrophobic motif called the OCIA domain. This domain alone is sufficient to target proteins to vesicles. Lack of the OCIA domain results in general cytoplasmic distribution of Asrij and Padosan. *asrij* chimeric mice generated using ESCs carrying a mutant allele of *asrij*, have cardiovascular defects. The *asrij* promoter is GC rich and transgenic mice carrying a lacZ reporter under the control of asrij express beta-galactosidase in the heart and blood vessels. We have also shown that *Drosophila asrij* is expressed in hemocytes and mutants lacking asrij are temperature-sensitive lethal.

Rudhira: A novel marker for ES cells, the erythroid lineage, and tumors.

Using a functional genomics approach we identified a novel murine gene rudhira that is expressed at high levels in embryonic stem cells and is restricted to blood islands and the erythroid lineage during embryonic development. Rudhira is expressed in angiogenic precursors but is excluded from the differentiated endothelium. Rudhira-expressing cells are seen in close proximity to endothelial cells in angiogenic blood vessels. Rudhira encodes a predicted cytoplasmic WD40 protein that is 98% identical to human BCAS3. The gene encoding BCAS3 maps to a breakpoint of hematological neoplasms on human chromosome 17q23, but its expression and function remain to be determined. We demonstrate that mouse *Rudhira* is a novel marker for analysis of the erythroid lineage. *Drosophila rudhira* also encodes a cytoplasmic protein and is expressed in post-embryonic pericardial cells. Hence *Drosophila* Rudhira is a useful marker to analyze pericardial cell lineage and function.

Comparative Vascular Biology

Our analysis suggests that *asrij* and *rudhira* have important roles in the developing vertebrate and invertebrate circulatory system. Our current efforts are aimed at understanding the regulation, function and developmental role of these genes using valuable reagents that we have generated, such as fluorescent-labeled proteins, mutant ES cells, mutant mice, mutant *Drosophila,* transgenic mice and transgenic *Drosophila.* As molecules and mechanisms in development are often conserved, studying development of circulatory systems in various models has given insights into mammalian vascular development. The current focus is on comparative studies between vertebrate and invertebrate models to elucidate common themes in the development of circulatory systems.

Figure 2: Reporter gene expression (blue) in an E11.5 transgenic embryo bearing *arj2-lacZ* promoter-reporter construct.

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Transcription Regulation in Humans with Special Emphasis on Diseases

The major focus of the Transcription and Disease Laboratory is to understand the mechanisms of regulation of chromatin transcription in humans, with a special emphasis on diseases that result from their dysfunction. My group is interested in deciphering the role of histone chaperone NPM1, in the regulation of chromatin transcription and in the gene expression in response to stress. NPM1 is a multifunctional dynamic nucleolar protein and is dramatically over expressed in several cancerous cells. Recently, our group has shown that NPM1 enhances the acetylation dependent chromatin transcription. The role of nonhistone chromatin proteins in the regulation of p53 function and structural organization of chromatin by these proteins is another area that we are investigating. We have discovered that human positive transcriptional coactivator, PC4, is a bonafide chromatin-associated protein and can activate the cellular function of the tumor suppressor p53.

The reversible acetylation of histone and nonhistone chromatin proteins is one of the key regulators of gene expression. Imbalance in the Histone Acetyl Transferase (HATs) and Histone Deacetylase (HDACs) functions has a causal relationship with different disease manifestations. Therefore these enzymes are new targets for therapeutics. Our laboratory is screening different natural and synthetic compounds for small molecule modulators (activator and inhibitors) of the HATs and HDACs. Recently, we have found several HAT inhibitors and one p300/CBP specific HAT activator, CTPB. CTPB is the only known small molecule activator of HAT. Screening for specific modulators of Histone Methyl Transferases (HMTase) is also in progress. These molecules may serve as lead compounds for therapeutics and may also be useful to probe the molecular function of histone modifying enzymes.

Tapas K Kundu obtained his PhD (1995) in Biochemistry from the Indian Institute of Science. He did postdoctoral work at the National Institute of Genetics, Japan (1995-96) and The Rockefeller University, USA (1996-99), before joining JNCASR (1999).

Transcription regulatory proteins as functional component of chromatin

Several transcription regulators, remain attached to the chromatin even after the transcription termination for a quite long period of time during the cell cycle. These proteins act as a "book mark". Apart from these, there are increasingly large number of nonhistone chromatin associated proteins that directly or indirectly play a significant role in transcriptional regulation. These include HMG proteins, heterochromatin proteins (HP1) and PARPs. Recently, we have found that multifunctional, human transcriptional coactivator PC4 is a chromatin-associated protein that plays an important role in chromatin organization. We wish to find out the functional coordination of PC4 in chromatin organization and transcriptional coactivation.

Nonhistone chromatin proteins in the regulation of p53 and its homolog's function

p53 a tumor suppressor protein and a transcription factor controls cell cycle check points, apoptosis and DNA repair via the regulation of several genes. p53 function is regulated by the post-translational modifications of p53 and several proteins which directly interact with p53. These protein factors include histone chaperone, which induces p53 degradation, and nonhistone chromatin associated proteins. We have demonstrated the role of acidic C-terminal domain and A-box of HMGB-1 (a dynamic chromatin interacting proteins) in p53-mediated transcriptional activation and its further downstream effect. Recently, we have shown that human transcriptional coactivator PC4 is a unique activator of p53 function. Interestingly, we have found that PC4 is a p53 inducible gene, thus establishing the first report of a positively regulated feed back loop to control p53 function. Currently, we are investigating the role of PC4 on p53-mediated repression of transcription and also p63, p73-mediated gene regulation.

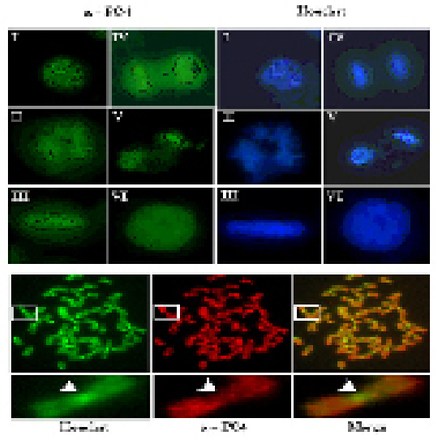

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Figure 1: Association of PC4 to the chromosome in different stages of mitosis: (A) HeLa cells were fixed and subjected to immunofluorescence study using PC4 antibody. Representative cells at different stages during mitosis: prophase (I), prometaphase (II), metaphase (III), anaphase (IV), telophase (V) and interphase (VI) are shown. (B) Distribution of PC4 on mitotic chromosomes.

Histone chaperones in the regulation of chromatin transcription

Regulation of transcription on a chromatin template has long been thought to be a result of the interplay between the modifying and remodeling factors. However, these factors are insufficient to explain the removal of histones. Moreover, the regulation is also achieved with the replacement of 'bulk' histones with histone variants. Among a plethora of histone-interacting proteins present in the nucleus that could carry out these functions, histone chaperones seem the most suitable candidates. Recent work from our laboratory has established that nucleophosmin (NPM1), an abundant nucleolar phosphoprotein, has a crucial role to play in the activation of acetylation-dependent chromatin transcription, and that it gets translocated into the nucleoplasm in response to DNA damage. We would like to elucidate the exact mechanism of transcriptional activation with particular reference to its histone interacting ability. We will also investigate the effect of post-translational modifications of core histones and NPM1 on the transcriptional enhancement brought about by NPM1. The genes regulated by NPM1 will be identified by microarray analysis. We also intend to identify the different interacting partners of NPM1, in an endeavour to network the functional modulators of the protein. Our preliminary data suggests that NPM1 interacts with linker histone H1. We plan to see the effect of NPM1 on the higher order chromatin structure and on transcriptional regulation from an H1 containing template.

Histone modifying enzymes as new targets for therapeutics

Human genes are organized into a highly compact dynamic nucleoprotein complex called chromatin, which consists of histones and associated nonhistone proteins. Though apparently repressive, the precise organization of chromatin is essential for all DNA templated phenomena inside the cell. Alteration in chromatin organization modulates the expression of underlying genes. The posttranslational modifications (e.g.: reversible acetylation, methylation and phosphorylation) of chromatin proteins play crucial roles in the dynamic organization of the chromatin template for all cellular phenomena including transcription. Dysfunction of these enzymes is often associated with several diseases like cancer, asthma, diabetes and several genetic disorders. Small molecule modulators of HATs, HDACs and HMTases thus are new potential therapeutic molecules. We have discovered several small molecule modulators of acetyl transferases, which include anacardic acid, garcinol, curcumin as HAT inhibitors and CTPB and its derivatives, DTK9-14 as HAT activators. The effects of these modulators on gene expression are being studied in vitro and in vivo. Furthermore, we have recently found a potent inhibitor of histone methyl transferase (HMTase). These compounds could be useful as biological switching molecules for probing into the role of HATs, HDACs, HMTases in gene regulation and may also serve as new chemical entities for the development of new drugs.

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HIV-1 Subtype-C Strain: Success Story of the Fittest Viral Subtype?

The Molecular Virology Laboratory focuses on the subtype-C viruses of HIV-1. Depending on the genetic variation, HIV-1 is classified into nine primary subtypes (families). In addition to the primary viral subtypes, there are several recombinant forms circulating in the world. The viral subtypes are distributed across the globe in a non-uniform fashion. Of these various subtypes of HIV-1, subtype-C viruses alone cause more than half the infections in the world and nearly 99% of the infections in India. Subtype-C viruses have also been identified from countries like Brazil with progressively increasing incidence, and from countries like the UK where they had not been identified previously.

Are subtype-C viruses endowed with unique biological properties that make them successful in establishing rapidly spreading epidemics worldwide? Are subtype-C viruses replacing other subtypes in a gradual and progressive fashion? Do we need a vaccine targeting specifically subtype-C? Can vaccines made against one subtype offer broad protection against other subtypes? Answers for these important questions are difficult to find. It is, however, widely believed that subtype-C viruses are more infectious and less pathogenic than other viral subtypes (a smart bug, isn't it?). A successful parasite should not cause rapid elimination of the host before it itself is transmitted to other hosts. Many researchers believe that subtype-C virus has already taken one step in this direction and become adjusted to the host to a greater extent.

Diverse research themes in our laboratory are directed essentially towards finding an answer to this elusive and challenging question: Are subtype-C viruses of HIV attenuated to a greater degree?

Udaykumar Ranga has obtained his PhD in Life Sciences (1990) from SLS, JNU, New Delhi. He worked as a Post-doctoral fellow at Food and Drug Administration, USA and the University of Michigan, USA before joining JNCASR in 1997.

1) The Indian epidemics are dominated by HIV-1 subtype-C strains: We developed a novel subtype-C specific PCR and applied this technique to more than 600 primary clinical samples collected from various rural villages, towns and urban centers spanning across all the four southern states of India. Our study identified subtype-C strains of HIV-1 as responsible for nearly 99% percent of the infections in the southern Indian states (602/608). This study is not only the first report from southern India but also the largest one to appear from India to date.

2) Identification of unique HIV-1 B/C recombinant viruses in India: For the first time we identified three unique B/C recombinant viruses in India. The env sequence of one of the three recombinant strains is phylogenetically associated with Thai-B viruses that are common in China and Thailand, while those of the other two are associated with the subtype-B viruses found in the USA and Europe. Presently it is not known if an independent epidemic is emerging in India due to B/C recombinants. Work is presently in progress to extend the analysis to a few thousand samples collected from all over the country to determine the real incidence of recombinant strains in India. We are also isolating the molecular clones of these recombinant viruses to determine their molecular and biological properties. In pair-wise competition experiments, we will determine if the recombinant viruses have a competitive advantage over pure subtype -B or -C viruses.

3) Are subtype-C viruses defective in inducing dementia?
The incidence of HIV-associated dementia in India (1–2%) is significantly different compared to what has been reported from the USA and Europe (up to 35%) where subtype-B viruses are in circulation. We tested the hypothesis that unique biological properties of different subtypes are one of the possible reasons for the difference observed in the incidence of dementia between these two clinical contexts. We identified a natural variation in the Tat protein of subtype-C (C-Tat), a cysteine to serine variation at position 31. We experimentally demonstrated loss of chemokine property in C-Tat and hypothesized a correlation between this natural variation in Tat and low incidence of HIV-associated dementia in India. Interestingly, the variant serine in C-Tat is phosphorylated, suggesting the acquisition of novel signaling properties for C-Tat. We are presently evaluating subtype differences in Tat transgenic mice and by injecting infected monocytes into mouse brains to study encephalitis, monocyte migration and other pathological manifestations. We are also generating isogenic full-length C-viruses that differ only in the cysteine 31 residue. The replication fitness of these viruses will be evaluated in pair-wise competition experiments.

4) Optimization of DNA vaccines through engineering molecular adjuvants:
DNA vaccines offer the great technical advantage that the encoded antigens are introduced into the MHC class-I pathway. This unique property of the DNA vaccine efficiently induces the cell-mediated immune responses that are required for protection against viruses including HIV. DNA vaccines, however, haven't been successful in inducing strong immune responses in larger animals. Using Tat as a model antigen, for the numerous advantages this HIV antigen offers, we have been engineering molecular components into expression vectors with an objective of improving the performance of DNA vaccines. We have demonstrated enhanced immune responses to Tat by means of codon-optimization of Tat, targeting Tat for rapid antigenic processing by ubiquitin-tagging, and enhanced antibody generation by linking Tat to multiple copies of C3d. We are presently optimizing EF1α promoter as a possible alternative for the popular CMV promoter. Additionally, we are also evaluating the effect of engineering various regulatory elements into Tat-expression vectors for enhanced immunogenicity.

5) Development of immune and molecular diagnostic techniques for HIV
For optimal disease management of HIV/AIDS, the availability of efficient and affordable diagnostic tests is as important as access to chemotherapy. Two tests are highly important, (1) the viral load assay and (2) CD4/CD8 count. Our laboratory is actively collaborating with national (Microtest Innovations, Bangalore) and international (ReaMetrix) Biotechnology companies to develop such molecular diagnostic techniques.

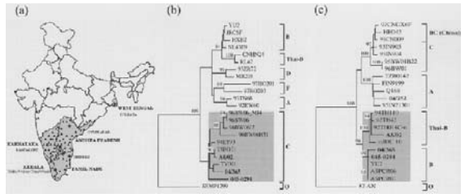

Figure 1: (a) Geographical distribution of various rural and urban towns of India from where the clinical samples were collected. (b) and (c) are phylogenetic relationship of the three novel B/C recombinants with the reference viral strains in the LTR and env genes. The Indian B/C strains and the newly identified subtype-A strain are shown in bold.

Key Publications

1) Siddappa NB, Dash PK, Mahadevan A, Desai A, Jayasuryan N, Ravi V, Satishchandra P, Shankar SK, Ranga U. Identification of unique B/C recombinant strains of HIV-1 in the Southern State of Karnataka, India. *AIDS,* 19 (13), 1426–1429, 2005.

2) Siddappa NB, Dash PK, Narayana J, Mahadevan A, Hoffman B, Keefe R, Satish KS, Satish B, Sreekanthan K, Venu K, Satishchandra P, Ravi V, Shankar SK, Shankarappa R, Ranga U. Identification of Subtype C Human Immunodeficiency Virus Type1 by Subtype-Specific Polymerase Chain Reaction and Its Use in the Characterization of Viruses Circulating in the Southern Parts of India. *Journal of Clinical Microbiology,* 42 (6), 2742–2751, 2004.

3) Ramakrishna L, Anand KK, Mohankumar KM, Ranga U. Codon optimization of an inherently non-immunodominant HIV-1 antigen generates strong immune responses in mice following genetic immunization, *J. Virol.*, 78, (17), 9174–9189, 2004.

4) Ranga U, Shankarappa R, Siddappa NB, Lakshmi R, Nagendran R, Mahalingam M, Mahadevan A, Narayana J, Satishchandra P, Shankar SK, Prasad VR. Tat protein of Human Immunodeficiency Virus Type-1 subtype C viruses is a defective chemokine. *J. Virol,* 78 (5), 2586–2590, 2004.

5) Ramakrishna L, Anand KK, Mahalingam M, Mohankumar KM, Shilpa R, Siddappa NB, Ranga U. Codon optimization and ubiquitin conjugation of Human Immunodeficiency Virus-1 Tat lead to enhanced cell-mediated immune responses. *Vaccine,* 22 (20), 2586–2598, 2004.

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From NIMHANS: Nagadenahalli Byrareddy Siddappa

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Mechanism of Chromosome Segregation: A Molecular Approach

Centromeres are cis-acting DNA elements that occur once per chromosome. A centromere, the chromosomal binding site of spindle microtubules, controls chromosome segregation during mitosis and meiosis. A kinetochore is the proteinaceous structure formed by trans-acting factors (centromeric proteins) at the centromeric DNA. While the baker's yeast *Saccharomyces cerevisiae* contains a small 125 bp region with full centromeric activity ("point" centromeres), most other eukaryotes including humans have much larger centromeric regions rich in repeated DNA sequences ("regional" centromeres). However, only a very few proteins are found to be functionally conserved between point and regional centromeres.

Candida albicans is the most frequently isolated human fungal pathogen. It causes opportunistic infections in immunocompromised patients (such as AIDS patients). *C. albicans* is a polymorphic organism that can grow in budded, hyphal and pseudohyphal forms. Most of the drugs used as antifungals have severe side effects since they inhibit processes that are common to humans and the fungal pathogens. Therefore, it is necessary to identify molecular drug targets that are unique to the pathogen and such drugs should be safer and more potent to combat infections.

We have previously identified centromeres of each of the eight chromosomes of *C. albicans*. Interestingly, centromeric DNA sequences are all unique and different in this organism, a centromeric property previously unobserved in other organisms. Our aim is to perform a structure-function analysis of *C. albicans* centromeres. This analysis should identify some kinetochore proteins, unique to *C. albicans* (and/or related species). Identification of such species-specific kinetochore proteins will have biomedical applications as they can be used as targets to develop specific anti-fungal drugs.

Kaustuv Sanyal obtained his PhD from the Bose Institute (Jadavpur University) and was a post-doctoral researcher at the University of California, Santa Barbara. He joined JNCASR as a Faculty Fellow in October 2005.

Centromere Function in *Candida albicans* may be Regulated by an Epigenetic Mechanism

How centromeres are recognized and propagated in most eukaryotes is a subject of much conjecture. The failure to identify any common DNA sequence motif that distinguishes centromeres from non-centromeric DNAs suggests that a non-DNA sequence element may be involved in the marking event. A family of histone H3-like proteins (called Cse4p in yeast/ CENP-A in humans) is found to be common in the functional centromeres of all organisms studied to date. These proteins (also known as centromeric histones/CenH3) are known to replace canonical histone H3 at the centromeric DNA. We have shown that the CaCse4p molecules replace most of the histone H3 molecules at *C. albicans* centromeres to make a specialized centromeric chromatin. But attempts to discover a mechanism for how CenH3 recognizes centromeres were often unsuccessful. Moreover, in the fission yeast, some plasmids with centromere DNA are the subject of epigenetic activation after introduction into cells by standard transformation procedures. The centromere of these plasmids initially is in an inactive state, but switches to a stable active form after a few generations.

The centromeric DNA sequences of *C. albicans* not only lack conserved DNA elements of point centromeres and repeated elements of regional centromeres, but also each chromosome of *C. albicans* contains a different and unique CaCse4p-rich centromeric DNA sequence. We have also observed that in *C. albicans,* the chromosomal context of the centromeric DNA, rather than the primary DNA sequence per se, is most important in the formation of a functional kinetochore and its subsequent propagation through many generations. Studies on human neocentromeres and the centromere of rice chromosome 8 have shown that functional centromeres can form on ordinary unique DNA sequences carrying transcribed active genes. These observations strongly suggest that rather than the DNA sequence, an epigenetic marking event determines centromeric identity, and this process could be evolutionarily conserved. We are now investigating the role of epigenetic processes in regulating centromere activation in *C. albicans*. This study should have broad implications in understanding centromere function in diverse organisms.

Characterization of Kinetochore Proteins of *C. albicans*

It is apparent that centromere sequences are more divergent than kinetochore proteins in different organisms. Although centromeres of different eukaryotes form on diverse DNA sequences of varying length, they all perform a highly conserved function of chromosome segregation. Identification of several kinetochore proteins of budding yeasts and other organisms including vertebrates suggests that some of the kinetochore proteins or protein complexes are structurally and functionally conserved. Three of the most important and evolutionarily conserved kinetochore protein families are Cse4p/CENP-A, Mif2p/CENP-C and Mtw1p/Mis12p/hMtw1p. We have cloned and characterized CENP-A (CaCse4p) and CENP-C (CaMif2p) homologs of *C. albicans* in our previous studies. We have also identified and in the process of characterizing the Mtw1 homolog in C. albicans (CaMtw1p). By using the following biochemical and genetic techniques we will identify other components of *C. albicans* kinetochores:

i) Purification of proteins complexes by expressing TAP-tagged version of known kinetochore proteins. Tandem affinity purification (TAP) technique has been used extensively in various systems to identify proteins interacting with a protein of interest. This technique uses expression of the protein of interest with two different epitope tags—usually a calmodulin-binding peptide and an IgG-binding domain. The TAP-tagged versions of each of the 3 known kinetochore proteins discussed above will be expressed in *C. albicans*. Subsequently, by a two-step purification procedure, a complex of interacting proteins can be purified and identified by mass spectrometric analysis.

ii) Centromere-DNA affinity chromatography. DNA affinity column using centromere DNA sequence has been used previously to isolate kinetochore proteins in various organisms including *S. cerevisiae* and *S. pombe*. Streptavidin-coupled beads will be used as the matrix that efficiently binds biotinylated DNA (CaCse4p-rich centromeric DNA). Protein preparations from *C. albicans* whole cell extracts will be passed through this centromere-DNA affinity column. Bound proteins will be eluted by appropriate buffers, separated on a SDS-PAGE gel and identified by mass spectrometric analysis.

iii) Suppressors of *ts* mutants of known kinetochore proteins. Analysis of gene products that can suppress a temperature-sensitive *(ts)* mutation is an effective way of identifying genes that are believed to have overlapping functions. The *ts* alleles of both Mif2/CENP-C and Mtw1 family of proteins were sequenced and critical amino acids were identified. Thus, by changing the conserved amino acids we will generate *ts* mutants of corresponding homologs in *C. albicans*. An expression genomic library of *C. albicans* will be constructed to express cloned genes from a strong but regulated promoter (such as the *PCK1* promoter). Any clone that will allow the *ts* mutant strain to grow at a restrictive temperature will either carry the gene itself or its suppressor.

The genes of the interacting proteins thus identified by biochemical and genetic screens will be cloned and characterized.

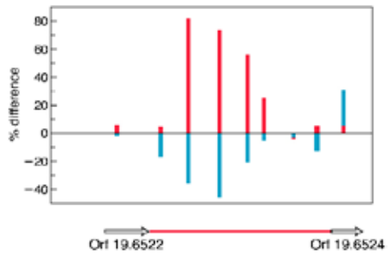

Figure 1: Centromere-specific histone CaCse4p replaces histone H3 at the 3 kb putative centromere locus. Chromatin immunoprecipitation followed by PCR performed with antibodies against CaCse4p (red bars) or histone H3 dimethyl-Lys4 (blue bars). Positions are aligned above a schematic of the open reading frames (ORFs; arrows) that flank the non-ORF region (red line). ORFs are numbered according to Assembly 19 conventions of the *Candida* Genome Database. Enrichment values are presented as the percent difference from a non-centromeric region Ca*LEU2*.

Recent publications

1) Sanyal K, Carbon J. The CENP-A homolog CaCse4p in the pathogenic yeast *Candida albicans* is a centromere protein essential for chromosome transmission. *Proc. Natl. Acad. Sci.* USA, 99, 12969–12974, 2002.

2) Sanyal K, Baum M, Carbon J. Centromeric DNA sequences in the pathogenic yeast Candida *albicans* are all different and unique. *Proc. Natl. Acad. Sci.* USA 101, 11374–11379, 2004.

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Plasmodium falciparum: Functional Genomics of Metabolic Pathways, Antimalarial Drug Development and Molecular Epidemiology

Malaria, which infects an estimated 500 million people and kills 3 million people a year is caused by the protozoan parasite *Plasmodium*. There is currently no vaccine against malaria, and the frontline drugs like chloroquine used for treatment are losing their effectiveness, now that resistant strains of *Plasmodium* have arisen. Additionally, the drugs themselves can have highly undesirable side effects. For these reasons there is a need to identify novel targets for developing new and more effective antimalarials. Research in my laboratory focuses on (i) identifying novel pathways operating in a relict chloroplast termed 'apicoplast' (when present in apicomplexans) of the parasite; (ii) characterizing various enzymes of these pathways through molecular biology, biochemical and cell biology approaches, and also by analyzing their structure-function relationship. From the structural details, the specificity of the *Plasmodium* enzyme paves the way to design and develop inhibitory molecules. My laboratory discovered a novel 'apicoplast' metabolic pathway, namely fatty acid synthesis (FAS II), which is essential for the survival of the parasite. This type II FAS pathway operating in 'apicoplast' is intrinsically different (because of its prokaryotic nature) from the eukaryotic type I FAS, present in humans, and thus is a unique target for developing new therapeutics for treating malaria. We also found that a very widely used antibacterial, 'Triclosan' (a component of toothpastes, anti-acne creams and deodorants) acts as an 'antimalarial', both *in vitro* and *in vivo*. This lead molecule has now become the 'template' molecule for multimillion-dollar industrial efforts worldwide, to develop therapeutic molecules not only for malaria but also for diseases such as tuberculosis and sleeping sickness; and (iii) Molecular epidemiology of the disease.

Namita Surolia has a PhD in Biochemistry from Allahabad University. She was a post-doctoral fellow at IISc before joining the JNCASR in 1996. She is a fellow of the Indian Academy of Sciences as well as the National Academy of Sciences.

Discovery and Delineation of Fatty Acid Biosynthesis for Developing New Antimalarials.

The 35 kb circular genome of *Plasmodium* 'plastid' encodes mostly house keeping genes and no information can be obtained from its sequence about its functions, raising questions such as: what is this organelle doing in the parasite and is there any pathway, operating in the 'plastid', essential for the survival of the parasite? While pursuing our efforts to answer such questions, we discovered the type II *Plasmodium* fatty acid synthesis pathway.

To understand the role of FAS in *Plasmodium,* all the enzymes of the pathway are being characterized in great detail and their interactions with other players of the pathway as well as *in vivo* pools are currently being dissected. The crystal structures of some of these proteins have been solved, which has led to the designing of molecules that are to be tested for their antimalarials effects, *in vitro* as well as *in vivo*.

My laboratory also study the roles of various "apicoplast" genes by making parasite 'knock-outs' and dissecting the targeting of these nuclear encoded, plastid targeted genes by constructing various GFP fusion proteins.

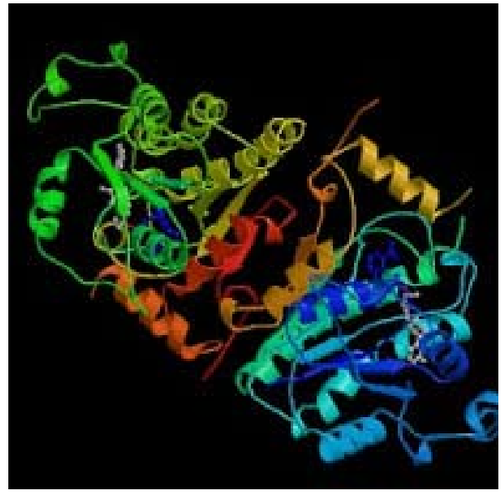

Figure 2: Ribbon diagram of Pf FabI (the target of triclosan with NADH)

Figure 1: Expression of GFP-FabG in *Plasmodium* (schizont stage)

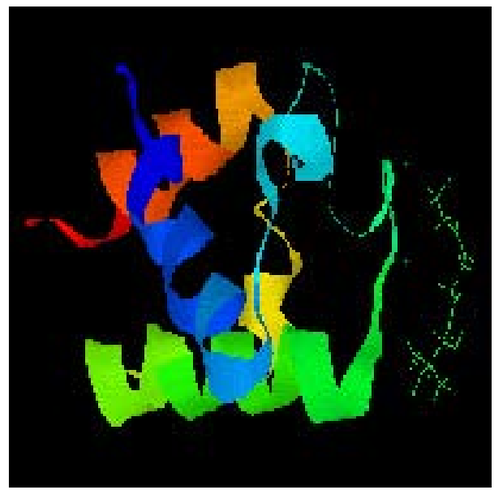

Figure 3: Solution structure (NMR) of holo-PfACP.

Molecular Epidemiology of Malaria

Malaria is the strongest known force for evolutionary selection in the recent history of the human genome. There is growing evidence of ethnic differences in the susceptibility to malaria, and of the diverse genetic adaptations to malaria that have arisen in different populations. We are interested in the epidemiological confirmation of the hypotheses that G6PD deficiency and hemoglobinE protect against malaria mortality. This effort would help us to understand mechanisms of protective immunity that can be used in the development of an effective malaria vaccine.

Key Publications

1) Surolia N, Surolia A. *Nature Medicine,* 7, 167–173, 2001.
2) Surolia et.al. *Biochem J.,* 383, 401–412, 2004.

PhD Students

Krishanpal Karmodiya, Rahul Modak, Pankaj Sharma

Theoretical Sciences Unit

Chairman
Rahul Pandit

Faculty
Shobhana Narasimhan
Swapan K Pati
Srikanth Sastry
Umesh V Waghmare

Fellow
NS Vidhyadhiraja

In the Theoretical Sciences Unit, we use the tools of theoretical and computational physics and chemistry to address, explain and understand the rich diversity we observe in the physical world. We also aim to use the knowledge thus gained to design new materials with desired properties, and to study the behaviour of matter under conditions that are difficult or impossible to achieve in a laboratory.

In the very early universe, matter was homogeneous, but this is clearly no longer so. Due to "spontaneously broken symmetries" and sequences of phase transitions, the world around us now displays variety and complexity: carbon is ultrahard as diamond or soft as graphite; ice contracts when it melts, whereas copper expands; DNA replicates easily and protein molecules coil into complex structures; chewing gum stretches when stepped on, while glass shatters ... why?? In order to understand this fascinating yet perplexing range of behaviour, we have to examine the structure and properties of matter at a nanoscopic level, and consider the complex consequences of having large numbers of electrons, atoms or molecules that interact strongly with one another.

Research in the physical sciences usually falls into one of two categories: either one is looking for universality, or one is exploring diversity. In our unit, we are motivated by both these research philosophies: We find it intellectually gratifying (and useful) when we are able to develop a unified framework for handling many materials or explaining many phenomena; at the same time, we are excited by the prospects offered by exploiting diversity. To cite some examples of recent and ongoing work: we have explored general principles by which glass-formers can be classified; we have formulated a comprehensive argument that explains why some nanoclusters melt at higher temperatures than bulk crystals, while for others the opposite is true; we are searching for molecules which can function both as nano-transistors and as memory devices; and we are designing better piezoelectric materials that are environmentally-friendly.

We use a variety of approaches to look at the kinds of questions mentioned above, including classical and quantum mechanical treatments of condensed matter theory and statistical mechanics, such as *ab initio* density functional theory, quantum many body theory, dynamical mean field theory, quantum chemistry, molecular modeling, molecular dynamics and Monte Carlo simulations. We combine analytical calculations with extensive state-of-the-art computation. The techniques we use have a wide range of applicability, not just to inanimate matter, but also to biological systems.

Some of the systems that have been of recent interest to us are: organic molecules, polymers, colloids, glass-forming liquids, network-forming liquids, simple, noble and transition metals and their surfaces, transition metal oxides, ferroelectrics, magnetic and dilute magnetic semiconductors, Kondo insulators, heavy fermion metals, nanoclusters, nanotubes, nanowires, fullerenes and biomolecular systems. The range of phenomena we have studied is similarly comprehensive: relaxation processes, phase transitions, phase transformation kinetics, transport, vibrations, excitations, charge transfer, surface reconstruction, and catalysis. Specific themes and properties of interest include metal-insulator transitions, magnetic phase transitions, phase transitions in liquids, the glass transition, melting in nanoparticles, stability and excitations in solids, electronic transport, bonding, structure and thermodynamics of biomolecules, properties of relaxor ferroelectrics, and piezoelectricity.

The atmosphere in our unit is interactive and informal. We are engaged in multiple collaborations, amongst ourselves as well as with theorists and experimentalists at JNCASR and worldwide. We also have access to sophisticated computational resources, both within our unit and at the central computational facility of JNCASR.

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Equilibrium and Nonequilibrium Statistical Mechanics of Condensed-Matter Systems

My research interests cover a wide variety of problems in the statistical mechanics of condensed-matter systems, phase transitions, and nonlinear dynamics including the statistical properties of fluid and plasma turbulence, spatiotemporal chaos in extended, deterministic dynamical systems such as models for cardiac arrhythmias, the statistical mechanics of quantum antiferromagnets and models for the colossal magnetoresistive manganites, superfluid, Mott-insulator, and other phases in systems of interacting bosons, complex fluids like microemulsion, micellar, lamellar, and sponge phases in oil-water-surfactant mixtures and bilayer systems, and the statistical mechanics of systems with surfaces, interfaces, and membranes including wetting, roughening, and surface melting.

Recent work in my group has concentrated on the following problems:

- The systematization of the multiscaling of time-dependent structure functions in fluid and passive-scalar turbulence.
- Detailed numerical investigations of the role of conduction inhomogeneities in cardiac tissue on arrhythmias such as ventricular fibrillation; these are carried out by using partial differential equations for cardiac tissue.
- The elucidation of the natures of and transitions between superconducting and Mott-insulating states in systems of interacting bosons on a lattice; such lattices can be realised by optical means in cold-atom systems.

Rahul Pandit obtained his PhD in Physics from the University of Illinois at Urbana-Champaign, and was a Postdoctoral Associate at Cornell University. He is also a Professor in the Department of Physics at the Indian Institute of Science

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Condensed Matter Theory: *Ab Initio* Investigations of Low-Dimensional Systems

I am primarily interested in using theoretical techniques to explore novel physics and chemistry at the nanoscale. The properties of finite, low-dimensional systems often vary drastically from those of infinite three-dimensional solids, though the chemical composition might remain unaltered. For example, even a material like gold (chemically inert and structurally simple in its familiar three-dimensional form) displays complicated structural rearrangements and unexpected chemical and transport properties when one looks instead at a two-dimensional gold surface, a one-dimensional nanowire, or a zero-dimensional gold cluster. Understanding the science behind these novel phenomena, and predicting how this behaviour will change under different conditions, presents a formidable but fascinating theoretical challenge.

To address such issues in a precise way, I mainly use the techniques of ab initio density functional theory (DFT), a very successful approach towards predicting and computing the properties of quantum mechanical many-electron systems from "first principles". This powerful method makes use of no empirical input apart from the atomic numbers of elements; everything else emerges naturally from the calculation. Crucially for the systems we are interested in, this method accurately reproduces the effects of reduced atomic coordination. We are also interested in using DFT calculations to parametrize models that can be used to explore physics at large length-scales and time-scales that may not be amenable to a fully *ab initio* calculation.Though the work in my group is primarily motivated by intellectual curiosity and a desire to understand basic underlying mechanisms, much of our work has important implications for, and potential applications in, the emerging field of nanotechnology.

Shobhana Narasimhan has a PhD in physics from Harvard University. She was a postdoc at Brookhaven National Laboratory and the Fritz-Haber-Institut, Berlin, and has held visiting positions at the University of Cambridge, the University of Paris, and the Max-Planck-Institut, Stuttgart.

Vibrational and Thermal Properties of Nanosized Objects:
Will a really small object (composed of tens to hundreds of atoms) melt more easily than a large object or not? Until recently, it was believed that small atomic clusters would melt at lower temperatures than bulk samples of the same material, but recent experiments and simulations have questioned this. Using DFT and density functional perturbation theory (DFPT) techniques, we find that small clusters of some elements do indeed melt at temperatures above the bulk melting temperature; for other elements the opposite is true. By examining vibrational properties, we are able to formulate simple physical arguments that can explain this variation in thermal properties, and have come up with a rule-of-thumb that can be used to predict how different materials will behave.

Surface Structures and Growth:
Many surfaces "reconstruct", i.e., the arrangement of atoms at and near the surface differs from that in the bulk. We are particularly interested in the reconstruction of close-packed metal surfaces (e.g., Au(111) and Pt(111) and various heteroepitaxial systems), where the reconstruction consists of a tiling of domains where surface atoms occupy different sites. This results in beautiful ordered patterns with a regular periodicity of tens of nanometres. We have performed *ab initio* DFT calculations to parametrize classical models, which we have then used to study the surface reconstruction. Our simulated scanning tunneling microscopy (STM) images (see picture) show a striking resemblance to experimental ones. We are currently extending this work to the study of the reconstruction of vicinal (stepped) surfaces.

We are also interested in the use of these patterns as templates for the growth of self-ordered nanostructures: upon depositing another metal on the reconstructed surface, one can obtain a regularly-spaced lattice of monodisperse (uniformly sized) islands of the overlayer material. These nanostructures constitute novel model systems for the investigation of the intriguing electronic and magnetic properties of small, finite systems. They could also lead the way towards the development of more compact magnetic memory storage devices.

Surface Vibrations:
The shaking and rattling of atoms can serve as a useful tool for understanding interatomic interactions, and also have an impact on thermal properties, chemical activity, etc. Atoms at surfaces vibrate differently from those in the bulk, due to the different environment they sit in. We have used both the "frozen phonon" technique and DFPT to look at such issues, and to calculate the surface phonon spectrum of different surfaces. For example, we have found that certain bonds at the surfaces of face-centered-cubic (110) surfaces are twice as stiff as corresponding bulk bonds. This surprising finding provides a simple explanation for many counter-intuitive phenomena observed on these surfaces: e.g., some interlayer distances contract (rather than expand) upon raising the temperature, and atoms in the outermost surface layer have been found to vibrate with a smaller amplitude than atoms in the second layer.

Catalysis:
Catalysts are used to selectively promote desired chemical reactions; they work by reducing the energy barrier for the "rate limiting" step in a reaction. Of vital importance in industry and environmental protection, they have hitherto been selected and developed largely by trial-and-error. We are using DFT to understand catalytic processes, with the ultimate goal of designing new and better catalysts. We are currently interested in the effects of reduced atomic coordination (e.g., at rough surfaces or in nanoclusters) in changing reaction barriers for the catalytic oxidation of carbon monoxide, or in "three-way" catalysts, where there is a simultaneous oxidation of carbon monoxide and reduction of nitrogen oxides. We are also examining the intriguing way in which the atoms on some surfaces switch back-and-forth between square and hexagonal arrangements during catalytic cycles.

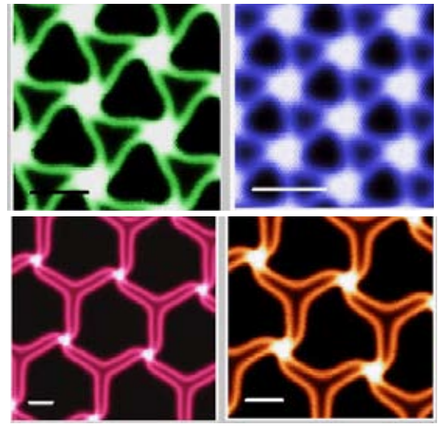

Figure 1: This sequence of simulated STM images shows how the domain patterns on the reconstructed Pt(111) surface change, as the density of atoms in the topmost layer is increased. The horizontal black/white lines represent a length of 50 Å.

Other Projects:
We have long been interested in anharmonic properties, i.e., the consequences of the fact that atoms vibrate in potential wells that are not perfect parabolas. It is crucial to take this into account when describing many common physical phenomena, such as thermal expansion. We have explored the implications of the existence of enhanced anharmonicity at surfaces, and have also shown that "exchange-correlation errors" (one of the main sources of error in DFT calculations) are reduced considerably when one computes anharmonic properties, rather than harmonic properties. We are also interested in calculations of surface stress (e.g., in heteroepitaxial growth), and in the structure and properties of one-dimensional nanowires.

Collaborations:
We have ongoing collaborations with the experimental groups of David King (Cambridge) and Sylvie Rousset (Paris), and the theoretical groups of Stefano Baroni and Stefano de Gironcoli (Trieste) and Umesh Waghmare (Bangalore).

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Advanced Quantum Theory: From Molecules to Extended Materials

Our research interest encompasses a broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum systems. Including the relevant orbital, spin, charge and molecular/lattice degrees of freedom, we try to understand the microscopic structure-property relationship for a wide spectrum of applications in transport, optical, magnetic, electrical and mechanical behavior. We use a variety of quantum mechanical methods ranging from empirical to semi-empirical, mean field methods and perturbative to non-perturbative formalisms. The systems of interest include molecules, clusters, solids, polymers and biomaterials in their isolated forms or their variants in experimental conditions.

Our state-of-the-art numerical methodology involves developing effective theories based on appropriate recognition of relevant states that are responsible for the particular application. With a few to a very large number of states, the effective theory considers quantum-many body interactions in the most appropriate manner through random-phase approximation, configuration interactions with one or a few reference states, zero-T many-body perturbation theory to very high orders, finite temperature methods with statistical averaging, and non-perturbative renormalization group based on density matrix formalisms. Apart from numerical tools, we also develop analytical tools in certain limits for a host of quantum many-body models like the Heisenberg and Hubbard Hamiltonians, etc. Above all, in our work, chemistry and physics meet each other to provide a better insight into, and a clearer understanding of, the whole system.

Swapan K Pati has a PhD (1998) from the Indian Institute of Science. He was a post-doctoral fellow in Physics at the University of California, Davis and in Chemistry at Northwestern University, before joining JNCASR in 2000.

Quantum Magnetism and Related Phenomena:
Quantum Magnetism is as old as quantum mechanics. There have been a number of celebrated models in this area, and although the field was initially completely theoretical in nature, the last couple of decades have witnessed the synthesis of an innumerable number of novel systems with far-reaching applications in magnetic recording, data storage and magneto-electronics circuitry. This field offers the promise of manipulating purely quantum objects like spin for applications in fields such as quantum computing, spintronics and quantum qubit technology.

Our interest lies in the interface of structural aspects and quantum ordering: mostly in insulating oxides, sulphides and related materials. Different structural manifestations of magnetic ions, together with the interactions among the spin degrees of freedom in various forms, open up a host of possibilities. This is more evident in low-dimensional systems, where quantum effects may give rise to completely unconventional and exotic quantum phases. We have been involved in developing quantum many-body theories to accurately calculate several static and dynamic properties of low-dimensional magnetic systems. In particular, the effects of competing exchange interactions and lattice dimerizations have been analysed in detail for a large class of systems including Kagome antiferromagnets, sawtooth lattices and ladder structures. We have also been extending our theory to design novel magnetic clusters with desired technological applications in magneto-electronics.

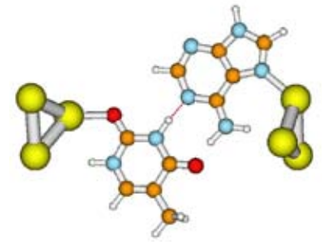

Figure 1: Trapping DNA bases and base-pairs within gold clusters results in overall deconfinement

Optical and Opto-electronic Properties:
Materials with large non-linear optical absorption and emission properties find tremendous applications in lasers, optical switches and optoelectronics. To fully realize the potential offered by optically active materials, one has to be able to optimize properties of individual molecular species at a microscopic level, as well as come up with efficient ways of arranging molecules macroscopically, so as to achieve maximum density and acentricity.

Our interest lies in developing theories that can help in understanding and predicting *a priori,* the optical response functions in a wide variety of systems ranging from organic crystals composed of charge-transfer species to dipolar crystals and inorganic materials. We design strategies that enhance the opto-electronic response functions at the molecular as well as at the crystalline aggregate level.

Using semi-empirical and density-functional formalisms, coupled with our effective exciton theory, we are able to describe dynamical phenomena in various constrained geometries of molecular and supra-molecular assemblies. Invoking dipolar interactions and topological features, we have analysed odd-even oscillations in optical features and chirality-induced optical transitions. We have also been studying the non-linear optical responses in inorganic charge-transfer salts. All-metallic sandwich type aluminium complexes have been proposed for the first time, together with strategies for future experimental synthesis.

Transport in Nanostructures:
Due to possible applications in miniature circuits, the study of charge conduction through single molecules and nanosystems has gained tremendous impetus. Our theoretical investigations focus on the parameters that critically influence conductance across such systems. We consider real experimental systems that exhibit such phenomena. We have been involved in developing effective theories that describe the spatial electrostatic potential across electrode-nanosystem interfaces as well as nonequilibrium dynamical properties like conductance, current and capacitance. Landauer-Buttiker equations together with mean-field configuration interactions methods have been successfully applied through non-equilibrium Green function formalisms to understand various transport characteristics in a number of nanosystems.

Our analyses of current-voltage characteristics, with and without electron-phonon coupling, and various donor-acceptor characteristics have been able to explain a large number of experimental observations in many molecular devices. We have been developing theories to design nanomaterials for molecular memory and switching devices. Long-range charge-transfer between two terminal components is also being actively pursued.

H-Bonding, Aromaticity and related phenomena:
Hydrogen bonding is one of the most important interactions at the supramolecular scale. Although well known and recognized for more than 50 years, the exact nature of H-bonding interactions is still not very clear: are H-bonds purely electrostatic in nature or do they have significant charge-transfer that may lead to covalency? Our major goal has been to develop a unified theory for the H-bonding interactions in gas-phase structures, solid state clusters like ice, organic/inorganic crystals and also in many biomolecular systems. We are also investigating the interplay between H-bonding and Coulomb stacking interactions in biological systems such as RNA and DNA. We have extended the concept of aromaticity from the molecular scale to supra-molecular scale, where this concept has been used to explain the formation of cyclic closed-loop H-bonded H_2O clusters inside open-framework and related crystal structures

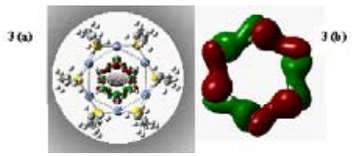

Figure 2: (a) Aromaticity in cyclic tiara Ni-thiolates (b) Aromaticity leading to s-electron delocalization in cyclic water hexameric cluster (H2O)6

PhD Students
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Dynamics and Phase Transformations in Disordered Systems: Liquids, Glasses and Biomolecules

The research interests of my group are in the area of statistical mechanics, with a focus on understanding a variety of properties of liquids and other disordered substances. The systems of interest include glass forming liquids, amorphous solids, water, liquid and amorphous silicon, polymers and biomolecules such as RNA and proteins. The types of properties and phenomena whose understanding is sought include intermolecular structure, phase transitions, metastability, kinetics of phase transformation, flow in confined geometries, structural relaxation and other time dependent phenomena and structural arrest. Specific questions along these lines are addressed by various theoretical and computational methods, by analyzing realistic as well as idealized models of the systems of interest.

A variety of physical systems exhibit *glassy behaviour* including supercooled molecular liquids, polymers, disordered magnetic systems (spin glasses), and granular materials. Such behaviour involves a strong change in transport properties such as viscosity for relatively small changes in external conditions such a temperature, complex relaxation dynamics, loss of ergodicity, aging and memory effects on experimental time scales. The study of these phenomena forms a significant component of our research. We are also interested in the study of novel phase transitions such as a liquid-liquid transition that has been studied in silicon, and in the application of ideas and methods employed in these studies to systems that exhibit more complex molecular detail such as polymers and biomolecules.

Srikanth Sastry has a PhD (1993) in Physics from Boston University. He was a postdoctoral fellow at NIH and Princeton University, USA, before joining JNCASR in 1998.

Glass forming liquids and the glass transition:
Important questions in studying glass formers concern the nature of the *glass transition* (when, e.g., a supercooled liquid transforms to an amorphous solid, or *glass*), the explanation of the complicated dynamics above the glass transition, and the description of thermodynamic and dynamic features of glasses. For supercooled liquids, an understanding of structural changes related to glassy behaviour and the relation to the crystalline state are also important aspects of the problem.

One of the main approaches to elucidating these issues has been the *energy landscape approach,* which attempts to address thermodynamic and dynamic behaviour in terms of knowledge of the statistics and properties of local energy minima, saddle points and such descriptions of the energy landscape of the glassy system. The energy landscape approach has also found application in studying other complex systems such as evolving populations and biomolecules. Our work has attempted to employ the energy landscape approach in combination of extensive computer simulations of realistic and model liquids to address glassy behaviour.

Figure 1: **(Left)** The distribution of local energy minima vs. their energy for a glass forming liquid, for different densities. The shape of the distribution is related to the *fragility* of the glass.
Figure 2: **(Right)** Schematic is the liquid-gas mechanical stability limit (spinodal) and the glass transition line, which intersect at a finite temperature.

One of the problems to which this approach has been applied is the understanding of *fragility,* which quantifies the rapidity of change of transport properties in glass formers. Our analysis has led to relating the fragility to the distribution of local energy minima in glass forming liquids. My work has also lead to the recognition of the role of the energy landscape in glassy dynamics, and the identification of the onset temperature of slow dynamics in these terms.

Another problem that has been studied is the relationship between the liquid-gas mechanical stability limit and the glass transition line, which together form ultimate bounds to the liquid state. Analysis of this relation from computer simulations and theoretical calculations has led to a metastable *phase diagram* with intersecting glass transition and mechanical instability lines, and a glass-gas limit of stability. In addition to molecular liquids, this phase diagram is also of interest in relation to gelation and vitrification of colloidal fluids.

Ongoing work also addresses the nature of the glass transition, the role of structure and configuration space geometry in determining glassy dynamics, and vibrational modes in amorphous solids, and involves the development of new computational methods to analyse energy landscapes and structure, and improved simulation techniques.

Liquid-liquid transitions:
Another theme of interest is the study of a novel liquid-liquid phase transition in network forming liquids, such as water, silica and silicon. From computer simulations, the existence of such a transition has been established for silicon, an estimate of the location of the critical point has been made, and it has been shown that this transition also marks a metal to semi-metal transition. Ongoing theoretical and computational work is aimed at developing a better understanding of the transition. A related theme is the development of a better understanding of glass forming ability of different substances, and establishing the connection between interatomic interactions and the nature of the dynamics.

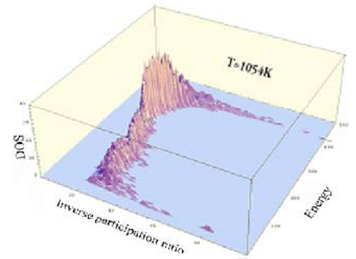

Figure 3: The electronic density of states of liquid silicon in the low temperature phase displaying localization of states near the Fermi energy.

Biomolecular systems:
The ideas and methods developed in the above studies are also being applied recently to the study of systems with more complex molecular detail, such as polymers and biomolecules. Work along these lines includes the application of novel simulation techniques to calculate polymer free energies, geometric analysis of protein strcture, three dimensional structure of RNA molecules, dynamics of transitions between RNA secondary structures, and the application of statistical mechanical methods to understanding protein aggregation.

Key Publications

1) Ashwin SS, Waghmare UV, Sastry S. Metal to non-metal transition in supercooled liquid silicon. *Phys. Rev. Lett.,* 92, 175701, 2004.
2) Sastry S, Angell CA. Liquid-liquid phase transition in supercooled silicon. *Nature Materials,* 2739, 2003.
3) Sastry S. Relationship between fragility, configurational entropy and the potential energy landscape of glass forming liquids. *Nature,* 409, 164, 2001.
4) Sastry S. Liquid limits: The glass transition and liquid-gas spinodal boundaries of metastable liquids. *Phys. Rev. Lett.,* 85, 590, 2000.

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Computational Materials Theory: From Electronic Motion to Macroscopic Properties of Materials

The central theme of research in my group is to determine properties of materials on the macroscopic and intermediate length and time scales through a non-empirical description of their chemistry and microscopic structure. It usually starts with computational solution of electronic motion treated within a quantum mechanical density functional theory and identifies the lowest energy degrees of freedom and their interactions. An effective (model) Hamiltonian is then derived by integrating out the rest of the degrees of freedom. This *first-principles* Hamiltonian is then used in large-scale simulations that yield properties of materials at different scales. Owing to continuing advances in computers and algorithms, it is now possible to characterize and design new materials, particularly at the nano-scale, based mostly on such simulations.

Research in my group has three-fold goals: (a) understand aspects of chemical bonding and microscopic couplings that are essential to the specific properties of a material, (b) obtain information about the atomistic structure and electronic states that may be hard to access experimentally, and (c) design new materials or modify existing materials to yield desired properties, or narrow down the choices of new materials for design by experiment. We are interested in materials that exhibit novel phenomena and are of technological importance. They include *smart materials* such as ferroelectrics, multiferroics, dilute magnetic piezoelectrics and electroactive polymers. We are exploring new functionalities of materials with nano-scale structure, such as super-lattices, clusters, nano-wires and nano-tubes. While applying state-of-the art techniques to studies of these systems, we are also engaged in developing new computational tools and programs in my group.

Umesh Waghmare has a PhD (1996) in Applied Physics from Yale University. He was a post-doctoral fellow in Physics at Harvard University, USA, before joining JNCASR in 2000.

Smart Materials: Ferroelectrics and Multiferroics

Ferroelectrics, which exhibit macroscopic electric dipole moment spontaneously, are useful as *smart* materials in micro-electro-mechanical systems (MEMS) and in non-volatile computer memories. The dipole moment of these materials couples with mechanical changes in the environment, making them useful as sensors and actuators. Most ferroelectrics used in technological applications today contain lead, which makes them toxic and hazardous to the environment. My group is involved in designing environment-friendly ferroelectrics that are lead-free and have properties comparable to those of the lead-based materials. Our efforts are directed towards tuning their properties by changing chemistry and structure (for example, superlattices).

Recently, many groups have shown that ferroelectricity is preserved in ultra-thin (a few nano metre thickness) films, contrary to the expectation that surface charge on films would kill ferroelectricity. My group is probing the possibilities of stripe (domains) formation that may stabilize ferroelectricity at the nano-scale, and their impact on properties and usefulness of these films. Our work involves use of *first-principles* effective Hamiltonians in molecular dynamics simulations, and is presently focusing on the dynamics of these domains as a function of temperature.

Multiferroics, which exhibit both electric and magnetic dipoles spontaneously, hold promise of much wider range of functionalities and applications, as both electric and magnetic fields can be used to drive their response. However, such materials are not very common in nature. In collaboration with experimental groups at JNC, we are engaged in understanding multiferroics and their properties. Our activities encompass related materials, the dilute magnetic piezoelectric semiconductors, which are crucial to the emerging field of spintronics.

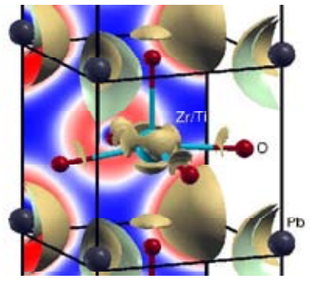

Figure 1: Electron localization functions of ferroelectric $PbZr_{0.2}Ti_{0.8}O_3$; shells surrounding Pb atoms correspond to the lone-pair of 6s electrons, which are important contributors to ferroelectricity in Pb-based materials.

Nano-structures and molecular systems:

Our work on nano-structures complements experimental efforts in the Centre. In particular, we determine structures and electronic properties of nano-clusters and nano-wires from first-principles. We are presently studying vibrational properties of nano-clusters and carbon nano-tubes, and their implications for thermal stability and properties.

Nano-structured materials are bulk materials obtained as aggregates of nano-size units or grains and exhibit rather interesting mechanical properties. We use first-principles calculations to understand the microscopic origin of their macroscopic mechanical behavior and are trying to identify signatures of these properties in the nature of bonding characterized with topological analysis of electron density.

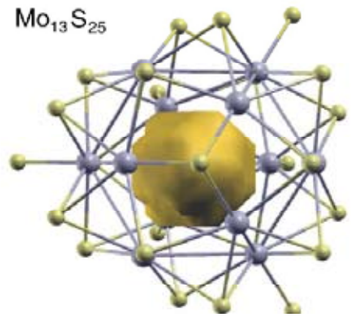

Figure 2: A stable cluster of $Mo_{13}S_{25}$. Yellow colored volume shows the void space inside its cage-like structure.

Development of methods:

A new technique to evaluate quantitatively the charge transfer, covalency, centricity and multiplicity of bonds has been developed based on geometric phases of Bloch electrons, generalized localized bond orbitals (Wannier functions), and a Bond Orbital Overlap Population. Our computer program interfaces with a density functional theory code *ABINIT* and is available as free software.

In the near future, we plan to use the generalized localized orbitals developed in my group to construct models for larger-scale simulations of bio-molecules interacting with inorganic nano-structures.

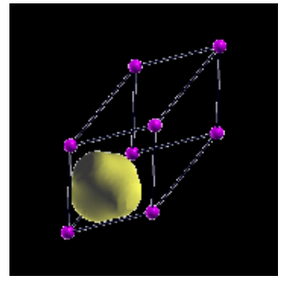

Figure 3: A bonding orbital of aluminium in the face centered cubic crystal, revealing a 4-center bond.

PhD Students

From JNCASR: Joydeep Bhattacharjee, Gargi Dutta, Prasenjit Ghosh, Mousumi Upadhyay Kahaly
From IISc: Aditi Datta

CSIR Centre of Excellence in Chemistry

Head
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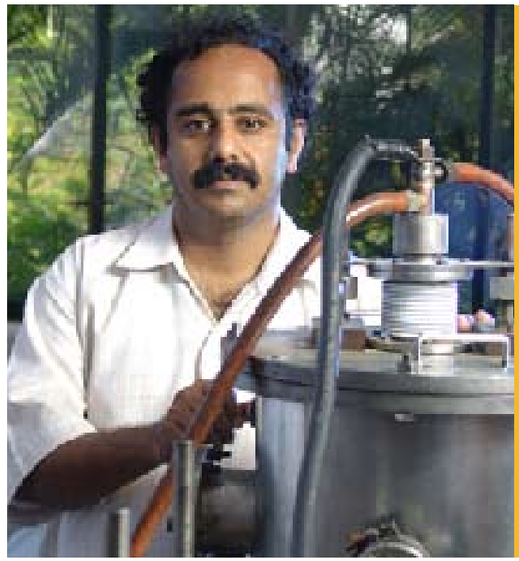
A Govindaraj



A Govindaraj

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The Council for Scientific and Industrial Research (CSIR) has a programme to establish Centres of Excellence devoted to frontline, interdisciplinary areas of research to recognize, promote and support outstanding individuals or groups and to generate trained R & D personnel in the areas of interest. In January 1991, the CSIR established this person-based Centre of Excellence in Chemistry. The Centre works on various aspects of solid state and materials chemistry. The main activities of this CSIR-Centre deal with the following aspects.

- Synthesis and characterization of designer solids (molecular solids) with novel structures and properties, supramolecular chemistry, porous solids having framework structures, crystal growth and Raman & Brillouin scattering.
- Developing new strategies for the synthesis, purification, functionalization and solubilization of nanotubes [multi-walled and single-walled carbon nanotubes, junction nanotubes, core-shell nanostructures such as fullerene encapsulated nanotubes ("peapods", C_{60}@SWNTs)] to study the electrical transport, optical and other confinement properties.
- Synthesis, characterization and properties of nanotubes and nanowires of various inorganic materials including elements, metal oxides, nitrides, carbides and chalcogenides using new synthetic strategies.
- Synthesis of composites of nanotubes and nanowires with various polymers to enhance their properties for potential applications in mechanical, electronic, sensor and other devices.
- The study mainly in phenomena and properties exhibited by transition metal oxide systems, including high temperature superconductivity, colossal magnetoresistance, metal-insulation transition and multifunctionality.
- Synthesis of metal and semiconductor nanocrystals/nanoparticles in colloidal sols as well as at liquid-liquid interfaces, ligand-shell modification, core-shell nanocrystals, magic nuclearity nanocrystals, mesoscalar assemblies.

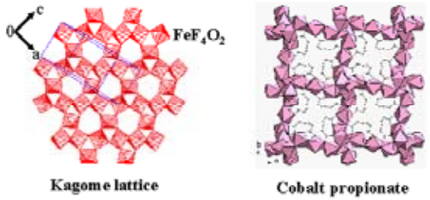

Figure 1: Framework solids

Chemical Biology Unit

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The Chemical Biology Unit is located on the campus of the Indian Institute of Science. The work carried out in this unit by the Honorary Faculty Members of JNCASR covers many of the emerging areas of chemical biology.

Recent and Current Work

Isolation and Structure Determination of Unusual Peptides from Fungal Sources: For example, two new cyclohexadepsipeptides, Isaridin A and Isaridin B, were recently isolated from the fungus *Isaria*, and characterized by a combination of ESI MS, 500MHz ^{1}H NMR and single crystal X-ray analysis.

Effect of Signal Peptide on the Stability and Folding Kinetics of Maltose Binding Protein : While the role of the signal sequence in targeting proteins to specific sub-cellular compartments is well characterized, there are fewer studies that characterize its effects on the stability and folding kinetics of the protein. Detailed characterization of the folding kinetics and thermodynamic stabilities of Maltose Binding Protein (MBP) and its precursor form, preMBP have been achieved.

Design of Temperature Sensitive Mutants: Temperature sensitive (Ts) mutants are powerful tools to study gene function in vivo. Ts mutants are typically generated by random mutagenesis followed by laborious screening procedures. Using the *E. coli* cytotoxin CcdB as a model system, simple procedures for generating Ts mutants at high frequency through site directed mutagenesis have been developed.

Total Synthesis of Complex Bioactive Natural Products: The idea is to explore these natural products as lead or 'privileged' structures for drug discovery by creating molecular diversity around them. The protocols developed for the total synthesis should lend themselves to ready adaptation to generate small molecule libraries. Recently, the total syntheses of over a dozen molecules of varying degree of complexity were achieved, which exhibit activities ranging from the inhibition of angiogenesis to promotion of apoptosis. Some of these natural products are of great contemporary interest.

Cationic Surfactants, Novel Lipids and Nucleic Acid Analogs: Novel Cationic Surfactants with multiple pyridinium headgroups provide a number of opportunities for application in diverse areas. Such molecules have been synthesized, and their aggregation properties have been investigated using spectroscopic and small-angle neutron scattering studies. A new class of lipids with oxyethylene linkages have been developed and their biophysical properties after membrane formation have been investigated. Cationic Gemini micellar media have been shown to enhance dephosphorylation and deacylation reactions suggesting possible applications for detoxification (nerve gases, pesticides) and enzyme mimics. Using novel strategy distamycin-linked oligonucleotides with chosen sequences have been synthesized. Their duplex formation and related physical characterization has been completed.

Bile Acid Chemisty: The study of novel analogs of bile acids have led to the design of unusual gelators which have diverse applications. Thus, such bile gels have been used for the design of thermochromic materials, as templates for the design of inorganic nano structures, and also for the anchoring of stabilized metal nanoparticles. A variety of phosphonobile acids are being developed for examining their effect on bile acid metabolism *in vivo*. Cationic analogs of bile acids are being investigated for cholesterol gallstone dissolution.

Condensed Matter Theory Unit

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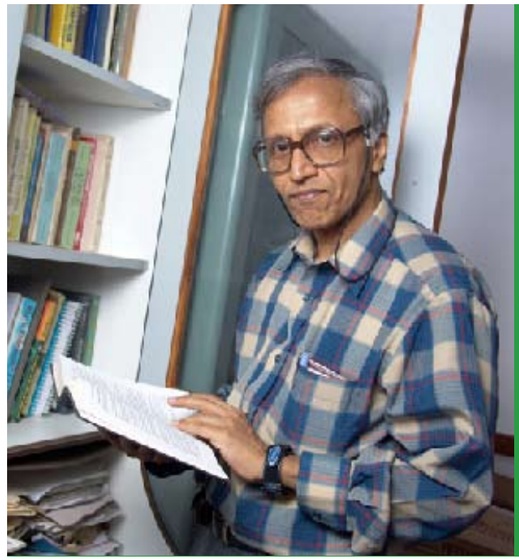

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This Unit consists of 14 Honorary Faculty Members of JNCASR and several R&D Assistants. This unit receives support from JNCASR in the form of funds for Research Associates, R&D assistants and Visitors, Computational Facilities and a contingency grant for day-to-day expenses and domestic travel. The members of CMTU are engaged in theoretical research on a variety of topics in the general area of Physics and Chemistry of Condensed Matter systems, some of which are as mentioned below:

Electronic Structure, Especially Strongly Correlated Electron Systems:
Dynamical effective medium theories; *d*-wave superconductivity in cuprates; Luttinger liquids and quantum wires; Molecular Magnetism and Photomagnetism; Electron-hole recombination, Triplet-triplet Annihilation and Excitation Transfer in Organic Light Emitting Diodes; Calculation of Auger spectra including matrix element effects; Calculation of X-ray magnetic circular dichroism spectra from compounds; Kinetically-driven magnetism in a class of magnetic compounds (double perovskites, dilute magnetic semiconductors); Spin-wave dispersions in double perovskites; Electronic structure of semiconducting nanomaterials by real space calculations; Study of a spintronic material, *Mn*-doped *GaAs,* in the nanometric size regime; Theories of doped manganites, including spin, charge and orbital ordering effects; Studies of low-dimensional interacting quantum systems using the density-matrix renormalization group and other numerical methods.

Equilibrium and Non-equilibrium Statistical Mechanics of Soft Condensed Matter and Other Complex Systems:
Systems of vortex lines in high-T_c superconductors in the presence of pinning; Frustrated magnetic systems; Study of Portevin-Le Chatelier effect through time series analysis and modeling; Study of martensitic transformations; Multiscaling in fluid and magnetohydrodynamic turbulence; Spatiotemporal chaos and spiral turbulence in excitable media, including models for ventricular fibrillation; Semiflexible polymers; Dynamic scaling in driven systems; Orientational and solvation dynamics in complex liquids; Phase diagrams and dynamics of charged micellar systems; Dynamics of ions in complex porous networks and biomembranes; Laser-induced freezing in colloidal systems; Numerical studies of the glass transition and slow dynamics in models of simple liquids; Equilibrium properties of classical fluids in a random potential; Complex networks in chemical, biological and social systems; Evolution of complexity in adaptive systems; Analytic and numerical studies of neural network models; Modeling of the growth of thin films under chemical vapour deposition and molecular beam epitaxy; The statistical mechanics of sedimentation; Dynamics and rheological chaos in surfactant solutions; Theory and experiments on ordered nonequilibrium steady states in agitated monolayers of granular rods; Statistical hydrodynamics of self-propelled organisms, from fish to bacteria to cell-membranes coupled to motors, filaments, and ATP; Rheology of the living cell.

ResearchFacilities
Network of workstations, personal computers and peripherals.

Academic Activities

Academic Programmes

Graduate Student Programmes

JNCASR has a bright and diverse student body. At present, there are 113 students registered in the various academic programmes of the Centre. While the majority of these students are pursuing a PhD degree, we also have students enrolled in our Integrated PhD, MS, and MS (Engineering) programmes. The student population at JNCASR is drawn from across the length and breadth of the country; in addition, we frequently have foreign students visiting the Centre under various exchange programmes.

The majority of new students join the Centre during the August semester each year; they are admitted based on their performance in interviews carried out in the early summer. Certain programmes also consider admitting students halfway through the academic year (i.e., at the start of the January semester). In order to be eligible for consideration in these interviews, students have to meet various academic criteria, as specified below. Admission in these programmes is fairly competitive eg., in 2005, 715 students applied, 480 were called for interviews, and finally 31 were admitted.

All students who are admitted to the Centre's programmes receive stipends that are more than adequate to cover their tuition and living expenses, including hostel fees, etc., and they get an opportunity to attend international meetings/ workshops through partial funding for travel from the Centre. Our students have recently attended conferences in countries such as Korea, Iran, France, Singapore, USA, Japan, Sweden, and Italy.

We generally expect students to take five years to complete a regular PhD programme, and seven years to complete the Integrated PhD programme; however, several students have completed their research and obtained their degrees in a shorter time than this. Students who are admitted to the Integrated PhD programme also get an MS degree, typically two years into their programme of study.

In addition to carrying out research, students take a combination of required and elective courses. The majority of courses are held on-campus, and taught by the Centre's faculty members. However, students can also choose to attend a few courses at other scientific institutes in the Bangalore area. In addition to regular academic courses, there are also seminar courses, and we have recently introduced a course on scientific writing. After completing two years in their PhD programmes, students have to pass an oral comprehensive examination, where they present and are quizzed about their research as well as the material covered in their coursework.

Since 2002, the Centre is recognized as a "Deemed University" by the University Grants Commission, and students' degrees are awarded directly by JNCASR. Since the inception of the Centre, 42 degrees have been awarded; these include 24 PhD's, 13 MS degrees, 4 MS (Engg.) and 1 MSc (by research) (Biological Sciences).

Students who are alumni of the Centre have gone on to enjoy successful academic careers, and are currently spread out across the world.

Eligibility Requirements for PhD / MS / MS (Engg.) Programmes

Candidates with an MSc, BE, BTech, ME, MTech or MBBS are eligible to apply; the specific requirements for each Unit are listed below. They should have at least 50% in their highest University examination, and should also have qualified in the GATE/UGC-CSIR-NET, JRF/ICMR, JRF/JEST/competitive advanced national level examination. Candidates with a Master's degree in Engineering/Technology/Medicine, however, do not require a qualifying exam.

Integrated PhD Programme

This programme is offered only in the Chemistry and Physics of Materials Unit (CPMU) and admits two or three students per year. Selection is based on a competitive entrance examination, followed by an interview, conducted in Bangalore. Candidates with a first class BSc in physics, chemistry or mathematics are eligible to apply. They take chemistry oriented courses to get an intermediate MS degree in chemical sciences.

Prospective students can use the following table to see which programmes they are eligible to apply for:

Candidate's Degree	PhD	Integrated PhD	MS	MS (Engg.)
BE/BTech/ME/MTech	CPMU		EOBU	CPMU*
	EMU		MBGU	EMU
	EOBU			TSU
	MBGU			
	TSU			
BSc: Physics, Chemistry, Mathematics		CPMU		
MBBS, MD	EOBU		EOBU	
	MBGU		MBGU	
MSc: Biosciences, Life Sciences, Bioinformatics, Statistics	EOBU			
MSc: Chemistry, Materials Science, Electronics	CPMU			CPMU
	EOBU			
	MBGU			
	TSU			TSU
MSc: Physics, Mathematics	CPMU			CPMU
	EMU			EMU
	EOBU			
	MBGU			
	TSU			

*including specialisation in nano science and nano technology

Scholarships/Fellowships/Assistantships

All Integrated PhD students receive a stipend of Rs.4,000 in their first two years; this is raised to Rs.8,000–9,000 in subsequent years. All PhD and MS/MS (Engg.) students receive scholarships of Rs.8,000–10,000. [Typically, perhaps 20% of this goes towards paying hostel and mess fees, while the annual tuition fee is Rs.4,000 for PhD and Rs.3,000 for MS/MS (Engg.)]. Students are automatically enrolled in a Group Insurance Scheme and a comprehensive medical scheme and have access to an on-campus doctor, as well as to medical facilities elsewhere.

The following merit-based awards are also awarded to outstanding students each year:

- The Babu Matru Prasad Scholarship is available for an Integrated PhD student.
- The Smt & Sri Bapu Narayanaswamy Prize is given to the best MS thesis of an Integrated PhD student.
- The Prof CNR Rao Medal will be awarded to the best physical and biological science PhD thesis of the year.

Graduate Courses

The students admitted to PhD, MS and MS (Engg.) degrees undergo a one-year course programme in their respective disciplines, whereas students working towards an Integrated PhD follow a two-year long course programme. Though the majority of courses are taught on-campus by the Centre's faculty members, students may also choose to attend a few courses at neighbouring institutes. Currently, the following courses are offered at JNCASR:

JC 201	Fundamental Concepts in Chemical Physics
JC 202	Experimental Techniques for Materials
JC 204	Special Course in Chemistry and Physics of Materials
JC 205	Seminar Course
JC 206	Physical Chemistry
JC 207	Solid State Chemistry
JC 208	Organic and Inorganic Chemistry Lab.
JC 209	Basics in Nanoscience
JC 301	Photonics: Properties, Materials and Devices
JC 302	Introduction to Surface Science and Thin Films
JC 303	Selected Topics in Materials Science
JC 304	Chemistry of Materials
JE 201	Population and Quantitative Genetics
JE 202	Chronobiology
JE 203	Introduction to Population Dynamics
JE 204	Basic Quantitative Tools in Biology
JE 301	Evolutionary Genetics of Fitness
JE 302	Chronobiology: Advanced Aspects
JF 201	Mathematical Methods
JF 202	Nonlinear Dynamics: Applications to Fluid Dynamics
JF 301	Advanced Topics in Fluid Dynamics
JN 201	Scientific Writing
JM 201	Introduction to Genetics
JM 202	Basic Biological Chemistry
JM 203	Advanced Molecular Biology & Genetics
JM 204	Basics in Immunology
JM 205	Cell Biology
JM 206	Gene Expression and Development
JM 207	Advanced Course in Regulation of Gene Expression
JM 301	Advanced Molecular Genetics
JT 201	Solid State Physics
JT 202	Computational Methods
JT 203	Advanced Theoretical Chemistry
JT 204	Statistical Mechanics
JT 205	Quantum Mechanics I
JT 301	Computational Methods for Electronic Structure
JT 302	Topics in Condensed Matter Theory
JT 303	Quantum Mechanics II

Degrees Awarded

The Centre is a Deemed University, and awards PhD, MS, and MS (Engg.) degrees. Since the inception of the Centre, 45 students have obtained degrees. The universities, research institutes and corporate research laboratories where our alumni have gone on to pursue their career include: Rockefeller University; University of California, Santa Barbara; National Institute of Health; New York University; Queen's University, Kingston, Canada; University of Liverpool; SISSA, Trieste; GE, Hindustan Lever and University of Heidelberg.

Below, we list all the students who have been awarded degrees during 1997 to 2005.

MS IN CHEMICAL SCIENCES

Meciya Kalaiselvam, *An Investigation of Submicron Particles of Oxidic Materials Prepared by Nebulized Spray Pyrolysis and by the Sonochemical Method* (Advisor: CNR Rao)

R Srinivas Gopalan, *Investigations of Rare Earth Manganites and Metal Nanoparticles* (Advisors: CNR Rao and GU Kulkarni)

S Neeraj, *Investigations of Mesoporous Solids* (Advisor: CNR Rao)

K Vijaya Sarathy, *Metal Nanoparticles and Their Crystalline Arrays* (Advisor: CNR Rao)

TR Anupama, *Design of Organic Solids Based on Supramolecular Hydrogen-Bonded Assemblies* (Advisor: CNR Rao)

Sachin Parashar, *Investigations of Thin Films of Metals and Metal Oxides Deposited by Nebulized Spray Pyrolysis* (Advisors: CNR Rao and AR Raju)

P John Thomas, *Investigations of Metal Nanocrystals* (Advisors: CNR Rao and GU Kulkarni)

R Vaidyanathan, *Investigations of Open-Framework Metal Oxalates and Phosphates* (Advisors: CNR Rao and S Natarajan)

Gautam Gundiah, *Investigations of Macroporous and Mesoporous Materials* (Advisor: CNR Rao)

K Shivashankar, *Studies of Supramolecularly Organized Chemical Systems and of Open-Framework Metal Squarates and Organic Amine Squarates* (Advisor: CNR Rao)

S Vijayalakshmi, *Molecules Co-adsorbed on Metal Surfaces: Investigations Using X-ray Photoelectron Spectroscopy* (Advisor: GU Kulkarni)

Ayan Datta, *Quantum Chemical Investigation of Linear and Nonlinear Polarizabilities in Organic Molecular Aggregates and Inorganic Clusters* (Advisor: Swapan K Pati)

SRC Vivek Chand, *New Strategies for the Synthesis and Characterization of Nanotubes and Nanowires* (Advisor: CNR Rao)

N Arun, *Electric Field Effects on Surface Patterns and Hybrid Structures Based on Bacteriorhodopsin/Conjugated Polymers* (Advisor: KS Narayan)

KP Kalyanikutty, *Investigations of Inorganic Nanomaterials* (Advisor: CNR Rao)

MS IN ENGINEERING

Binaya Kumar Dhar, *Unsteady Aerodynamics of Flapping Flight* (Advisor: KR Sreenivas)

Kirti Chandra Sahu, *Numerical Computation of Spatially Developing Flows by Multigrid Technique* (Advisor: Rama Govindarajan)

Ashwin S Sampangiraj, *Study of Dynamics and Electronic Structure of Supercooled Liquids,* (Advisor: Srikanth Sastry)

Antina Ghosh, *Simulation of Nano-scale Flows by Molecular Dynamics Methods* (Advisors: Rama Govindarajan and Srikanth Sastry)

MSc (BY RESEARCH)

G Praveen Bhat, *Cloning and Characterization of the Eukaryotic Initiation Factor 2α from the Malarial Parasite Plasmodium falciparum* (Advisor: Namita Surolia)

PhD

S Neeraj, *Investigation of Open-Frame Work Metal Phosphates and Mesoporous Solids* (Advisor: CNR Rao)

R Srinivas Gopalan, *Investigations of Molecular Crystals Using Experimental Charge Density* (Advisor: CNR Rao)

AA Alagiri Swamy, *Defect-Induced Transport Studies of Semiconducting Polymers* (Advisor: KS Narayan)

V Sheeba, *Probing the Adaptive Significance of Circadian Rhythms using Drosophila melanogaster* (Advisor: Amitabh Joshi)

IN Sujay Subbaiah, *Investigations on the Plasmodium falciparum, Human and Chimeric Hypoxanthine Guanine Phosphoribosyltransferases* (Advisor: Hemalatha Balaram)

B Vadhiraja Bhat, *Bio-Modulatory Properties of: (i) C-Phycocyanin, A Biliprotein from Spirulina Platensis, (ii) Novel Analogues of Uric Acid* (Advisor: KM Madyasta)

K Vijaya Sarathy, *Charge Ordering and Related Phenomena in Rare Earth Manganates and Metal Nanoparticles and Their Assemblies* (Advisor: CNR Rao)

P John Thomas, *Mesoscopic Organization and Properties of Nanocrystals of Metals, Metal Oxides and Other Materials* (Advisors: CNR Rao and GU Kulkarni)

Lakshmi Ramakrishna, *Engineering and Evaluation of Molecular Adjuvants for DNA Immunogens Based on the HIV Transactivator (Tat) Proteins from Indian Isolates* (Advisor: Udaykumar Ranga)

Priyaranjan Pattanaik, *Protein Structure and Dynamics: Studies on the Plasmodial Proteins—Triosephosphate Isomerase (TIM) and Hypoxanthine Guanine Phosphoribosyltransferase (HGPRT) and Plasmepsin II* (Advisor: Hemalatha Balaram)

Sachin Parashar, *Investigations of Thin Films of Rare Earth Manganites, Magnetoferroelectrics and Related Materials* (Advisors: CNR Rao and AR Raju)

Sourav Banerjee, *Regulation of p53 Function By Non-Histone Chromosomal Proteins, HMGB-1 and PC4* (Advisor: Tapas Kumar Kundu)
L Sudheendra, *Colossal Magnetoresistance, Charge Ordering, Phase Separation and Related Properties of Rare Earth Manganates* (Advisors:CNR Rao and AR Raju)
P Vinmathi Vanitha, *Ferromagnetism, Metallicity, Charge Ordering and Related Aspects of Rare Earth Manganates and Cobaltates* (Advisor: CNR Rao)
TR Anupama, *Investigations of Hydrogen-Bonded Organic Solids by X-ray Crystallography and Experimental Charge Densities* (Advisors: CNR Rao and GU Kulkarni)
Th Birendra Singh, *Novel Organic Polymer Based Photodetector Structures* (Advisor: KS Narayan)
Gargi Raina, *Investigations of Molecular Clusters and Other Species Employing a Cluster Beam Apparatus* (Advisors: CNR Rao and GU Kulkarni)
AG Manoj, *Photoelectric Properties of Hybrid Conjugated Polymer Based Bilayer Structures* (Advisor: KS Narayan)
Saji Varghese, *Band Model Computation of Near-surface Longwave Fluxes* (Advisor: R Narasimha)
R Vaidhyanathan, *Metal Carboxylates with Open-Architectures* (Advisors: CNR Rao and S Natarajan)
R Jayalakshmi, *Structure-function Studies on Successive Purine Salvage Pathway Enzymes-Hypoxanthine Guanine Phosphoribosyltransferase and Adenylosuccinate Synthetase* (Advisor: Hemalatha Balaram)
Gautam Gundiah, *Investigations of Nanomaterials and Porous Materials* (Advisor: CNR Rao)
M Krishnan, *Phase Behaviour of Linear Molecular Crystals in Bulk and on Graphite: A Molecular Dynamics Simulation Study* (Advisor: S Balasubramanian)
Mohd Jamal Dar, *Studies on Plasmodium falciparum Enoyl-ACP Reductase (FabI)* (Advisor: Namita Surolia)
NG Prasad, *Life-history evolution in Laboratory Populations of Drosophila melanogaster Subject to Selection for Faster Development and Early Reproduction* (Advisor: Amitabh Joshi)

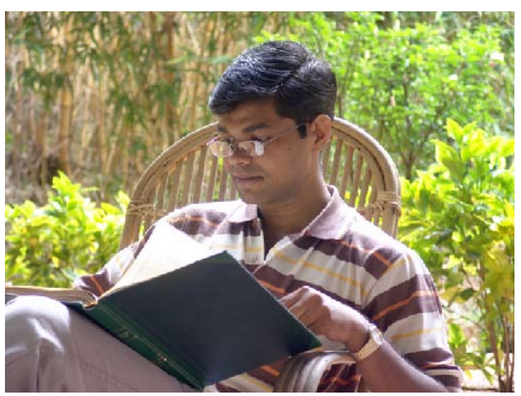
Student Life

At JNCASR, a willingness to engage echoes throughout student life, both in and outside of the laboratory. The students are accommodated in two modern, spacious and architecturally striking hostels. At the students' hostel, one can find students chatting in their double or single rooms, snacking in the well-catered mess, absorbing the latest programmes in the TV room, or thrashing an opponent at table tennis. The hostel's kitchenette encourages students to develop their gourmet instincts, and the Laundromats ensure that more time can be spent reading the latest additions to the hostel's student-run book club. Moreover, the athletic facilities—volleyball court, cricket ground, and the current construction of a well-equipped gymnasium, badminton and basketball courts—only add to the richness of student life.

This engagement is fostered through the multifarious expressions of student voices. For example, the student's movie committee arranges the screening of a new or popular movie every Saturday night. The mess committee receives input from the student body to decide the monthly mess menu. The sports committee arranges athletic activities and suggests improvements to the existing facilities. Organizers of the Hostel Day celebration, held during the third week of January, arrange a showcase of students' cultural, art, musical, and athletic talents. Participants in 'Dhavani' have rousing discussions on anything from quantum mechanics to post-modernism and oftentimes brainstorm on their latest vexing research problems. Indeed, it appears that the same passion for pursuing the intricacies of scientific issues is responsible for the enriching and stimulating extra-curricular life.






Extension Programmes

Visiting Fellowships

www.jncasr.ac.in/extn_prog/vf

To foster collaborations with the Centre's faculty and to provide research opportunities, the Centre offers Visiting Fellowships to research scientists working in educational institutions and R&D laboratories in India. Visiting fellows are associated with faculty and honorary faculty of the Centre, and the research work is in the broad areas of *Life Sciences* (including molecular and developmental biology, chronobiology, genetics, ecology, behaviour); *Materials Sciences* (including nanoscience); *Chemical Sciences* (including solid-state chemistry, theoretical/computational chemistry, and inorganic, physical and organic chemistry); *Physical Sciences* (including experimental and theoretical condensed-matter and materials physics, statistical physics, organic electronics and experimental nanobiotechnology); *Engineering Sciences* (including fluid dynamics, nonlinear dynamics, and thermal and chemical engineering); and *Atmospheric Sciences*. The fellowship is tenable for 2 or 3 months and carries a suitable honorarium. The place and period of work may be decided according to mutual convenience. So far sixty-two scientists have visited the Centre under this programme from various parts of India, e.g., from Davanagere, Garhwal, Jammu, Kollam, Lonavala and Aizawl.

The announcement for these fellowships appear in Current Science and on our website around July every year. Application forms may be downloaded at any time from **http://www.jncasr.ac.in/extn_prog/vf** or obtained by writing to the Assistant Coordinator, JNCASR, Jakkur, Bangalore 560 064.

Short-Term Courses

www.jncasr.ac.in/extn_prog/stc

These are of 2 or 3 days duration and are offered by the Centre's faculty or honorary faculty along with other resource persons. Each course consists of a series of lectures in a chosen area at a University outside Bangalore. The target audience is typically the scientific community of the region, including students and teachers.

The Centre bears the travel costs of the speakers, and pays them an honorarium, while the host institution takes care of local hospitality and arrangements for the course work. Twenty-two courses have been conducted so far and many more are being planned. Among the courses that have been conducted so far are *Concepts in Chemistry* at Guru Nanak Dev University, Amritsar, *Finite Element Methods and Applications* at the Siddaganga Institute of Technology, Tumkur, *Frontier Lectures in Molecular Biology & Genetics* at Mangalore University, Mangalore, Nanomaterials at SV University, Tirupati. A complete list is available on our website.

A University interested in the possibility of conducting such a course may contact the faculty member whose research interests match closely with the proposed course content.

Summer Research Fellowships Programme

www.jncasr.ac.in/extn_prog/srfp

The Centre offers summer fellowships for two months to bright undergraduate and MSc students (renewable for a second year for selected students). This programme has proved to be popular and competitive; each year, about 5000 students from all over India apply for the 120 fellowships awarded. Fifty fellowships are supported by the Department of Science & Technology, Government of India, fifteen by the Rajiv Gandhi Institute for Contemporary Studies, New Delhi, and the rest by the Centre. Students are placed with research groups at the Centre or with scientists elsewhere in India. They are paid travel expenses and a monthly stipend of Rs. 4000. Selected students get the opportunity to participate in cutting-edge research, and several summer projects have led to publications in leading journals. A random sample of projects pursued in past years is: *Preparation of* $La_{0.5}Sr_{0.5}Co0_3$ *by Sol-Gel spin coating method; Study of correlated response to selection on faster development and early reproduction in Drosophila melanogaster; A study of the chaotic nature of flow in the neighborhood of vortices; Statistical analysis of fatal mining accidents in eight companies of Coal India Ltd.* Many of the summer students of past years have gone on to pursue graduate studies and a research career, at the JNCASR or at another leading university.

The announcement for these fellowships appear in the media and on our website in October/ November every year. At the appropriate time, application forms may be downloaded from **http://www.jncasr.ac.in/extn_prog/srfp** or obtained by writing to the Assistant Coordinator, JNCASR, Jakkur, Bangalore 560 064. Selected students are intimated by regular mail or e-mail, and the list is announced on our website, during the last week of February.

Project Oriented Chemical Education

www.jncasr.ac.in/extn_prog/poce

In 2004, the Centre initiated the Project Oriented Chemical Education programme (POCE), to give an opportunity to young bright undergraduates who are interested in chemistry to discover their potential. The programme, spread over three consecutive summers for 6-8 weeks each year, is planned so as to nurture a scientific temper in the participants and equip them to take up research as a career.

About 10 students from anywhere in the country, in the first year of their BSc, are selected to participate. They are offered a monthly scholarship of Rs.4000.

In the first summer, students attend lectures, carry out experiments and participate in seminars and discussions. During the second summer, each student works with a faculty member on a small project, in addition to attending academic lectures and giving seminars. During the third summer students do research work.

We have received a very good response to this programme; in fact, several participating students have expressed a desire to spend even more time at the Centre (such as during the winters), to continue work on their research projects. Those who complete the programme successfully are given certificates by the Centre.

The announcement appears in the newspapers and on our website around December each year. At the appropriate time, application forms may be downloaded from **http://www.jncasr.ac.in/extn_prog/poce** or obtained by writing to the Coordinator, Science Outreach Programme, JNCASR, Jakkur, Bangalore 560 064.

The programme is being coordinated by Professor SN Bhat with Dr A Govindaraj.

Project Oriented Biological Education

www.jncasr.ac.in/extn_prog/pobe

As part of Science Outreach, the Centre is initiating the Project Oriented Biological Education programme (POBE) for undergraduate students. The programme will be conducted during summer for a period of 6 to 8 weeks. Students are expected to work at the Centre for three such periods and upon completion will receive certificates from the Centre. Those currently studying in I year BSc (any science stream) are eligible to apply. Selected students will be paid a monthly scholarship of Rs. 4000.

The programme is conceived of as an adjunct to, and not a replacement for, the body of factual information students typically imbibe during their undergraduate curriculum in biology. In POBE, our focus is on equipping students with the conceptual, experimental and inferential tools that will help them in subsequent research work. We will introduce students to an integrated view of living systems, highlighting common underlying concepts and mechanisms, and emphasizing that interesting questions in biology can be approached simultaneously at various levels of structural organization, using a whole range of tools and techniques. Practical work will be integrative and emphasize the use of modern tools, data analyses, and experimental design to solve problems. An attempt will also be made to tie up this programme with some exposure to active research areas in biology today, as the students will undertake a research project in their third year under the direct supervision and mentoring of our faculty members.

The announcement will appear in the media and on our website around December each year. Students who are interested to apply can download the application form from **http://www.jncasr.ac.in/extn_prog/pobe** or obtain it by writing to the Coordinator, Science Outreach Programme, JNCASR, Jakkur, Bangalore 560 064. The programme is organised by Prof. Anuranjan Anand and Prof. Amitabh Joshi, and will be conducted by biology faculty at JNCASR, with participation from faculty of other institutions.

Lectures and Meetings

Special Lectures

The Centre organizes a few special lectures and hosts brief visits by eminent scientists from all over the world. Interaction with these scientists and their account of some of the important developments in science benefit the researchers at the Centre. Speakers of these special lectures have been:

THE LINUS PAULING LECTURE

- **YT Lee**, Nobel Laureate, *Steering chemical reactions through laser excitation* (1994)
- **Jean-Marie Lehn**, Nobel Laureate, *Supramolecular chemistry: Scope and perspectives* (1995)
- **James D Watson**, Nobel Laureate, *Human genome project* (1997)
- **Patrick Bateson**, *Genes, instincts and identity* (2001)
- **Anne Mclaren**, *Pluri potent stem cells, and the ethical and legal implications of their use* (2003)

THE MICHAEL FARADAY LECTURE

- **Lord Porter**, Nobel Laureate, *Electron and energy transfer in photosynthesis* (1995)
- **Sir John Meurig Thomas**, *In-situ methods in the study of catalysts* (1996)
- **Roald Hoffmann**, Nobel Laureate, *Molecular beauty* (1998)
- **Michael Sela**, Wolf Laureate, *From synthetic antigens to synthetic vaccines against infections and autoimmune diseases* (1998)
- **Ahmed H Zewail**, Nobel Laureate, *Femtosecond realm* (2002)
- **Alan J Heeger**, Nobel Laureate, *Plastic electronics and optoelectronics* (2005)

THE ISAAC NEWTON LECTURE

- **P de Gennes**, Nobel Laureate, *Principles of adhesion* (1996)
- **P Nozieres**, *Elastic effects at surfaces: A model of dry friction* (1997)
- **Phillip A Griffiths**, *Mathematics at the turn of the millennium* (1999)
- **Jacob Palis**, *Chaotic and complex systems* (2001)

Endowment Lectures

The Centre organizes a series of lectures named after individuals who have contributed significantly to the science and engineering research in India. These lectures are endowed by various departments of the government of India or scientist/foundation. Topics of these lectures span a broad spectrum from art, social and natural sciences to technology. Speakers of these lectures have been:

ISRO-SATISH DHAWAN LECTURE

The Department of Space, Government of India has instituted this lecture series in 1999.

- MGK Menon, *Place for values in the world of science* (1999)
- Thomas Odhiambo, *Science scenario in Africa: Preparing for a quantum jump* (2000)
- Deepak Nayyar, *Globalisation and development* (2002)
- Rajnish Mehra, *Equity premium: Current estimates and prospects for change* (2003)
- UR Anantha Murthy, *On being an Indian writer* (2004)
- Montek Singh Ahluwalia, *Growth, equity and poverty: What are the prospects?* (2005)

DAE-RAJA RAMANNA LECTURE SERIES IN PHYSICS

The Department of Atomic Energy has instituted this lecture series in 1999.

- BV Sreekantan, *Physics, the universe and consciousness* (1999)
- R Chidambaram, *The May 1998 Pokhran tests—Scientific aspects* (2000)
- TV Ramakrishnan, *Why are the colossal magneto resistance manganites so strange?* (2001)
- N Kumar, *Quantum zeno effect: C-axis transport in high-tc layered materials* (2002)
- SS Kapoor, *Frontiers in nuclear fission, superheavy nuclei and nuclear energy* (2003)
- SK Joshi, *C axis normal state transport in Cuprates* (2004)
- AK Sood, Dynamics of surfactant solutions: *Super diffusion and rheochaos* (2005)

Prize Lectures

- Chandan Dasgupta, *Universal concepts in the theory of glassy systems* (1999)
- HR Krishnamurthy, *Dynamical cluster approximation for strongly correlated systems* (2000)
- Bikash Sinha, *Micro and the macro cosmos* (2001)
- S Dattagupta, *Coherence versus decoherence* (2002)
- Anil Kumar, *Quantum computing by nuclear magnetic resonance* (2003)
- Mustansir Barma, *Phases and fluctuations in nonequilibrium systems* (2004)
- NV Madhusudana, *Liquid crystals made of banana shaped molecules* (2005)

AV RAMA RAO FOUNDATION LECTURES IN CHEMISTRY

The Rama Rao Research Foundation has instituted this lecture series in 1999.

- MM Sharma, *Innovative momentum of chemical industry* (1999)
- RA Mashelkar, *On putting life into gels* (2000)
- G Mehta, *Natural product synthesis: Is it relevant any more?* (2001)
- A Chakravorthy, *Some reflections and a few results* (2002)
- BM Deb, Being and becoming: *Quantum systems in intense external fields* (2003)
- JP Mittal, *Laser photons as specific reagents in organic chemistry* (2004)
- G Vijay Nair, *Novel C-C bond-forming reactions and their applications in organic synthesis* (2005)

Prize Lectures

- Darshan Ranganathan, *Designer peptides for supramolecular tubular structures* (1999)
- SS Krishnamurthy, *Journey into the organometallics continent with the torch of phosphorus* (2000)
- H Ila, *From synthons to bioactive molecules: Efficient strategies for heterocycle synthesis* (2001)
- Swapan K Ghosh, *Density functional theory in chemistry* (2002)
- J Gopalakrishnan, *Turning solids into materials: Chemistry plays a key role* (2003)
- Kalidas Sen, *Electronic structure calculations of confined atoms and molecules* (2004)
- RN Mukherjee, *Iron and copper complexes of varying nuclearity, inorganic and bioinorganic perspectives* (2005)

V RAMALINGASWAMY MEMORIAL LECTURE IN BIOLOGY

The Department of Biotechnology, Government of India has instituted this lecture series in 2002.

- Ananda M Chakrabarty, *Microbial pathogens and cancer: Using one ancient enemy against the other* (2002)
- MS Valiathan, *Caraca-Physician-Extraordinary of India* (2003)
- G Padmanaban, *Newer facets of malarial parasite biology and biochemistry* (2004)
- Miroslav Radman, *Mutation, recombination and evolutionary biotechnology* (2005)

CNR RAO ORATION AWARD LECTURE

Professor CNR Rao, the Linus Pauling Research Professor at the Centre contributed funds to institute an Oration Award for the faculty at the Centre. The awardees have been:

- Amitabh Joshi, *Development and competition in fruit flies: A tale of two densities* (2000)
- Srikanth Sastry, *Slow dynamics and the glass transition in liquids* (2001)
- Anuranjan Anand, *On genetic aspects of non-syndromic deafness in humans* (2002)
- KS Narayan, *Photoelectric activity bacteriorhodopsin–conducting polymer interface* (2003)
- Rama Govindarajan, *Unconvering patterns in the laminar-turbulent transition* (2004)
- Hemalatha Balaram, *Malaria: Understanding Plasmodium falciparum biochemistry* (2005)

Annual Faculty Meeting Lectures

An annual get-together of Faculty and Honorary Faculty is held in November every year at the Centre. In addition to a discussion on academic matters among faculty, a programme of lectures by five faculty members on their recent research activity is organized. The latter is open to all members of the Centre.

The lectures delivered in 2004 and 2005 are listed below:

- Umesh V Waghmare, *Computational studies and design of materials: A first-principles approach* (2004)
- Meheboob Alam, *Granular fluid* (2004)
- S Yashonath, *Size dependence of self diffusivity: Stokes-Einstein relation and levitation effect* (2004)
- Diptiman Sen, *Conductances of quantum wires: The effects of interactions, scattering points and junctions* (2004)
- R Varadarajan, *Rational design of temperature sensitive mutants* (2004)
- SB Krupanidhi, *Ultra-low dimensional ferroelectrics* (2005)
- G Rangarajan, *Linear and nonlinear causalitym measures* (2005)
- A Sundaresan, *Multiferroic oxides* (2005)
- Seyed E Hasnain, *Mycobacterium tuberculosis: Molecular epidemiology new diagnostics and drug discovery* (2005)
- Satyajit Mayor, *Rafts, nanoclusters and endocytic pathways of GPI-anchored proteins* (2005)

Meetings

The Centre provides a forum for scientific meetings and in-depth discussions on important and exciting topics in science and engineering. These are aimed at promoting interaction and collaboration among scientific community. The Centre supports its Faculty, Honorary Faculty, IISc Faculty and distinguished scientists in India to organize meetings. So far 415 meetings have been held.

The meetings held at Bangalore during 2004 and 2005 are listed below:

- *International Conference on Nonlinear Phenomena,* January 5–10, 2004, G Rangarajan (IISc).
- *3rd Global meet on Parasitic Diseases,* January 12–16, 2004, NJ Shetty (Bangalore University).
- *International Symposium on Cellular and Molecular Biophysics,* January 14–17, 2004, NB Joshi (NIMHANS).
- *IV Annual Meeting of the Indian Society for Study of Reproduction and Fertility,* January 23–25, 2004, PB Seshgiri (IISc).
- *Short Course on Cell Biology,* January 29–February 5, 2004, Manju Bansal (IISc).
- *NCC 2004: Tenth National Conference on Communication,* January 30–February 2, 2004, GV Anand (IISc).
- *Materials for the Future MF 2004,* March 22–23, 2004, K Chottopadhyay (IISc).
- *Tenth Asian Congress of Fluid Mechanics,* May 17–21, 2004, TS Prahlad (NAL, Bangalore).
- *Summer Course on Understanding Science: Introduction to History and Philosophy of Science for College Students,* June 14–25, 2004, R Narasimha (JNCASR).
- *Workshop on Unifying Concepts in Glass Physics III,* June 28–July 1, 2004, Srikanth Sastry (JNCASR) and Silvio Franz (ICTP).
- *IUPAP International Conference on Statistical Physics STATPHYS 22,* July 4–9, 2004, TV Ramakrishnan (IISc), S Dattagupta (SNBCBS) and Rahul Pandit (IISc).
- *National Symposium on Advances in Geotechnical Engineering,* July 22–23, 2004, BR Srinivasa Murthy (IISc).
- *Perspectives in Minerals, Metals and Materials Research,* July 22–23, 2004, S Subramanian (IISc).
- *Seminar on Assessment and Management of Water Resources (AMWR-2004),* July 26, 2004, BK Raghuprasad and MS Mohan Kumar (IISc).
- *AIDS in India: A Workshop-Symposium on Research, Trials and Treatment,* July 31–August 7, 2004, Udaykumar Ranga (JNCASR), VR Prasad (AECOM) and V Ravi (NIMHANS).
- *Indo-US Workshop on Nanotechnology: Issues in Interdisciplinary Research and Education,* August 11–13, 2004, K Chattopadhyay (IISc).
- *Lecture and Panel Discussion on Nano Science and Technology,* August 26, 2004, (JNCASR and IISc).
- *In-house Brainstorming Meeting on Challenges to Indian Science and Scientists,* September 1, 2004, (JNCASR).
- *Consortium of Students in Management Studies 2004,* September 24–25, 2004, NJ Rao, (IISc).
- *Seminar on Science, Development and Education,* September 27–28, 2004, (TWASROCASA, JNCASR).
- *Asia-Pacific EPR/ESR Symposium,* November 22–25, 2004, SV Bhat (IISc).
- *International Workshop on Risk Assessment in Site Characterization and Geotechnical Design,* November 26–27, 2004, (Civil Engg Dept, IISc).
- *IUTAM—Symposium on Laminar Turbulent Transition,* December 13–17, 2004, Rama Govindarajan (JNCASR).
- *Symposium on Epigenetics,* December 22–23, 2004, V Nanjundiah (IISc) and Maneesha Inamdar (JNCASR).
- *6th Meeting of OP 2005—Optical Probes of Conjugated Polymers and Biosystems,* January 4–8, 2005, KS Narayan (JNCASR) and S Ramasesha (IISc).
- *25th International Symposium on Shock Waves,* July 17–22, 2005, KPJ Reddy (IISc).
- *Indo-Japan Workshop on Understanding of Chromatin Structure Function,* January 20–23, 2005, Tapas Kumar Kundu (JNCASR) and Masami Horikoshi (IMCB).
- *Recent Trends in Solid State NMR in Biological Systems,* January 24–26, 2005, KV Ramanathan (IISc).
- *Scientific Computation, Numerical Analysis and Application (Workshop 1),* January 24–February 4, 2005, G Rangarajan (IISc).
- *Advances in Spectroscopy,* February 21–24, 2005, S Umapathy and E Arunan (IISc).
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- *International Conference on Scientific Computation, Numerical Analysis and Application,* July 18–21, 2005, G Rangarajan (IISc).
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- *National Conference on Case Studies in Geotechnical Engineering (Geopractice 2005),* July 25–26, 2005, GL Sivakumar Babu (IISc).
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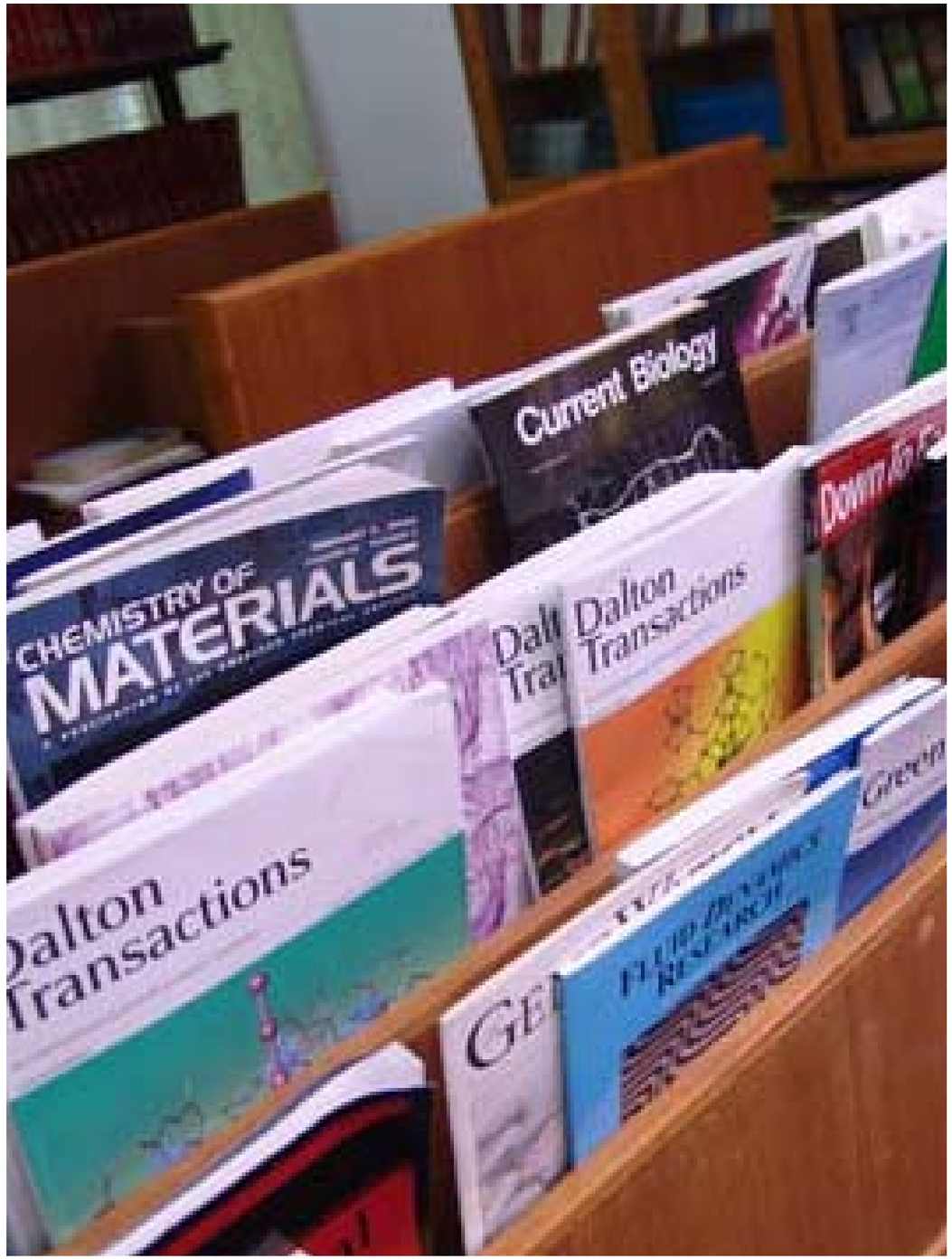

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Intellectual Property

The Centre values the creative and innovative research being carried out by its faculty and has an enabling mechanism for protecting novel innovations which can be usefully exploited by Industry. It has constituted an Intellectual Property Management Committee which addresses all issues concerned with securing, maintaining, protecting and valorizing the Intellectual Property created by its faculty. The Centre has not only filed and secured a very high per capita number of patents, but has also licensed a high percentage of them to Industry.

In addition, the Centre holds copyright over a number of educational monographs and multimedia packages on interesting areas in science and engineering.

Some of the patents already granted to the Centre and others at various stages of examination, have been indicated below:

Title of the Invention: Use of Hydroxydiphenyl Ether Class of Chemicals, as Exemplified by Triclosan, as an Antimalarial and Identification of Fatty Acid Synthesis at its Target
Inventors: Surolia N and Surolia A
Applicants: JNCASR and IISc
Entered National Phase at various countries. Australian Patent No. 780085. South African Patent No. 2001/2305.

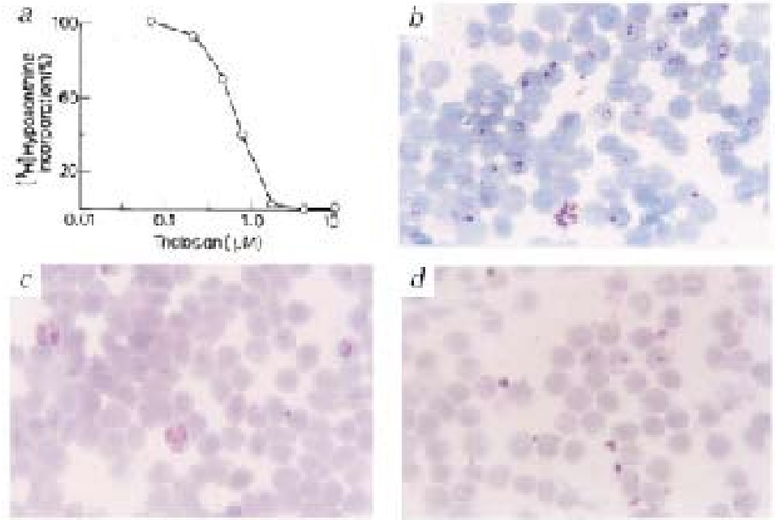


Figure 1: In vitro antimalarial activity of triclosan. a, [3H]hypoxanthine uptake by the parasite. b-d, Giemsa stained smears of triclosan untreated/treated parasites. b, control treated 48 h. c, Triclosan treated 24 h. d, Triclosan treated 48 h.

Title of the Invention: Modulators (Inhibitors/Activators) of Histone Acetyltransferases
Inventors: Kundu TK, Balasubramanyam K, Swaminathan V
Entered National Phase at various countries.

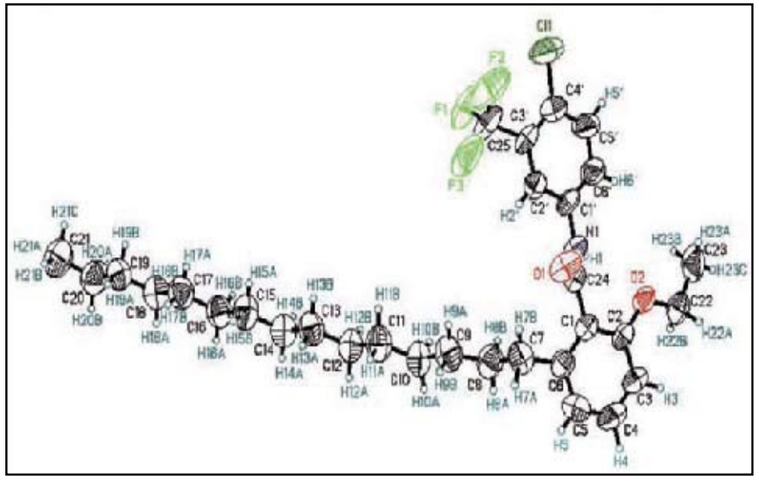


Figure 2: Based on the natural inhibitor of histone acetyltransferases (HATs), Anacardic acid, inventors have synthesized the first known small molecule activator of HAT that is specific to p300.

Title of the Invention: Process for Extraction of Superior Quality Plasmid DNA
Inventor: Ranga U
Indian Patent No.193223.

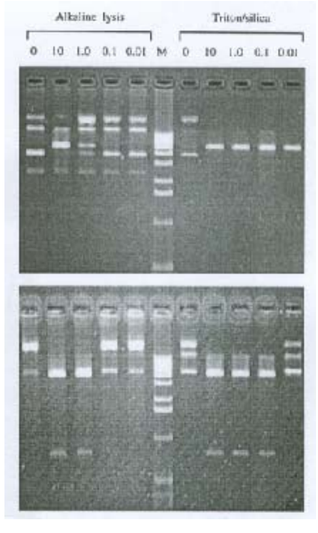


Figure 3: Comparison of the purity of the mpDNA isolated using the Triton/silica method with that of alkaline lysis. 5 ml of the mpDNA was incubated with varying concentrations of HindIII (top) or EcoRI (bottom) for 1 h at 37°C. The concentration of the enzyme (units/reaction) is shown at the top of the lanes. The following restriction patterns were expected after successful enzyme digestion: HindIII, linearization; EcoRI, 801 and 4425 bp. M, 1 kb.

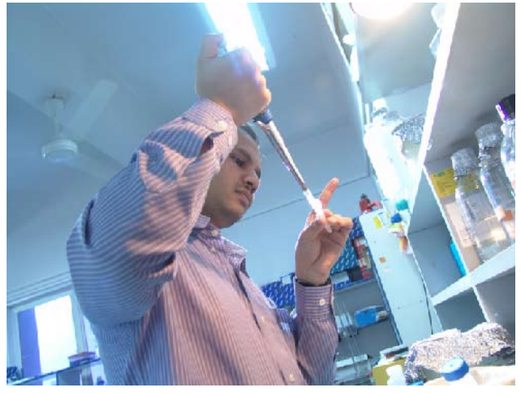
Title of the Invention: Photo Responsive Organic Field Effect Transistor
Inventor: Narayan KS
US Patent No. 6,992,322. Filed Continuation Patent Application.

Title of the Invention: Polyisoprenyl Benzophenones as Inhibitors of Histone Acetyl Transferases and Uses Thereof
Inventors: Kundu TK, Balasubramanyam K
Entering National Phase soon.

Title of the Invention: Use of Curcumanoids as Histone Acetyltransferases (HATs) Inhibitors
Inventors: Balasubramanyam K, Varier RA, Altaf M, Swaminathan V, Kundu TK
Filed in India and USA. Entering National Phase at various countries.

Title of the Invention: Highly Specific Polyclonal Antibodies of Individual Core Histone and Uses Thereof
Inventors: Kulangara FK, Varier RA, Kundu TK, Das C
Filed PCT (International Patent Application)

Title of the Invention: Specific Derivatives of 1,2,4-Triazolo-1,3,4-Thiadiazole Condensed Heterocyclic Nucleus Bearing Novel Small Molecule Compounds Induce Cancer Specific Cell Death: Lead Compounds for Anti-Neoplastic Therapeutics
Inventors: Kundu TK, Varier RA, Shivananju N, Basappa, Rangappa KS
Applicants: JNCASRA and University of Mysore
Filed in India



Central Facilities

Animal Facility

The Animal Facility is located in a secluded corner of the campus, away from noise and pollution, providing an excellent environment for animal care. The facility is equipped for small animal experimentation with quarantine, breeding and experimental rooms for rodents and rabbits.

The facility is registered with the CPCSEA (Reg.No. 201/CPCSEA). The procurement of animals from other sources is strictly controlled by animal facility management and users are required to adhere to the guidelines. The breeding centre can provide a small number of mice if required for approved experimentation at JNCASR. Animal experimentation is under the control of the Institutional Animal Ethics Committee of JNCASR and animal use is regulated as per the guidelines of the Government of India. Investigators obtain approval of the IAEC before initiating experiments. Member of the Animal Facility: Suresh.

Computer Laboratory

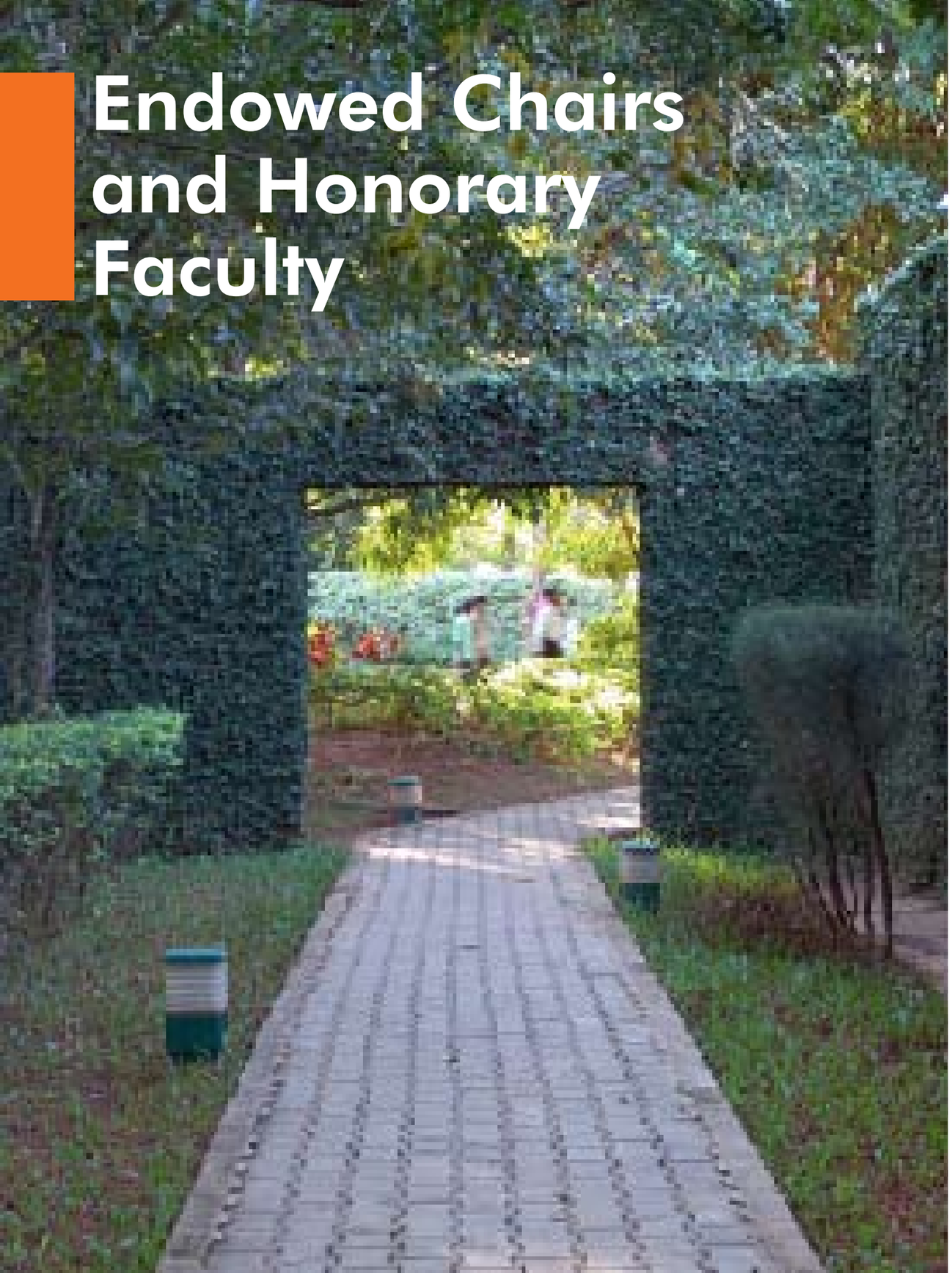
Say Bangalore—think IT. Given Bangalore's fame as the emerging icon of the world's burgeoning Information Technology industry, it may come as no surprise that the JNCASR community has round-the-clock access to well-maintained, world-class computational infrastructure. The Computer Lab at JNCASR houses heavy-duty number-crunching machines, and also looks after maintenance and updates for the numerous PCs and workstations scattered throughout the Centre. It is also responsible for maintaining our fast Internet links (through both satellite and phone lines).

The high performance computing (HPC) resource has a 0.325 TFLOPs capacity; recent acquisitions include an SGI Altix 350 shared memory machine, and two Sun Fire V60x and Sun V60z distributed memory machines. Additionally, the 24-hour central computing facility contains a terminal room with several desktop PCs—with both Linux and Windows operating systems—that are equipped with a wide range of the latest software. Moreover, all members of JNCASR have access to free print-outs from the computing facility's high-quality printers. The days when one had to wait, twiddling one's thumbs, while an image downloaded with glacial slowness, are long past! At present, all offices and laboratories have exceptionally fast Internet access through an optical fibre-based local area network (LAN). Members of the Computer Laboratory currently include: Computer Laboratory Head Umesh V Waghmare; Staff Members TK Shithal and M Vikash. To ensure maximum efficiency, an outside contractor also provides additional round-the-clock technical support.

Library

The Library at JNCASR serves as a repository and resource for books and journals, and manages electronic services such as online journal subscriptions and search / citation indices. It also provides a pleasant environment for those who would like to take a break from their laboratories for a while, and browse through the latest issue of "Nature" or "The Economist", while lounging in a comfortable armchair.

Steadily amassing books at the rate of several hundred per year, the library contains a comprehensive collection of documents that are available throughout the day. Currently, around 4000 documents—books, conference proceedings, monographs and theses—and over 80 journal subscriptions are housed in the library. In addition to catering to the specific scientific interests of individual groups at the Centre, there are also copies of textbooks that have been prescribed for courses, and books and journals of general interest, which have been bought at the suggestion of members of the JNCASR community. Apart from the standard on-site services and a document delivery service, the library provides an inter-library loan facility with neighbouring institutes such as IISc, RRI, NCBS and NIAS. Library staff members include: AR Jayamangala, Nagesh Hadimani and E Nandakumari.



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Endowed Chairs

Many scientific institutions and industrial houses have instituted endowment chairs at the Centre. Eminent scientists in India hold these chairs at the Centre.

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MM Sharma, Emeritus Professor of Eminence, Mumbai University, Mumbai.

Hindustan Lever Chair
A Chakravorty, Indian Association for the Cultivation of Science, Kolkata.
V Krishnan, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.

Linus Pauling Research Professor
CNR Rao, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.

Vikram Sarabhai Research Professor
BM Deb, S N Bose National Centre for Basic Sciences, Kolkata.

In additon, the Centre hosts AstraZeneca Chair, SS Bhatnagar Chair, Gharda Chair and IBM Information Technology Chair.

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In order to further our aims of scientific collaboration, outreach activities and extension programmes, several distinguished scientists, academics and administrators from across the country are associated with JNCASR in an honorary capacity.

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MK Bhan, Dept. of Biotechnology, New Delhi.
S Bhattacharya, Tata Institute of Fundamental Research, Mumbai.
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S Chandrasekaran, Indian Institute of Science, Bangalore.
Dipankar Chatterji, Indian Institute of Science, Bangalore.
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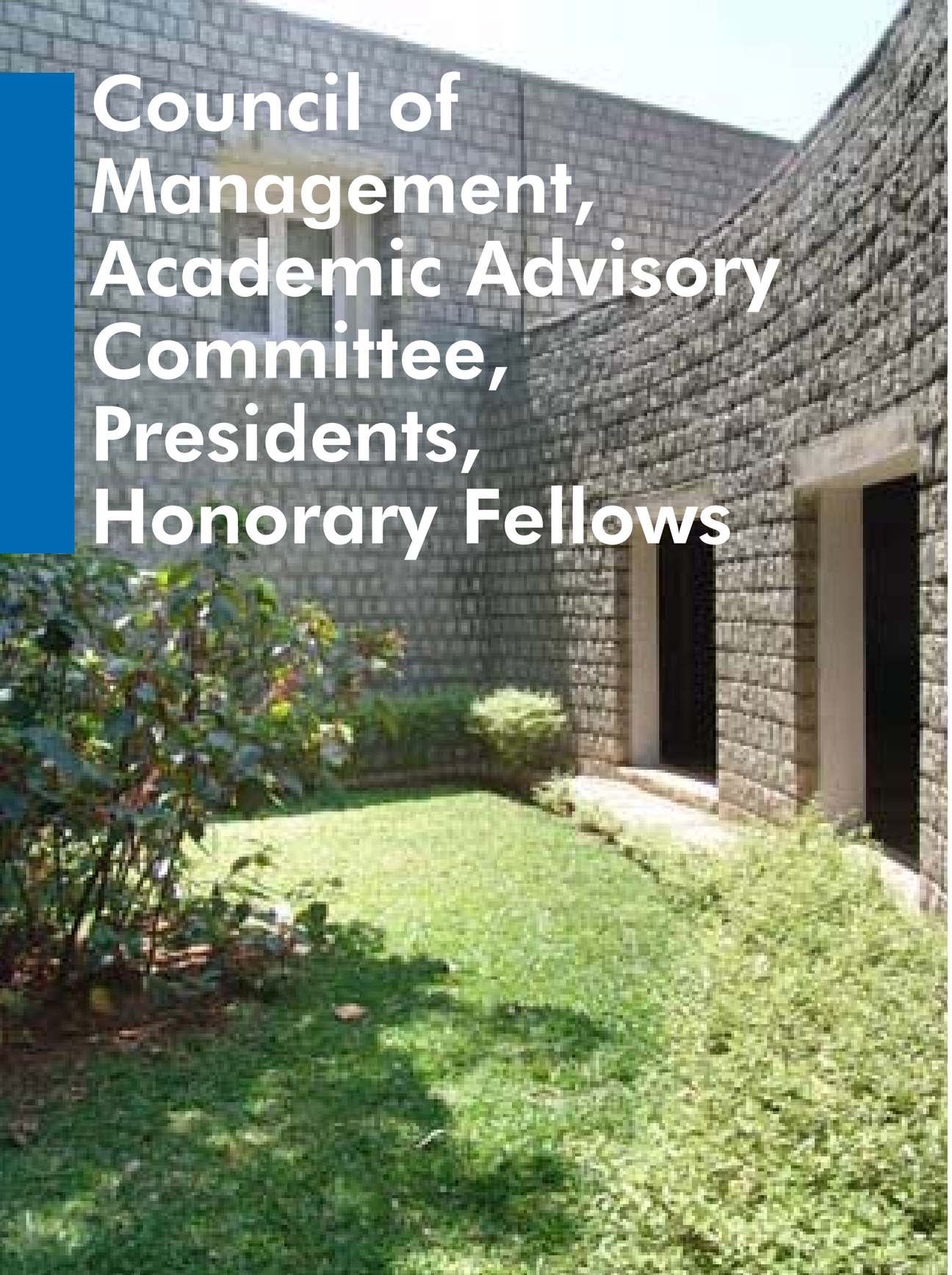
Organisation



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