Jawaharlal Nehru Centre for Advanced Scientific Research 2007–2008

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Contents

New Initiatives from JNCASR

New Chemistry Unit

Members of this Unit carry out research on important interfaces of chemical science with materials, biology and other areas. Some of the specific areas being pursued are asymmetric organic synthesis, peptide and protein chemistry, biomaterials, organic supramolecular chemistry, theoretical chemistry, carbon and oxide based materials and catalysis. The Unit admits students for the PhD degree programme which includes research and course work.

Facilities

400 MHz NMR Spectrometer
X-Ray Diffractometers
FT-IR, UV-Vis and Fluorescence Spectrometers
Parallel Peptide Synthesizer
Gas Chromatograph Mass Spectrometer (GC-MS)
Liquid Chromatograph Mass Spectrometer (LC-MS)
High Performance Liquid Chromatography (HPLC)
Gel Permeation Chromatography (GPC)
Digital Polarimeter
Nano research facilities
Various materials characterization facilities

Members

Chair

Professor CNR Rao	FRS, Hon. FRSC, National Research Professor and Linus Pauling Research Professor

Faculty Fellows

T Govindaraju	PhD
Subi Jacob George	PhD

Associate Faculty

M Eswaramoorthi	PhD, Faculty Fellow, CPMU
Tapas Kumar Maji	PhD, Faculty Fellow, CPMU
Swapan K Pati	PhD, Associate Professor, TSU
A Sundaresan	PhD, Associate Professor, CPMU

Honorary Faculty Fellow

A Govindaraj	PhD

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Organic synthesis (asymmetric), Peptide and protein chemistry, Bionanotechnology (Biomaterials)

Our research activities are at the interface of chemistry and biology. Currently we are involved in three different research projects which are interdependent and complementary. First we synthesize chiral unnatural amino acids with metal binding properties (metal binding ligands). These chiral-amino acid ligands will be used for the 'asymmetric induction' in metal mediated asymmetric syntheses. This provides us a novel methodology to access chiral biologically important natural products and synthetic organic molecules with diverse applications. New chiral-amino acid ligands obtained as mentioned above would also help us to develop 'sensors' for different metal ions in complex fluids and to assess their concentration levels. A new class of oligomers with metal binding ligands will be designed and synthesized. These synthetic oligomers serve as smart-building blocks for the design and synthesis of metal directed assemblies and will find applications as biomaterials.

PhD Student
Debabrata Maity

T. Govindaraju has obtained his PhD (2005) in Chemistry from National Chemical Laboratory (NCL), Pune. He was a postdoctoral fellow in Chemical and Biological Engineering, and Biochemistry at University of Wisconsin-Madison, Madison, USA. He was an Alexander von Humboldt Research fellow in Chemical Biology at Max Planck Institute of Molecular Physiology, Dortmund, Germany before joining JNCASR in 2008.

Subi Jacob George

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Organic and Supramolecular Synthesis, Functional Organic Materials, Chiral Nanotechnology

The underlying theme of our research lies at the interface between synthetic efforts on small molecules/polymers and macroscopic properties at the materials level, developing a macro-organic approach to chemistry. A major focus will be on the design of self-assembled functional systems from chromophores or π-conjugated oligomers, which are the key ingredients in the integration of electronic components for nano-sized electronics. Special attention will be given to the synthesis of multi-component self-assembled fibers with increased complexity and well-defined dimensions. Another focus will be on the design of supramolecular polymeric materials that are capable of sensing and reversible switching in response to external stimuli (stimuli responsive polymers). In an extension of this work novel supramolecular polymers with biodegradable functionality will also be investigated. Next to the wish to design new functional organic materials, we aim at 'Chiral Nanotechnolgy', where design of chiral polymeric/organic self-assembled nanomaterials for the enantioselective recognition, separation and asymmetric catalysis are targeted.

PhD Student
Venkata Rao Kotagiri

Subi Jacob George has obtained his Ph D in Organic Chemistry from National Institute for Interdisciplinary Science and Technology, NIST (CSIR) (formerly RRL), Trivandrum, India. He was a post-doctoral fellow at Eindhoven University of Technology, The Netherlands before joining JNCASR in August 2008.

International Centre for Materials Science

Members

Director

CNR Rao	FRS, Hon. FRSC, Hon. F Inst. P, Director

Professors

SM Shivaprasad	PhD (Karnataka)

Associate faculty from CCMS

Balasubramanian Sundaram	PhD (IISc.)
Shobhana Narasimhan	PhD (Harvard)
Swapan K Pati	PhD (IISc.)
Srikanth Sastry	PhD (Boston)
Umesh V Waghmare	PhD (Yale), FA Sc., FNA Sc.

Associate faculty from CPMU

Chandrabhas Narayana	PhD (IISc.), Associate Professor
M Eswaramoorthy	PhD (Anna), Faculty Fellow
GU Kulkarni	PhD (IISc.), Professor
KS Narayan	PhD (Ohio State), FNA Sc., Professor
A Sundaresan	PhD (IITB), Faculty Fellow
Tapas Kumar Maji	PhD (IACS), Faculty Fellow

Honorary faculty

AK Sood	FA Sc., FNA, FTWAS
A Govindaraj	PhD (Mysore), of SSCU, IISc

Incharge-Coordinator

Aruna V Mahendarkar

www.jncasr.ac.in/icms

ICMS is the first international centre of its kind devoted to research, education and extension in materials science, established in the confines of a scientific cum educational institution. The Centre was envisaged by the Department of Science and Technology (DST), Government of India. The plan to establish the Centre got crystallized in 2007, with the Jawaharlal Nehru Centre for Advanced Scientific Research taking the lead and necessary steps to establish it. An important and unique activity of ICMS is to provide global research opportunities and to support international exchange programmes. ICMS is establishing major scientific user facilities to serve both in-house researchers and researchers from other universities. This facility will house specialized instrumentation maintained and run by experts. The research facilities include: Ultra High Resolution Electron Microscope, Pulse Laser Deposition, Molecular Beam Epitaxy System, X-ray Diffractometer and others.

The Centre for Computational Materials Science (CCMS), a constituent of ICMS, is one of the most powerful academic computing resources in the country. The ICMS building design houses several well ventilated offices, well planned Labs, spacious meeting rooms with video conferencing facilities and huge foyer and luxurious halls for the researchers to relax and contemplate. An international Visitors' House is also being established to accommodate visitors especially from abroad. Although, the building is still coming up, ICMS has already started to carry out the research activities.

The Activities and Programmes of ICMS are listed below:

Fellowship programme

- Sheik Saud RAK-CAM Fellowship: Prof. KS Narayan (Senior Fellowship) and SRC Vivek Chand (Junior Fellowship)

Schools and Workshops (Past)

- ICMS-ICMR International Winter School 2007, Dec 6-13, 2007 (with ICMR, UC Santa Barbara)
- A joint India-US workshop on Scalable Nanomaterials for enhanced Energy Transport, convenience and Efficiency, August 19-21, 2008 (with Purdue University)

Schools and Workshops (Future)

- International Winter school 2008, Dec 8-13, 2008 (with ICMR, UC Santa Barbara)
- Chemistry of Materials meeting arranged in collaboration (with Swedish Academy of Sciences) Feb 2-3, 2009

Proposals for Collaboration

- e-Icoon (Mesa+twente) being discussed
- Science bridges RCUK
- India-Iran joint program on Nano and Science and Technology
- A Joint IUSSTF program of Purdue (with ICMS/JNCASR and GE for Exchange of Graduate Student and Postdoctoral Researchers in Advanced Materials for Nanoscale Science and Technology)
- US-India S&T Forum proposal (with North Western University)

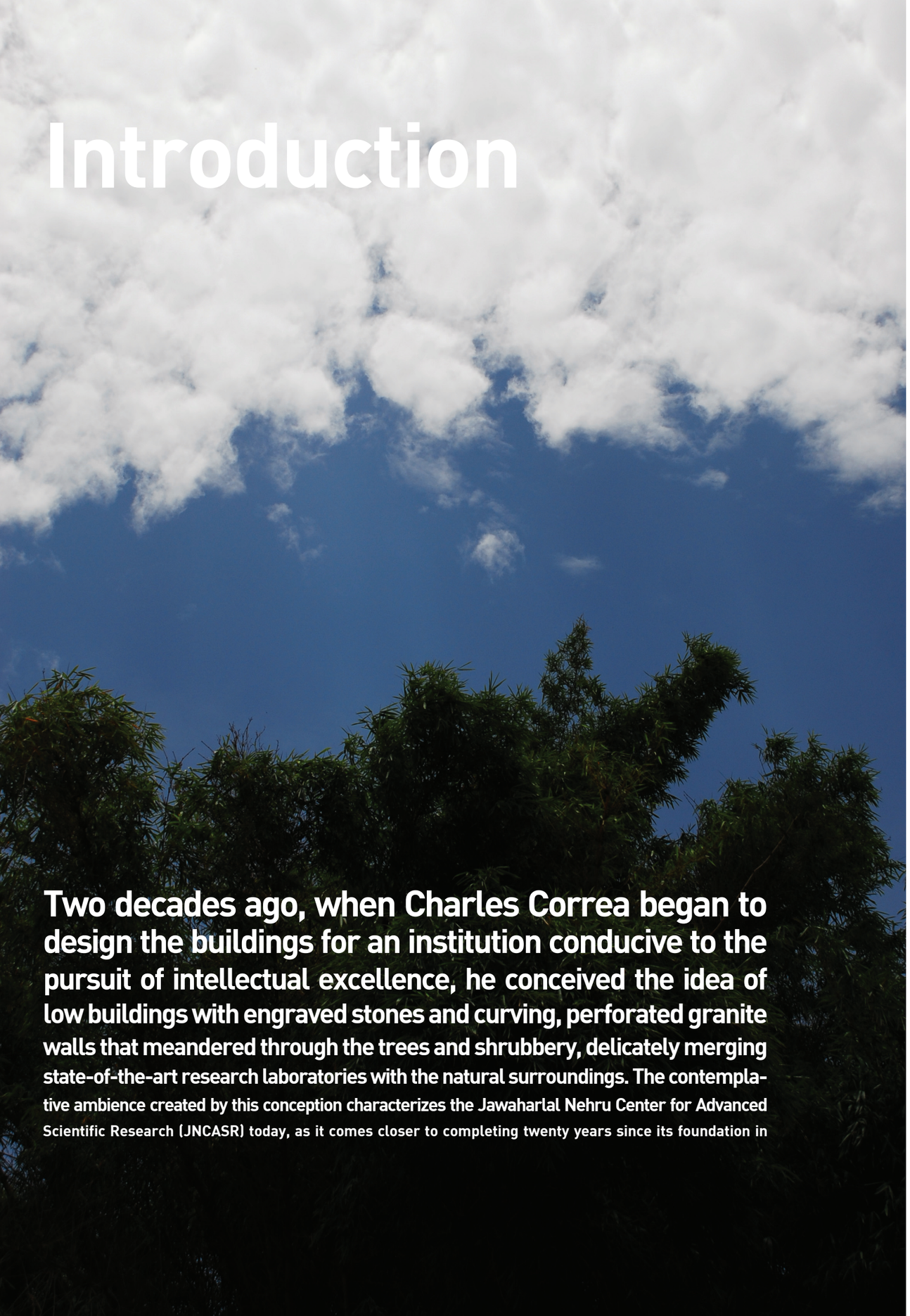
Visitors to ICMS (Past)

- Prof. Venkatesan Manivannan from USA
- Mr. Tran Duc Hoang from Vietnam
- Mr. Jafar Hoseini from Iran
- Ms. Nguyen Thi Mua from Vietnam

Visitors to ICMS (Future)

- Dr. Sharmin Kharrazi from Iran
- Mr. Md. Niyaifar from Iran
- Mr. Djafar Vatan Khah Dowlat Sara from Iran
- Mr. Joey Mangadlao from Philippines

Introduction



Two decades ago, when Charles Correa began to design the buildings for an institution conducive to the pursuit of intellectual excellence, he conceived the idea of low buildings with engraved stones and curving, perforated granite walls that meandered through the trees and shrubbery, delicately merging state-of-the-art research laboratories with the natural surroundings. The contemplative ambience created by this conception characterizes the Jawaharlal Nehru Center for Advanced Scientific Research (JNCASR) today, as it comes closer to completing twenty years since its foundation in 1989, under an initiative by the Department of Science and Technology, Government of India, to commemorate the centenary of Pandit Jawaharlal Nehru, the first Prime Minister of independent India.

As envisaged by its founders, research at JNCASR has seamlessly woven together diverse areas of science and engineering, fostering an extremely fruitful spirit of interdisciplinary collaboration. For instance, collaboration between a theoretical fluid-dynamist and an experimental physicist has helped develop femto cups, with potential applications ranging from nanoscale synthetic chemistry to single-cell biology. Similarly, a quantum mechanist has dedicated his thoughts to the mysteries associated with the transport properties of the DNA-helix, for applications in spintronics. 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-student ratio of about 1:5), and state-of-the-art experimental, computational and infrastructural facilities. Visitors to our campus are also invariably enamoured of our physical environment: the architecturally innovative buildings blend unobtrusively into several acres of lush landscape, with only the buckyball dome rising above the treetops; while kingfishers, cormorants 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, Education Technology and Geodynamics. We also have two off-campus units at the Indian Institute of Science focussing on Chemical Biology and Condensed Matter Theory. Though it is of course difficult to quantify scientific performance, by all numerical indications (number of publications, citations, grants, patents issued, 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, Naturwissenschaften, Evolution, Journal of the American Chemical Society, Angewandte Chemie, Journal of Fluid Mechanics and Physical Review Letters. The number of national and international patent applications filed and the technologies transferred has been steadily increasing. The work of the Centre's faculty is also being recognized by various awards. Prof. CNR Rao, our Honorary President and Linus Pauling Research Professor at the Centre, was recently awarded the Fellowship of University of Oxford, the only Indian scientist to receive this distinction. Prof. KS Valdiya received Padmashree from the Government of India, Prof. Rama Govindarajan was awarded the Shanti Swarup Bhatnagar Prize, Prof. Chandrabhas Narayana received MRSI Medal 2007, Prof. Balasubramanian Sundaram and Prof. Swapan K Pati received Swarnajayanthi Fellowship of DST, and Prof. Umesh V Waghmare received the BM Birla Science Prize in Physics and Prof. Meheboob Alam received the inaugural `Asian Young Fluid Dynamicist Award' (2007).

In addition to carrying out innovative scientific research, the Centre has a commitment towards fostering scientific education. We are a "Deemed University", and over a hundred graduate students are currently working toward 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 Education Technology Unit produces a range of teaching aids and educational materials; we organize and teach short term courses at universities across India; and promising young undergraduate students of Chemistry and Biology 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 enlivened by a regular stream of visitors from all over the world, who contribute to spirited scientific discussions at seminars, conferences and summer schools. Invited lectures by prominent researchers include Nobel laureates like YT Lee, Jean-Marie Lehn, James D Watson, Lord Porter, Roald Hoffman, Ahmed H Zewail, Alan J Heeger and P de Gennes. Apart from this, several endowment lectures, international conferences and workshops are organized every year to facilitate research and learning.

Chemistry and Physics of Materials Unit

Chairman
CNR Rao

Faculty
S Balasubramanian
N Chandrabhas
M Eswaramoorthy
GU Kulkarni
TK Maji
KS Narayan
SM Shivaprasad
A Sundaresan

Honorary Professors
AK Raychaudhuri
AK Sood

Distinguished Fellows
AK Cheetham
Gerard Ferey
Bernard Raveau

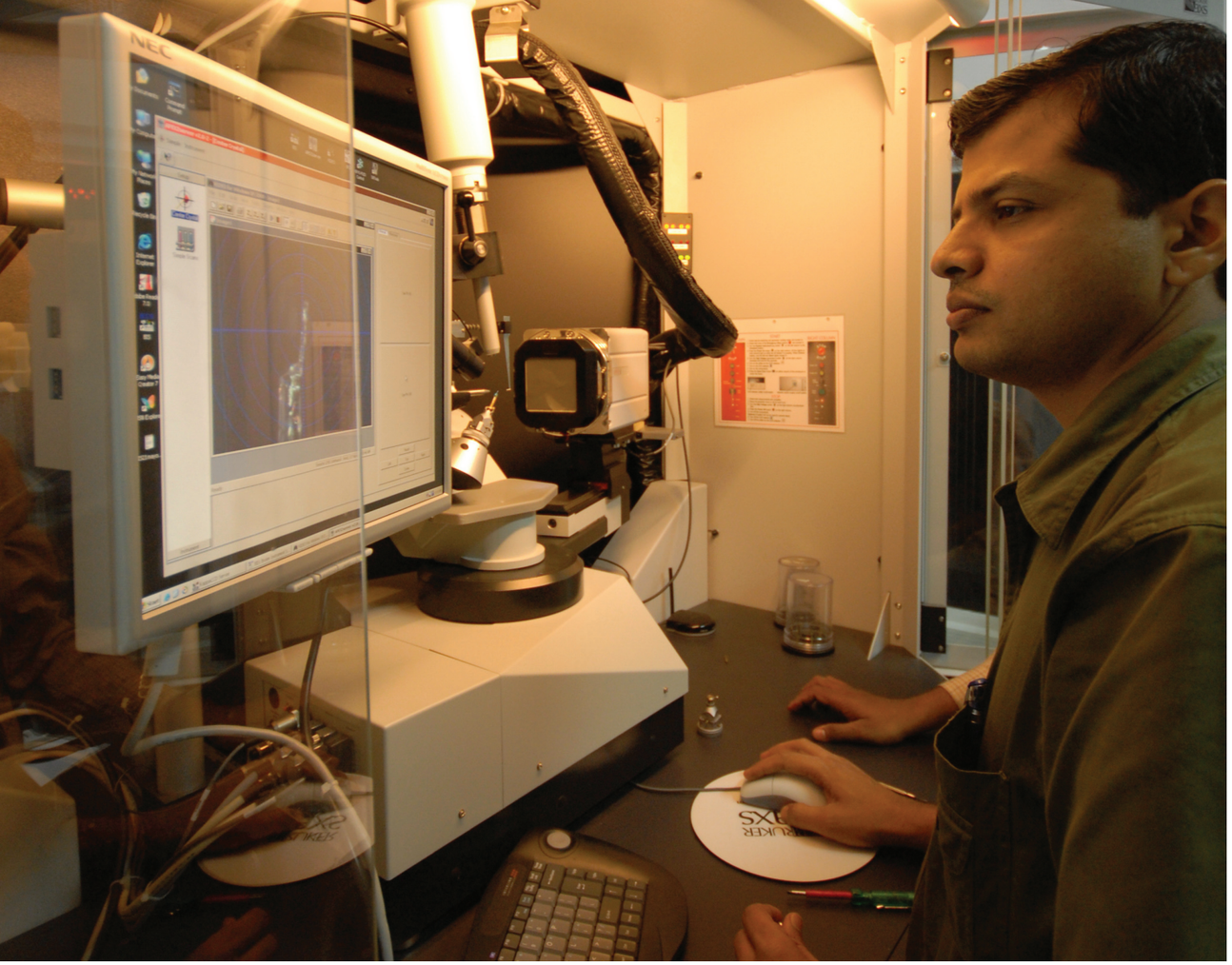
Materials research is at the frontiers of contemporary science and technology and thus constitutes major aspects of research investigations in both chemistry and physics. In recent years, biology has also become an essential component of materials research. This Unit is involved in the study of various facets of this interdisciplinary subject, with the primary goal being to understand and design the structure, properties and phenomena associated with advanced inorganic and organic materials. In the last few years, the Unit has acquired and developed sophisticated experimental facilities enabling state-of-the art methods to synthesize and characterize interesting properties and phenomena manifested in novel materials

Material synthesis forms a strong forte of this Unit where novel synthetic methods to produce organic and inorganic materials, including nanowires and nanotubes, have been developed. Materials at nanometer dimensions exhibit unique electronic, optical and magnetic properties that are different from their bulk forms, thus leading to potential novel technological applications. Nanotechnology being strongly dependent on the methods of synthesis, a variety of chemical and physical methods have been used to prepare nanoparticles of various metals, semiconductors and magnetic materials. Dip-pen lithography, electrostatic lithography using the AFM set-up and electron beam lithography have been employed to synthesize patterned nanomaterials on surfaces, as well as in the fabrication of nanocircuitry. Besides these techniques, pulsed laser deposition and RF magnetron sputtering methods have been employed to produce metal and metal oxide thin films, nanostructures and superlattices. Materials in different low dimensional forms are also being made by template-aided strategies, which are otherwise difficult to accomplish by conventional methods.

For example, supramolecular preorganization of organic molecules is used to synthesize functionalised clays, with spherical and tubular morphologies, which would find application in controlled drug release, ion sequestration and anisotropic composites. Work on heteroepitaxial structures and interfaces, is being initiated in the Unit. The materials synthesized in the Unit are probed by the state-of-the art characterization techniques (see page on Research Facilities).

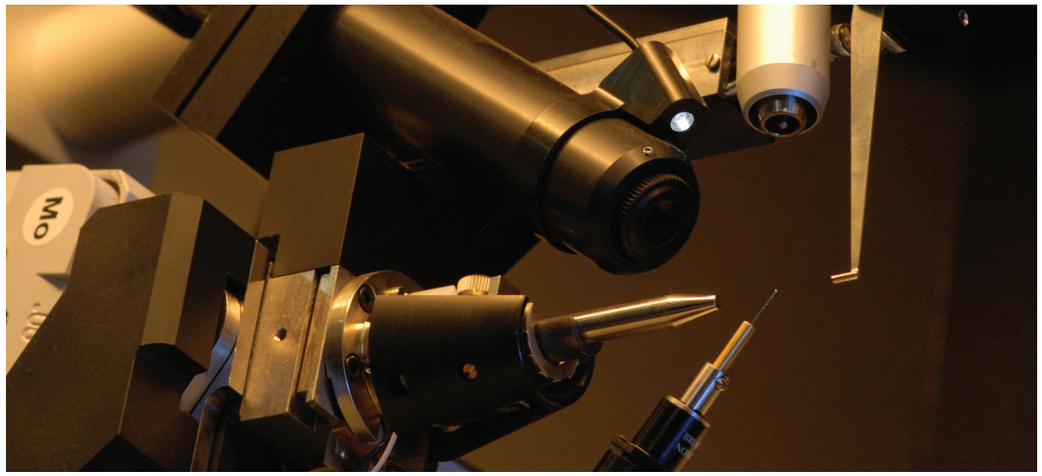
Studies of electronic, optical, photophysical and device aspects of organic, polymeric, nanoparticle and biomolecule based materials are being intensely pursued. This includes the study of the rich photophysics and electrical transport mechanisms in these systems, as well as probing new phenomena, and the development of devices such as Field Effect Transistors (FET), Light Emitting Diodes (LED) for flexible displays, Solar Cells and Image Sensors. Research innovations in the field of large area organic electronics are being actively pursued. Optical probes such as infrared, Raman and Brillouin scattering at ambient and extreme conditions, such as at high pressures, have been used to understand the structure, bonding and interactions in various materials, including those having technological importance. Recent research interest is on the surface enhanced Raman spectroscopy (SERS) by tagging gold and silver nanoparticles to proteins, polypeptides, etc., 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 activity focuses on the interdisciplinary area bridging physics and chemistry by employing simulation methods derived from classical, quantum and statistical mechanics. This group works closely with experimentalists and attempts to mimic the actual experimental conditions through simulations. A direct comparison of the simulations and experimental results enables the elucidation of the microscopic details underlying macroscopic phenomena.



Research Facilities

1. Single Crystal X-ray diffractometer with CCD facility (Bruker)
2. ESCA facility with UVPS, and LEED
3. Pulsed laser reactive ablation apparatus attached with mass spectrometer
4. Scanning Tunneling and Atomic Force Microscopes (STM/AFM) operating in air
5. Variable Temperature STM
6. Catalyst characterization with Gas chromatograph
7. Quadrupole Mass Spectrometer and Residual Gas Analyzer
8. Carbon arc-discharge Unit
9. Large number of furnaces for making samples in various atmospheres in the range 300°C to 1700° C
10. A closed cycle cryocooled 15 T superconducting magnet with a room temperature bore and an optical window
11. Floating zone melting crystal growth apparatus
12. High Resolution Transmission Electron Microscope (HRTEM) (300 kV, JEOL 3010)
13. Scanning Electron Microscope (SEM) with EDAX (Leica440I)
14. Magnetometer (VSM) and Faraday balance
15. Surface area measuring apparatus
16. Powder X-ray diffractometers (Bruker Siefert and Mini Rigaku)
17. Four Probe conductivity setup (15 K-325 K)
18. 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
19. Thermal characterization up to 1250 K (Mettler)
20. UV-VIS spectrometer (Perkin-Elmer)
21. Fluorescence spectrometer (Perkin-Elmer)
22. Mössbauer Spectrometer
23. Brillouin Spectrometer
24. Micro and Indigenously built Raman Spectrometers
25. Crystal polishing instrument
26. Diamond anvil cell for high pressure research
27. Optical stereo microscope with 200X magni□cation
28. Low temperature compressed Helium cryostat
29. Glove Box (← 2 ppm O_2 and H_2O environment) integrated with spin coating unit and accessories for device fabrication
30. Fabrication facilities for Light emitting diode (LED), photovoltaic (PV) diodes and solar cells, □eld effect transistor (FET)
31. Beowulf clusters for computational research
32. Device LED, PV, FET measurement facilities
33. Soft-lithography and Photolithography Implementation facilities
34. Time (→ 10 ns) and spatially (~ 50 nm) resolved photocurrent measurements
35. Photolumiscence emission and excitation spectroscopy
36. Physical Property Measuring System (PPMS, Quantum Design, USA) Evercool with 9T magnet (options: AC/DC susceptibility, AC/DC transport and heat capacity)
37. RF magnetron sputtering for making thin films and superlattices
38. Chemisorption - Physisorption Analyzer - Quantachrome Autosorb®-1-C
39. Zetasizer Nano ZS particle size analyzer- Malvern instruments
40. Precision Workstation (Radiant Technologies Inc) for dielectric measurements
41. Near field Scanning optical microscope
42. High pressure gas adsorption Unit (Belsorp HP)
43. Vapour adsorption Unit (Belsorp Aqua III)



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 constitute 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 $YCrO_3$. Multiferroic properties of charge ordered manganites are being explored.

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

CNR Rao is the National Research Professor as well as Linus Pauling Research Professor and founder and honorary president of JNCASR.

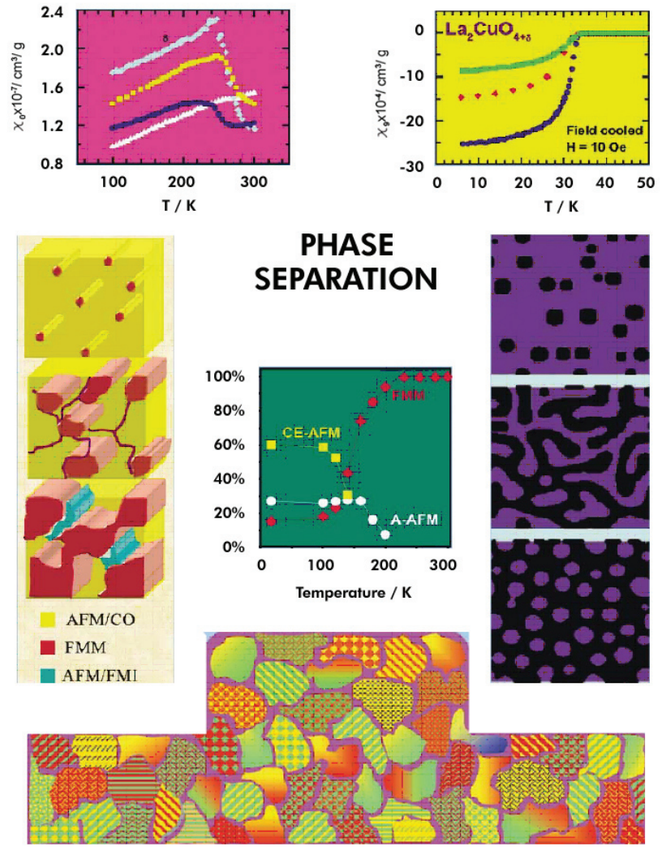

Figure 1: Phase separation in metal oxides

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. optical, magnetic, gas sensing) of the nanowires and their composites have been examined. Growth mechanisms of nanostructured material is being investigated by x-ray scattering and other techniques.

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, photovoltaic properties). Another unique material being investigated is nanographene. Functionalization and solubilization of nanostructures are being pursued.

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. Magnetic properties of Kagome structures are being investigated to understand their relation to the spin states of the transition metal ions.

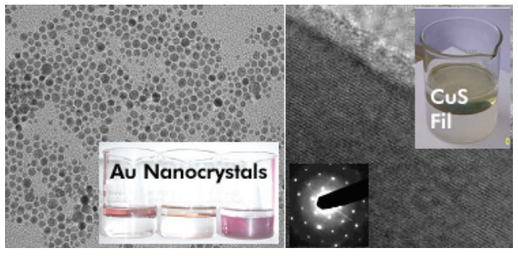

Figure 2: Organic-water interface for large scale syntheses of nanocrystals and single crystalline films

PhD Students

JNCASR: Venkata Prasad Bhat, SRC Vivek Chand, A Gomathi, KP Kalyanikutty, V Rakesh, Chandra Sekhar Rout, Jyoti Ranjan Sahu, Neenu Varghese

IISc: Anupama Ghosh, Basant Kanishka Biswas, Sandeep Ghosh, Claudy Rayan Serrao, Basant

MS (Engg.) Students

Leela Srinivas Panchkarla, Kalyan Raidongia, Subramanyam KS

Balasubramanian Sundaram

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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 are employed

Balasubramanian Sundaram is a 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.

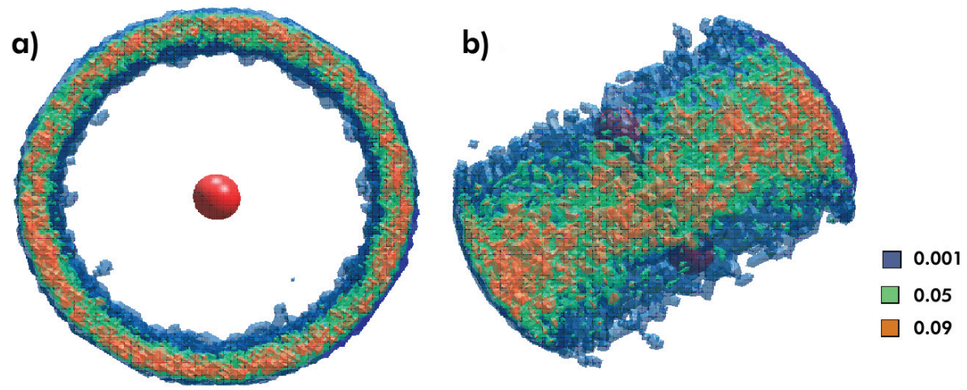

Figure 1: Ab initio MD simulations reveal the geometry of the first coordination shell of a carbon dioxide (CO_2) molecule in supercritical CO_2. Blue, cyan, and orange represent the increasing probability of finding an oxygen atom belonging to a neighbouring molecule in the first coordination shell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

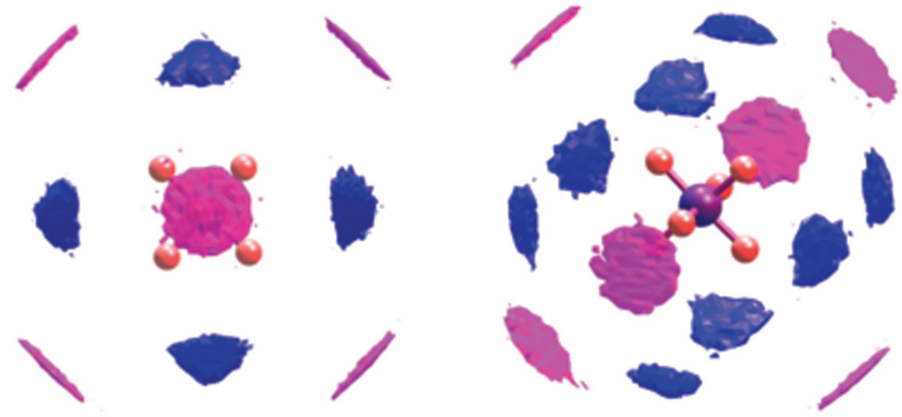

Figure 2: Atomistic molecular dynamics simulations show the location of cations (blue) and anions (pink) around an anion in the room temperature ionic liquid, 1-butyl,3-methylimidazolium hexafluorophosphate. Two views are shown.

Recent Publications

1. BL Bhargava, ML Klein and S Balasubramanian. Structural Correlations and Charge Ordering in a Room Temperature Ionic Liquid: The case of [bmim][PF6]. ChemPhysChem (Communication) 9, 67 (2008).
2. BL Bhargava, R Devane, ML Klein and S Balasubramanian. Nanoscale Organization in Room Temperature Ionic Liquids: A Coarse Grained Molecular Dynamics Simulation Study. Soft Matter 3, 1395-1400 (2007).
3. Bhargava BL, Balasubramanian S. Probing Anion-Carbon dioxide Interactions in Room Temperature Ionic Liquids: Gas Phase Cluster Calculations, Chemical Physics Letters, 444, 242-246 (2007).
4. BL Bhargava and S Balasubramanian. A refined potential model for atomistic simulations of an ionic liquid, [bmim][PF6]. Journal of Chemical Physics 127, 114510 (2007).
5. Bhargava BL, Balasubramanian S. Insights into the Structure and Dynamics of a Room Temperature Ionic Liquid: Ab Initio Molecular Dynamics Simulation Studies of [bmim][PF_6] and the [bmim][PF_6] - CO_2 Mixture, Journal of Physical Chemistry B, 111, 4477-4487 (2007).
6. Bhargava BL, Balasubramanian S. Intermolecular Structure and Dynamics in Supercritical Carbon dioxide with Pressure: An Ab Initio Molecular Dynamics Study, Journal of Physical Chemistry B, 111, 387-392 (2007).
7. Bhargava BL, Balasubramanian S. Layering at an Ionic Liquid-Vapor Interface: A Molecular Dynamics Simulation Study of [bmim][PF_6], Journal of the American Chemical Society, 128, 10073-10078 (2006).

Sponsored Projects

1. Towards an understanding of chemical reactivity, supramolecular ordering and protein thermostability in green solvents, DST, 2006-2011.
2. Computer simulation studies of room temperature ionic liquids, DST, 2005-2008.
3. Simulation studies of structure, dynamics, and solute-solvent interactions in supercritical carbon dioxide, CSIR, 2005-2008.
4. Computer simulations of aqueous protein solutions: A study on the role of biological water, DBT, 2003-2006.
5. Molecular modelling of discoid amphiphilic aggregates, CSIR, 1999-2002.

PhD student members of the group

Soumyasaswati Sarangi (Utkal), Srinivasa G Raju (SSIHL), Sandeep K Reddy (Osmania)

PhD students graduated

M Krishnan (currently at Oak Ridge Nat. Lab), M Saharay (currently at Oak Ridge Nat. Lab), BL Bhargava (currently at Univ. of Pennsylvania)

Chandrabhas Narayana

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SERS, Raman spectroscopy, Brillouin scattering and high-pressure research

The group is interested in study of materials using optical spectroscopy under ambient and extreme conditions. Primary activity of the group 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, elastic constants 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, (d) can one understand drug protein interactions and (e) is it possible to use spectroscopy in diagnostic applications in biology.

Recently, our group has developed techniques and focused on study of small molecule and protein interactions, improving immuno-assays to make it more sensitive for early detection of diseases and trying to develop PCR less detection of nucleic acid in collaboration with our biology colleagues.

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.

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.

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.

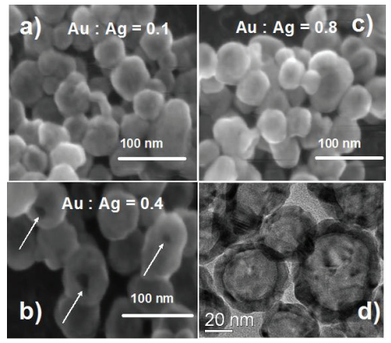

Figure 1: FE-SEM images of core-shell nanoparticles (NP) with Au to Ag ratio (a) 0.1, (b) 0.4, and (c) 0.8. (d) TEM image of core-shell NP shown in (b). The arrows in (b) point to the nanopores on the surface of the gold shell which act as hot spots in the present experiments. (G.V. Pavan Kumar et al Journal of Physical Chemistry C 111, 4388 (2007))

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.

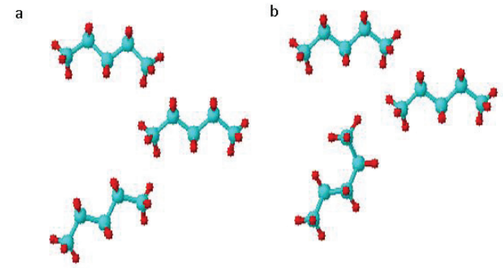

Figure 2: The schematic/cartoon representation of n-pentane molecular arrangement at (a) ←12.3 GPa, (b) → 12.3 GPa. (G. Kavitha et al Journal of Physical Chemistry B 111, 7003 (2007))

Brillouin scattering studies of pyrochlores, beryllium doped ZnSe/ZnTe chalcogenites: Pyrochlores are analogous to the spin ice. They demonstrate anisotropy in phonon behavior even though they are isotropic structurally, we have carried out Brillouin studies to elucidate these properties. ZnSe and ZnTe are wide bandgap materials and are used as nonlinear and IR detectors. With the addition of Beryllium one can increase the strength of these semiconductors. It is interesting to understand their elastic properties as well as how would this behave under the application of pressure and temperature. These are some of the questions we are looking into in these systems.

High pressure Raman spectroscopy

High pressure Raman scattering on mid chain hydrocarbons,flu orocarbon, oxides, low dimensional system: Our group has been actively pursuing the effect of pressure on materials to study the phase transition in materials. We have looked at normal alkanes to understand their behavior under pressure in the solid phase. It is important as many times these are used as hydrostatic or quasi-hydrostatic medium. In addition these mid-chain alkanes have been important in the petrochemical industries. We have seen solid solid transition in these liquids at high pressures, which suggest lack of mobility in high compaction. In the similar way we have carried out pressures studies on flurocarbons which are gaining importance due their use in solar cell as well as fuel cell applications using polymers. One question raised in these molecule is the inter-molecular interactions. Pressure is a very good probe to understand this. Our group has studied various oxides with properties ranging from colossal magnetoresistance to ferroelectric, and non-linear optical behavior to conducting oxides under pressure. Our group also looks at low dimensional materials like carbon nanotubes, metal nanospheres under pressure.

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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 such as tubes, rings, spheres and cups through different methods which are listed here.

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

Nanorings through self-assembly

Amorphous carbon nanorings from carbon nanostructures was derived from the carbonization of Pluronic P123 polymer inside mesoporous SBA-15 rods grown in a porous alumina membrane. The presence of the alumina and the silica walls restricts the diffusion of oxygen during calcination and facilitates the carbonization of Pluronic P123. The resulting carbonized nanostructures self- assemble around the water droplets in the presence of CCl4, and form ring structures with diameters between 2 and 10 μm and a rim thickness of ~50 nm.

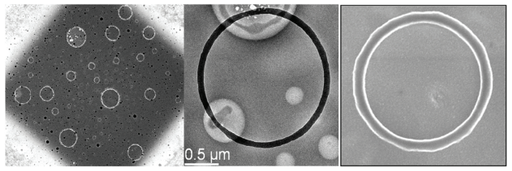

Figure 1: Amorphous carbon nanorings formed through self-assembly of carbon nanofibers

Zeptoliter bowls through self-assembly

The growing interest in single molecule detection and kinetics has given impetus to the technology of making many a complex morphologies like bowls and cups with Femto- or picoliter capacity. Such containers are useful when dealing with cellular systems and providing control on diffusion and kinetics, handling expensive reagents etc. However, it would be difficult to obtain a complex morphology like cup through direct template synthesis. Our observations in temperature-induced morphogenesis led us to successfully synthesize nano- and sub micron sized bowls of inorganic materials like ZnO, MnSO4, and Fe2O3 etc.

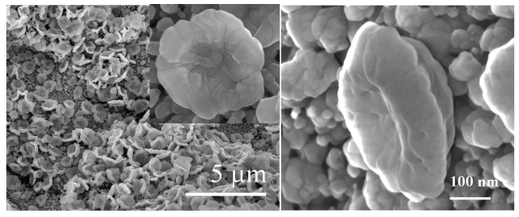

Figure 2: ZnO bowls formed through temperature induced self-assembly of ZnO nanoparticles

Nanotube brushes from glucose

We have been interested in low temperature synthesis of functionalized carbon materials that could be used for a variety of applications. Most of the carbon-based nanomaterials are synthesized by pyrolytic decomposition of hydrocarbons and organometallics. Such high temperature routes often end up being highly graphitic but poorly functionalized. However, there are a number of applications where the robust graphitic structure may not be as essential as the functionalized surfaces, in which case the high temperature synthetic routes can comfortably be circumvented. A sweeter alternative was to use 'glucose', a commonly available, non-toxic, inexpensive carbohydrate as the carbon precursor.

Glucose under hydrothermal treatment undergoes a polymerization reaction to form amorphous carbon structures with occasional graphitic regions. The most significant outcome of this method is the surface of the carbon material is highly functionalized with alcohol and carboxylic acid groups. These functional surfaces of carbon nanotubes were successfully exploited to synthesize Ga2O3, GaN and BCN nanotube brushes as well as a-Al2O3, MoO3 and ZnO nanorod brushes. Single crystalline ruby nanorods were obtained by introducing chromium ions during the synthesis of alumina rods.

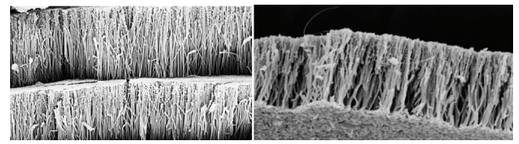

Figure 3: (Left) Amorphous carbon nanotube brush (Right) GaN nanotube brush

Materials for Tissue Engineering

Glass ceramics of composition CaO-P2O5-SiO2-MO (M = Na, Mg, etc) are highly bioactive and can be successfully used as a tissue engineering material for bone and tooth reconstruction and substitution because of their ability to form hydroxyapatite (HA) when implanted A hierarchically porous bioactive glass of composition 80 mol% SiO2 and 15 mol% CaO (MBGH) was synthesised using pluoronic P123 and glucose-derived amorphous carbon submicron spheres as templates. The negatively charged carbon spheres favour the local enrichment of calcium ions and favours the formation of amorphous calcium phosphate around the surface. On calcination, the walls of the macropores contain a crystalline hydroxycarbonate apatite nuclei. This hierarchically porous bioactive glass shows accelerated growth rate for hydroxycarbonate apatite in simulated body fluid (SBF).

Materials for Intracellular drug delivery

A number of factors that have to be taken into account while developing intracellular drug carriers include optimal hydrophilicity and hydrophobicity which will decide its entry, surface functionalisation which will act as a chemical handle to tag the drug, fluorescent tags for their visualization and finally their cytotoxicity. We are developing 'intracellular carriers that will have no barriers' across the cell membranes and even nuclear membranes. It is of immense interest to develop materials that possess all these qualities in a single step synthesis. We are using these intracellular carriers for delivering molecules inside the nucleus, which could find potential therapeutic applications.

Nanocomposites

We have been interested in exploring the synthesis and properties of clay-metal nanoparticle composites. Nanoparticles of metals such as Au, Ag, Pd and Pt embedded in exfoliated sheets of aminoclays of the type R8Si8Mg6O16 (OH)4, where R = CH2CH2NH2 are entirely water-soluble. These sheets of the composite come to the organic-aqueous interface on addition of alkane thiols to the aqueous layer.

Catalysis

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 nanomaterials and metal/metal oxide nanoparticles synthesized here would be used to test some catalytic reactions like NOx removal, methane conversion and selective oxidation of hydrocarbons.

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KKR Datta

MS (Engg.) student
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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) Exotic nanostructures from pulsed laser deposition, (c) Size dependent properties of individual nanoobjects, collective properties in a meso-assembly, (d) Patterned synthesis of nanomaterials for nanodevice fabrication and (e) Molecular properties from electronic charge density method.

Nanocrystals of Metals, (Au, Ag, Pt, Pd etc.) have been prepared employing soft-chemical routes and thiol derivatised to form extended 2D ordered lattices. The novelty of our work is that the obtained nanocrystals are essentially monodispersed and have the ability to self-assemble into an extended mesolattice. Structural parameters such as the particle size, length of the capping ligand and its conjugation have been varied easily. In a 'single-step' procedure, organic-water liquid-liquid interface has been exploited to synthesize ultrathin (~100 nm) nanocrystalline films of metals and alloys. These free-standing films may be extracted on flat substrates for various applications. Metal nanocrystals anchored to vertically standing organic spacers have been used as metal-organic heterostructures. Other interesting mesostructures include nanocrystal dimers and trimers linked by conjugated molecules- these are prototype molecular switches.

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

Nanocrystalline Au films have also been prepared on silicon substrates by the galvanic displacement method. By coating a thin layer of carbon on the substrate, the morphology of the substrates could be fine tuned to suit optical applications.

Pd nanocrystals have been prepared by the thermolysis of Pd alkanethiolates. The latter are soluble in organic media and exhibit lamellar structure with the bilayer thickness corresponding to nearly twice the hydrocarbon chain length. It is also demonstrated that a hybrid bilayer consisting of hydrocarbon chains of different lengths can act as an 'ion-trap'. The work is extended to magnetic Ni thiolates as well.

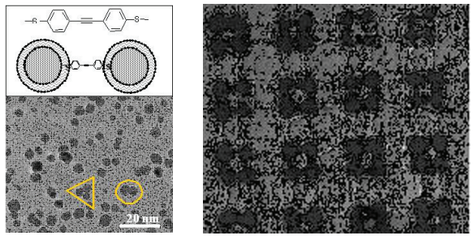

Figure 1: A molecular switch consisting of a conducting molecule held between nanocrystal electrodes.
Figure 2: Pulsed laser photolithography to create patterns of nanomaterials.

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. Micron sized alumina crucibles have been obtained by subjecting Al cups to careful oxidation.

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). A single molecular switch action from a nanocrystal dimer linked by a conjugated molecule has been realized. In the case of extended nanocrystal arrays, 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 apart by the adsorption of longer alkanethiols. The kinetics associated with the process also exhibits a trend dependent on the chain length.

Nanocrystalline Au films deposited on carbon coated Si substrates exhibit enhanced optical reflectivity and Raman scattering (over 10 million times). The application of these substrates in Raman studies (SERS) on biomolecules with very low concentrations, is demonstrated. The femtolitre metal cups obtained by pulsed laser ablation are also shown to be SERS active. 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 4 K, particularly when the interacting Ni-S backbones are held apart by short chain length spacers such as butanethiol.

Various nanolithography methods, electron beam (EBL) and AFM based, are being applied to create nanoscale patterns (below 100 nm) of nanomaterials on designated substrates, towards the ultimate goal of fabricating nanocircuits with functional circuit elements. In EBL, a focused electron beam is made to move over an electron sensitive precursor which instantly produces a nanomaterial in the regions exposed to the electron beam- the rest is washed away during developing. The novelty of such a direct write method has been demonstrated in the case of several important nanomaterials employing indigenously developed e-precursor resists. AFM is being used as a direct write lithography tool either by coating the tip with a nanomaterial ink (dip-pen lithography) or by applying electrical bias (electrostatic lithography). Well characterized metal sols and other colloidal dispersions are being used as inks for dip-pen raised patterns, the narrowest line being only 20 nm wide! The internal structure of the patterns has been studied using nanospectroscopy techniques on a synchrotron beamline. Electrostatic lithography technique has been used to ablate a polymer film with the biased tip to create nanoscale trenches. The obtained trenches act as a stencil that can be filled with nanocrystals or selectively adsorbed with active species like C60. In a new development, pulsed laser shots are being employed to perform optolithography over large areas, using suitable masks. A nanomaterial precursor undergoes thermolysis in regions exposed to the high energy nanosecond pulse, thus creating a patterned nanomaterial. Examples include gold, ZnO and polymers.

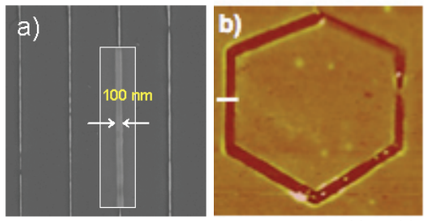

Figure 3: Direct write lithography: Pd nanowires by EBL **(a)** and **(b)** Nanotrenches in a polymer film by Electrostatic lithography using AFM.

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, conjugated conducting molecules as well as drug molecules.

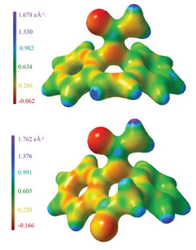

Figure 4: Electrostatic potential of Carbamazepine and Oxcarbazepine on the 0.5 eÅ^{-3} isodensity surface. The latter which is relatively more specific as an epileptic drug, is more polar (red regions).

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

My group has been actively involved in studying electronic, optical and optoelectronic phenomena and exploring device structures in polymeric/organic/nano and biomolecular based systems over the last decade. Our current research activities include (i) Photophysical studies of optically active soft-matter using a innovative combination of microscopy and spectroscopy methods (ii) Fabrication of field effect transistors; light emitting diodes and solar cells (PV) devices (iii) Large area patterning methods which includes studying and manipulating elastic/viscoelastic surface instabilities (iv) Photo-induced charge transport processes in membrane-protein/smart electrode systems (v) Modifying carbon nanotube transitors by controlling its environment. 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. Some of our noteworthy contributions to this research community and inventions are: (a) Polymer –Photo Field Effect Transistors (b) Efficient plastic solar celEls (c) Synergestic Processes at bacteriorhodopsin-conducting polymer interface (d) Flexible polymer based light- position sensor spanning sub-micron to few mm range (e) High resolution photocurrent imaging for estimating transport length scales and identifying active regions.

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.

The idea of solar cells based on carriers originating from thin polymer films, manufactured by printing and coating techniques from reel to reel, and packaged by lamination techniques is not only a novelty, but an attractive feature from a commercial-environmental-design aspects. A prerequisite for photo-induced charge generation and separation in these active layers is the presence of donor-acceptor moiety and a network which enables transport of the carriers. The underlying origin of the basic process of photoinduced charge separation process in a polymer/organics heterostructures and the tailoring of the optical and electrical gradients in these devices has been actively pursued in this research community. We have recently demonstrated a controlled-efficient low –cost method in depositing cathode of desired dimensions which are specifically relevant for polymer solar cells. We hope methods such as these can pave a potential paradigm change for fabricating low-cost polymer devices.

Doped conducting polymers offers a viable option of having a smart-electrode interface and provides a valuable gateway to monitor and control biological events. The possibility of linking well-defined and patterned organic electronic circuits to cellular activities has immense potential in applications ranging from nervous system to routine chemical sensing. We have explored the possibility of optically triggering changes in the conductivity of the conducting polymers in contact with the extracellular segments of a membrane protein, bacteriorhodopsin (bR).

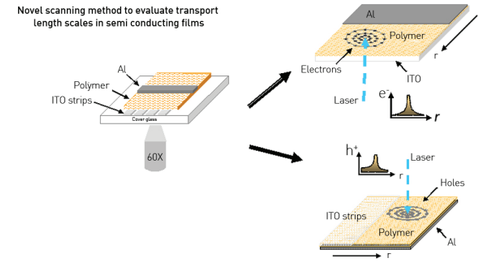


Figure 1: Novel scanning method to evaluate transport length scales in semiconducting films. Estimation of carrier mobility & diffusion lengths and its correlation with morphology is informative in the design of efficient solar cells. We have developed methods involving scanning probe photocurrent microscopy of films with asymmetric electrodes.

Figure 2: OLED fabrication technology without vacuum requirement
Figure 3: Flexible solar cells and detectors

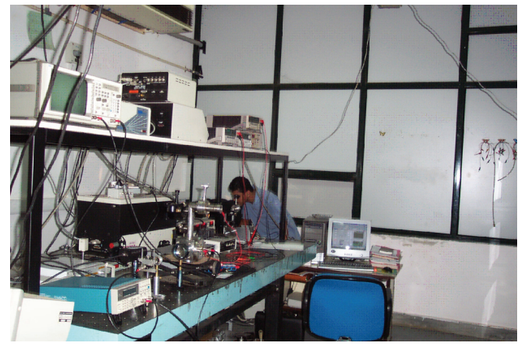


Figure 4: Spatially resolved, high speed optoelectronics measurements

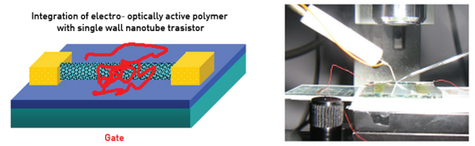
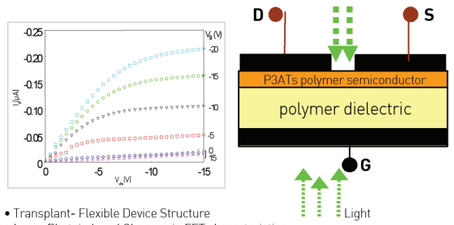


Figure 5: Integration of electro-optically active polymer with single wall nanotube transistor
Figure 6: Biochemical sensing using conducting polymers



- Transplant- Flexible Device Structure
- Large Photoinduced Changes in FET characteristics
- Gate controlled relaxation and spectral profit

Figure 7: Polymer PhotoFET. The laboratory has a U.S. patent on polymer field effect transistrors which can be controlled optically. The combination of electrical and optical gating of the drain source current opens a wide range of novel switching and memory devices.

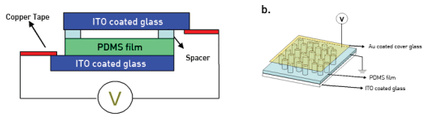


Figure 8: Large area patterning of elastomeric and viscoelastic films using electric field. This combination of pursuit of wide variety of problems in the area of optoelectronics and device physics of soft matter/molecular/nano systems using combination of microscopic, spectroscopic and electronic techniques provides an exciting ambience to aspiring researchers.

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Magnetism, superconductivity, and ferroelectricity

The goal of Dr. Sundaresan's research is to understand the relationship between the structure of a material and its properties. This involves both fundamental and applied aspects of chemistry and physics of solid state, and a spectrum of materials including superconductors, multiferroics and magnetic oxides. While continuing to work on bulk and thin film materials, he has recently explored a large number of inorganic materials at nano-scale and discovered that all these nanoparticles of inorganic materials exhibit ferromagnetism at room temperature and show how ferromagnetism is rather universal feature of the nanoparticles. He also made a new distorted perovskite oxide BiAlO3 under high pressure and demonstrated ferroelectricity in this material. The other important work is the study of multiferroics. In this study, he showed the importance of oxygen content in BiMnO3 and its structural and magnetic properties. Finally, his work on the fabrication of superconducting superlattices needs to be mentioned. In this work, he aims at achieving room temperature superconductivity in artificial material which can be prepared by layer-by-layer growth of metallic and insulating oxide layers.

In his work, he uses (a) solid state and chemical routes to synthesize bulk materials and physical methods to fabricate thin films, (b) X-ray, neutron and electron diffraction techniques for structural studies, and (c) physical property measurements of magnetic, electrical transport, heat capacity and dielectric response. The interdisciplinary research in Dr. Sundaresan's group is expected to yield understanding of materials that will facilitate design of environment-friendly materials with properties suitable for technological applications.

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

Universal Ferromagnetism in nanoparticles of otherwise nonmagnetic oxides

Nanoparticles of various oxides with no unpaired electrons such as CeO2, Al2O3, ZnO, In2O3, SnO2 and MgO were prepared using various chemical methods. Through a very careful and thorough analysis, these nano-materials were shown to exhibit ferromagnetism at room temperature. The origin of this unexpected ferromagnetism was shown to be confined only to the surface of the nanoparticles and suggested to be in the anion and/or cation vacancies at the surface. Based on this work, the ferromagnetism of nanoparticles was suggested to be universal feature not only of oxides but also of nitrides and chalcogenides. With its origin in the surface of nanoparticles, it was proposed that such ferromagnetism can coexist with any other functional properties of the bulk form. While incompatible with superconductivity, such ferromagnetism was demonstrated in the normal state of metal oxide and nitride superconductors.

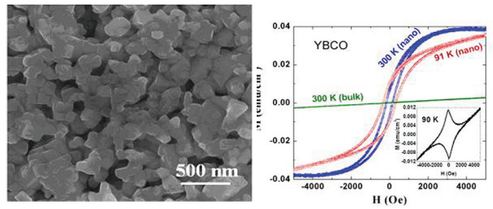

Figure 1: M(H) data of YBCO nanoparticles at 300 K and 91 K showing the ferromagnetic behavior. M(H) data of bulk YBCO is also shown for comparison. Inset shows the hysteresis at 90 K which is typical of a superconductor.

New lead free ferroelectric and multiferroic materials

Development of lead-free ferroelectric materials is important because of the toxicity of lead in the widely used material lead zirconium titanate (PZT) in devices. Recently, it has been predicted that the compounds, BiAlO3 with the hypothetical perovskite structure should have ferroelectric polarization higher than the PZT and we considered it would be really interesting and important to verify this experimentally. BiAlO3, prepared under high-pressure and high-temperature conditions has a rhombohedral perovskite-like structure (R3c with a = 5.3747(4) Å and c = 13.391(1) Å) and decomposes around 550 ºC to form the intermediate Bi2Al4O9 phase along with the Bi26-xAlxO40-y and Al2O3. Above 580 oC, the intermediate phase changes into the Bi26-xAlxO40-y. Dielectric measurements show an anomaly at the decomposition temperature and hysteresis at room temperature with a maximum polarization of ~ 16 μC/cm2. Raman scattering measurements suggest softening of optical phonon modes and are consistent with the occurrence of thermal decomposition of the rhombohedral phase to form the thermodynamically stable phase.

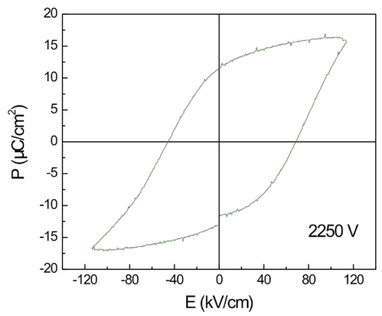

Figure 2: Room-temperature ferroelectric hysteresis of BiAlO3.

In recent years, there have been several reports regarding the structure of bismuth manganite. $BiMnO_{3-\delta}$ compositions differing in oxygen stoichiometry have been synthesized under high pressure. Interestingly, BiMnO2.99 crystallizes in an orthorhombic structure possibly with a small monoclinic distortion. Orthorhombic BiMnO2.99 and monoclinic BiMnO2.84 exhibit canted antiferromagnetism and ferromagnetism respectively. BiMnO2.94 and BiMnO2.89 are also monoclinic and show ferromagnetism, but it seems possible that they may contain domains of more than one phase.

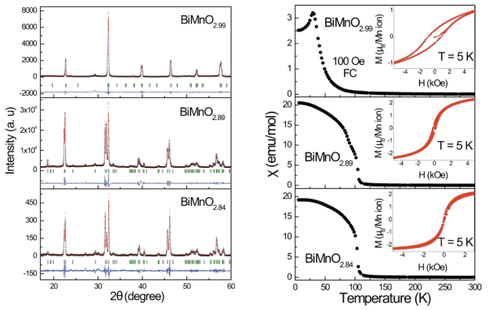

Figure 3: X-ray diffraction patterns and temperature-dependent field cooled (FC) susceptibility of three phases of $BiMnO_{3-\delta}$ (δ = 0.01, 0.11 and 0.16). Magnetic hysteresis curves are shown as insets. The magnetic behavior of BiMnO2.94 is quite similar to that of BiMnO2.89.

Atomic engineering of high Tc cuprate superconductors

The aim of this work is to prepare multi-layer high Tc superconductor thin films containing no toxic element with Tc → 100 K by an artificial superlattice method using rf magnetron sputtering. In this method, the infinite layers BaCuO2 and CaCuO2 are deposited alternatively to produce required number of CuO2 layers between the charge reservoir layers. These two layers are the building blocks of high Tc superconductors. Since BaCuO2 does not contain apical oxygen which is essential to create holes in the CuO2 layers, a partial substitution of copper by CO3 group could stabilize a tetragonal 1201 phase, (Cu,C)Ba2CuO4+y with c-parameter twice that of BaCuO2. This 1201 phase can accommodate apical oxygen and become superconducting (Tc ~ 40 K) with the resistivity showing semi-metallic behavior above Tc. Thus, the superconducting 1201 phase is suitable to form the charge reservoir layer for the fabrication of superlattice thin films and this work is being carried out.

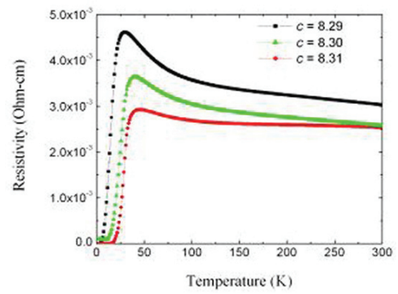

Figure 4: Temperature dependence of resistivity of (Cu,C)Ba2CuO4+y thin films showing superconducting transition.

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Surface Science, Heteroepitaxy and Nanostructures

Our research interests are in heteroepitaxial growth of thin films, characterization of low-dimensional materials by surface sensitive techniques and formation of nanostructures that are of interest in catalysis, semiconductors and nano-technology. Most of our materials development studies are performed in ultra-high vacuum conditions where ultra-thin metal films are adsorbed on well-defined substrates while monitoring the interface evolution in-situ by surface sensitive techniques such as X-ray Photoelectron Spectroscopy, Auger Electron Spectroscopy, Low Energy Electron Diffraction, Reflected Electron Energy Loss Spectroscopy and Scanning Tunneling Microscopy. The studies have enabled an atomistic view of the kinetics of surface processes and the stabilization of several novel surface phases. Our main aim has been to correlate the surface atomic arrangements to the chemical and electronic structure of the materials and elucidate the novel properties that arise due to the reduced dimensions. We have used surface orientation and reconstructions as templates to form novel nanostructures. We have formed several core-shell structures and studied their compositional and structural inter-relationships. In this process we have stabilized several novel phases and also observed some unusual properties in the nanophase. Combining our experience of forming low dimensional structures and in-situ characterization, we intend to direct our future activities towards addressing scientific issues that hinder the development of several heteroepitaxial structures of interest in various electronic and photonic applications using physical growth techniques such as Molecular Beam Epitaxy (MBE).

Shivaprasad obtained his Ph D in Thin Film Physics in 1982 from Karnatak University and served for 22 years at the National Physical Laboratory, New Delhi before joining JNCASR in 2007. He did his post-doctoral work at IIT-Delhi and as a Commonwealth fellow at the University of Sussex, UK. He has also been a visiting scientist at the National Institute of Standards and Technology (1987) and Rutgers University (1990-92), USA, Tohoku University, Japan (1994-95) and University of Ulm, Germany (1999-2000). He is a recipient of the CSIR Young Scientist Award and the MRSI Medal Lecture Award.

Metal/Metal Heteroepitaxy

We have studied metal/metal systems of catalytic interest by in-situ surface sensitive probes. The anisotropy in the surface free energy of the atomically rough W(111) surface drives to massive reconstruction with the adsorption of 1 ML Pd followed by annealing. The interface results in (211) faceted pyramidal structures, which are single-sized and self-organized and dependent on pre- and post-growth treatments. The adsorption of Ni on clean Ru(0001) substrate due to lattice mismatch, initially grows pseudomorphically at the hcp sites, but later strain relaxes by forming misfit dislocations. We have also observed that pre-adsorbing a low coverage of CO as a surfactant blocks hcp sites and causes the Ni atoms to occupy fcc sites, that results in a novel quartet (2x2) reconstruction. Of late, we have initiated some work on bimetallic alloys (Cu/Pd, Ag/Pd) that can cap rare-earth nanoparticles and enhance the hydrogen adsorption properties of the Gd particles while protecting it from oxidation. Our preliminary results hold promise for hydrogen sensing and storage applications.

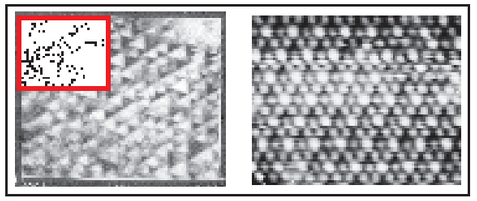

Figure 1: Pyramidal Faceting in Pt/W(111) and CO induced (2x2) quartet reconstruction in Ni/Ru(0001) system.

Metal/Silicon Interface

We have carefully studied the adsorption of Ag on Si(111) 7x7 and resolved coverage issue of the √3x√3 structure. Revisiting the Ag/Si(001) 2x1 surface has resulted in our reporting two novel energetically proximal surface phases of 2x3 and c(6x2). We have also adsorbed Mg and Mn on Si(111) and (100) surfaces to see several interesting surface modifications. Our extensive studies of the Sb/Si(111) 7x7 system has shown that the 7x7 reconstruction acts as a barrier to Schottky barrier formation, which is lifted by a structural phase transition. We have also revised the phase diagram existing in literature for this interface, showing the existence of novel surface phases that can play a significant role in buried layer technologies. We have provided a 2D-phase diagram for the Sb/Si(001) 2x1 and c(4x4) systems for the first time. Using the faceted and trenched morphology of the high index Si(5 5 12) surface we have been able to grow atom-wide nanowires and zig-zag 1D- nanostructures.

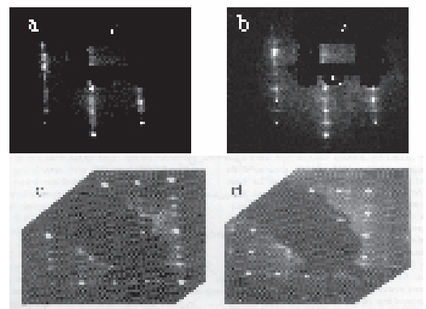

Figure 2: Depth profile of Core-level XPS spectra showing CuO/Cu_2O, and PbO/Pb core-shell nanoparticles.

Core-shell nano-structures

We have extensively exploited the combination of X-ray Photoelectron Spectroscopy and inert gas ion sputtering techniques to look into the compositional depth profile of nanoparticles. We have revealed the core-sell structures and related them to other observations and properties. We have shown that Cu_2O stabilizes in the nanophase by having a shell of CuO phase. We have reported the observation of cubic to hexagonal structural transformation in CdTe nanoparticles depending on the Te-oxide shell stoichiometry. Similar results are seen in case of In, Ag, CdS and Pb nanoparticles. Our recent work on the formation of organically capped CdSe and ZnSe capped CdSe have demonstrated the dominant role of surface modifications on the size dependent properties of nanoparticles.

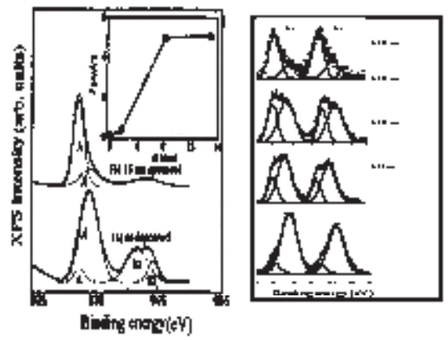

Figure 3: (a,b) Formation of Sb nanowires in trenches of on high index Si(5 5 12) surface. (c,d) Observation of single and double domain (2x3) and c(6x2) structures at the Ag/Si(100) 2x1 interface.

GaN Heteroepitaxy:

To obtain suitable substrates for GaN epitaxy with low defect densities, we have initiated ion-induced room temperature approaches. We have formed an epitaxial SiC overlayer by depositing C monolayers on Si(111) surface and subjecting it to Ar+ ion bombardment. We have also ni-trided the GaAs(001) surface to form a GaN by top layer by bombarding the surface by energetic N2+ ions. The better lattice matching between GaN and SiC and the isostructure of GaAs and GaN interface make these systems suitable as templates for growth of high quality epitaxial GaN overlayers with reduced defects.

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Self Assembled Molecular Materials Based on Metal-Organic Coordination Networks (MOCNs)

The research interest of our group is to design and synthesis of novel metal–organic coordination networks (MOCNs) with potential application of gas storage (H_2, CH_4 etc), heterogeneous catalysis, separation and exchange processes and to develop size- and shape-selective novel reactions in the porous framework and new approach towards the studies of the physico-chemical properties of the molecules in the adsorbed state. We are also interested in designing the frameworks with active metal site (unsaturated) to understand the chemisorptions processes and redox-active frameworks towards the formation nano-particles as well as the oxidation or reduction of the adsorbate results in the direction of novel functionalities. We are also involved in the studies of molecule based photo-, porous-, nano- and spin-crossover magnetic materials.

T. Maji has obtained his PhD (2002) in Inorganic Chemistry from Indian Association for the Cultivation of Science (IACS) (Jadavpur University). He did post-doctoral research at Kyoto University, Japan, and was Lecturer in Chemistry, Jadavpur University before joining JNCASR in 2006

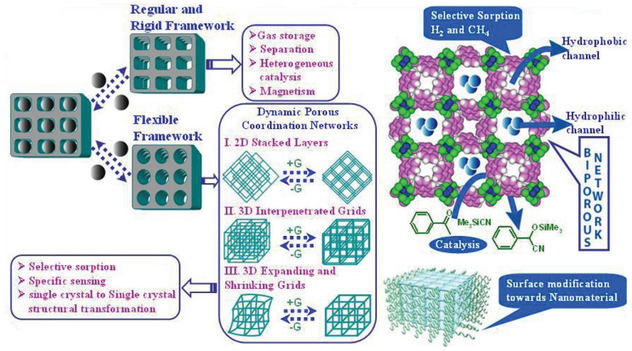


Figure 1: Functional Metal-Organic Coordination Networks

H_2 -Storage Materials

The systematic design and exploratory synthetic approaches have combined to offer a very broad range of metal-organic coordination networks (MOCNs) that are truly porous and their real advantages are springs directly from the modular processes by which they are constructed (Scheme 1). The most promising applications of MOCNs is storage of the small molecules such as H_2, O_2, N_2, NO, CO_2 and CH_4, considering not only important energy source and environmental hazards but also to understand the physico-chemical properties of the confined molecules which differs from the bulk state. Much interest and attention have been paid for efficient H_2 storage materials for replacement of current transportations energy source. The adsorption or storage of large amount of hydrogen is difficult as the polarizability and size of the hydrogen molecules is very small and the limited interactions with the pore surfaces of the adsorbent. Our efforts are directed towards the synthesis tailored framework with the small pore and high reactive or affinity sites which will be the potential candidates for the large amount H_2 storage.

Heterogeneous Catalysis

The use of chiral template molecules or the employments of the enantiomerically pure organic linkers are the options for the preparation of the functional chiral frameworks. But truly chiral microporous materials with enantio-selective sorption and catalysis are difficult to synthesis. The transformation of aldehyde to the chiral secondary alcohol and the enantio-selective transesterification in a chiral microporous framework are the most exciting example reported so far. Our activity encompass towards the design and synthesis chiral framework which will be crucial for enantio-selective sorption and catalysis (Scheme 1).

Porous Magnetic Materials

Next step is the bimodal functionality in MOCNs, like the strategic co-existence of multiple properties in same materials like, ferro / ferri- magnetism, conductivity, spin-crossover, optical properties and porous functionality. In order to achieve such functionalities, one of the approaches is to link the 0-D clusters or 1D (M-O-M) inorganic chains having high magnetic anisotropy by using the polycarboxylate to 3D robust framework compare to the long rigid linkers, as the magnetism have generic dependence of exchange coupling on distance. The introduction of the fluorescent guest or optically active molecules in the porous framework and combination with the diversity of pore structure and functionality would offer a versatile route to optical guest sensing. My group is involved in synthesis of such functional materials.

We are also currently engaged in synthesis of magnetic luminescent nanoparticles based on Prussian blue analogues or hybrid MOCNs coating with the organic or inorganic polymer. The magnetic nanoparticles further linked with the lanthanide luminescent probe by organic linker results a bifunctional nanomaterials.

Flexible Framework: Selective Sorption Flexible and dynamic MOCNs, in particular, those that reversibly change their structures and properties in response to external stimuli, so called "structural dynamism" would be a key principle for high selectivity, accommodation, and separation of a specific molecule (Scheme 1). These kinds of materials show bistable state with structural transformation, like single crystal-to-single crystal structural transformation. So, the design and synthesis of host framework, which can interact with the certain guest molecules in a switchable way has implications for the generation of advanced materials with potential application of molecular sensing and actuator. This kind of framework with selective sorption phenomenon will be used for the separation of different gases (like N_2, O_2, CO_2) and different organic molecules (like different alcohols, alkanes), which our group is also currently looking for.

Key Publications

1. KL Gurunatha, K Uemura, TK Maji, Temperature- and Stoichiometry-Controlled Dimensionality in a Magnesium 4,5-Imidazoledicarboxylate System with Strong Hydrophilic Pore Surfaces. Inorg. Chem. 2008, 47, 6578-6580.
2. TK Maji, R Matsuda, S Kitagawa, A Flexible Interpenetrating Coordination Framework with a bimodal porous Functionality; Nature Mater., 2007, 6, 142 [This article is also highlighted in News and Views of Nature Mater., 2007, 6, 92
3. TK Maji, G Mostafa, R Matsuda, S Kitagawa, Guest Induced Asymmetry in a Metal-Organic Porous Solid with Reversible Single-Crystal-to-Single-Crystal Structural Transformation ; J. Am. Chem. Soc., 2005, 127, 17152.
4. TK Maji, K Uemura, HC Chang, R Matsuda, S Kitagawa, Expanding and Shrinking Porous Modulation Based on Pillared-Layer Coordination Polymers Showing Selective Guest Adsorption; Angew. Chem. Int. Ed., 2004, 43, 3269 [This work has been considered as a VIP Paper and featured on the Cover Page of the Journal]

PhD students

Sudip Mahapatra, Prakash Kanoo

Project Assistant

KL Gurunatha, Sammer Vyasamudri

Education Technology Unit

Members
Prof. V Krishnan
Mrs. Indumati Rao
Ms. Jatinder Kaur
Mr. Sanjay SR 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)
- **Nanoworld** by **Prof. CNR Rao** (An Introduction to Nanoscience and technology)

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. In view of the increasing demand for these CD-ROMs from various institutions like the CSIR, National Science Museums, the Press and others, and considering the experiences of the end-users to make the learning experience easier for school children and more user-friendly for teachers to use these as reference material, the unit has revised the CD-ROM titles `Learning Science' volume 1&2', `Understanding Chemistry' and `Our Earth in the sky'. The Unit plans to translate, format and publish the book `Understanding Chemistry' in Hindi and Kannada.

National Book Trust, New Delhi has taken up the printing, publication and distribution of the `Learning Science' books in English and other Indian languages. The Kannada version of the books titled `Vignyana Kaliyona' `Samputa–1 to 4' was released at a function held on 18th August 2007 at Bangalore.

The CD-ROM titled `Nanoworld'- An introduction to Nanoscience & technology was developed and produced for students of high school and Pre-university levels. The interactive CD-ROM has nine topics. The script and narration was provided by Prof. CNR Rao. In the CD-ROM some basic aspects of nanoscience and technology are presented. The CD-ROM `Nanoworld' was released at the function `Children's Nano' as part of `Bangalore Nano-2007' held on December 7, 2007. 2000 CD-ROM's were procured by the Department of Information Technology, Biotechnology and Science & Technology, Government of Karnataka for distribution to the participants at the above function.

Figure 1: Multimedia CD-ROMs developed and produced by ETU

ETU is currently engaged in the translation, development of the CD-ROM's and books titled `Vigyan Seekhe'. The Learning Science series in Hindi is being brought out both as CD-ROMs and books. The books will be brought out by National Book Trust.

In the area of science popularization, `Celebration of Chemistry', `Learning Science' and `Vignyana Kaliyona' (a science popularization program in Kannada for the benefit of Kannada medium school children) programs were conducted at different places in the country. The unit has made presentations at various international fora using excerpts from the multimedia CD-ROMs Learning Science and Understanding Chemistry.

As part of National Science day celebrations, on 28th February 2007, Mrs. Indumati Rao gave a lecture on `Global Warming and Climate change'. ETU presented a multimedia presentation on the same theme from excerpts of the CD-ROMs `Learning Science' volume 1 & 2.

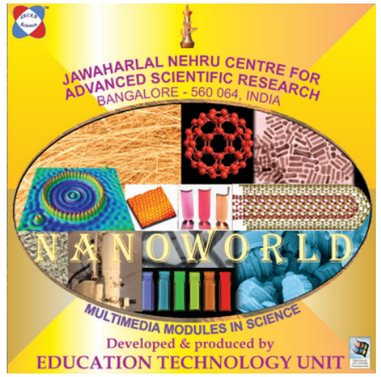


Figure 2: Nanoworld—A CD-ROM on Nano science and technology developed and produced by ETU

The unit presented a multimedia program "India @ sixty" as part of the Centre's program to celebrate 60 years of our independence. Children's Science Congress-2007 was organised at JNCASR on 27th November 2007. ETU presented multimedia presentation of excerpts from the CD-ROM `Nanoworld'. A short film titled `CNR Rao - A Life time Professor' was also screened at this function where students and teachers from various Navodaya Vidyalaya Schools participated. ETU presented the participating teachers with the books `Learning Science' and `Understanding Chemistry'.

As part of the global curriculum, the unit has plans to develop Mathematics, Geography and other subjects as multimedia packages. ETU plans to bring out a book titled `Nanoworld' authored by Prof. CNR Rao. This book is intended for students, teachers and others who have a interest in Nanoscience and technology. The book will cover various areas like technology, health and other aspects of Nano materials.

In addition the future plans of the unit involve bringing out the Kannada version of the CD-ROM `Nanoworld' called `Nanoprapancha'. The unit will be organizing a large number of science popularization programs for the school children and teachers.

Engineering Mechanics Unit

Chairman
Roddam Narasimha

Associate Professors
Meheboob Alam
Rama Govindarajan
KR Sreenivas

Faculty Fellows
Ganesh Subramanian

Senior Associate
SM Deshpande

Distinguished Fellows
Michael Gaster
Anatol 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.

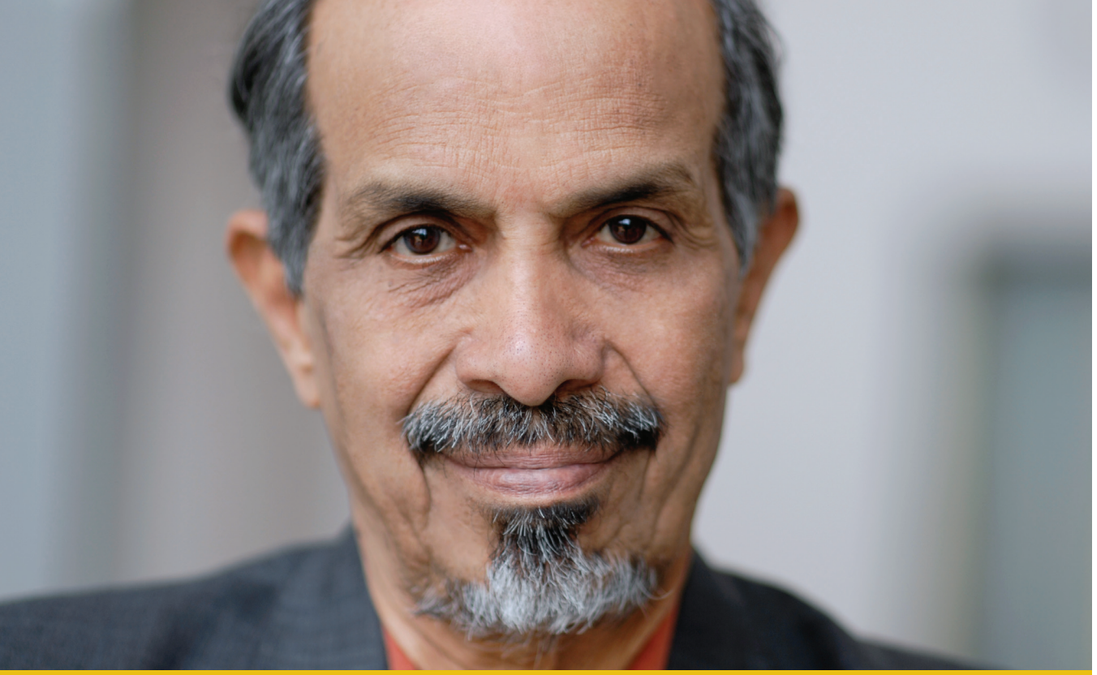
The Unit's technologically oriented studies primarily focus on aerospace and chemical applications. For example, studies on flow stability and transitions between laminar and turbulent states in a wide variety of situations have direct relevance to aerospace and chemical technologies. New insights into the action of polymers on turbulent flows - as well as the nature of transition on swept wings - have been obtained from such work. This work has shown that viscosity and density stratification have considerable influence on the transition to turbulence and on the flow near vertical structures. Research is being conducted also on discontinuities in the flow, such as hydraulic jumps, which are not caused by instability. It has been shown that a hydraulic jump driven by surface tension can be produced in the absence of gravity at small scales. Another area of special interest is computational fluid dynamics, chiefly in problems connected with aerospace technology.

Research on the dynamics of granular matter explores fundamental scientific problems and also has 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, facultyw 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), University of Twente (The Netherlands) and Max-Planck Institute for Marine Microbiology (Bremen, 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 m length and 0.6 m x 0.6 m 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. Work in experimental fluid dynamics is also carried out in several bench-scale set ups also 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 on 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 flow-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.

1. Transitions around a swept leading edge

Continuing work on a project carried out for Boeing, a special experiment has been devised in which an identical pressure distribution can be created on a flat and on a curved surface. It is shown that curvature hastens and intensifies reversion from turbulent to laminar flow, thus helping to explain how multiple transitions occur rapidly at high angles of attack. (With P R Viswanath, R Mukund, EAD/NAL).

2. Stability of a mixing layer

A mixing layer is the basic flow unit in fluid dynamical mixing problems. The stability of such a layer presents a paradox: if the flow is assumed parallel the layer is always unstable, which cannot be true at sufficiently low Reynolds numbers. Using the 'minimal composite theory' of non-parallel flows developed by us, we show that the mixing layer has a critical Reynolds number of about 30 when based on the velocity differential across the layer and the vorticity thickness. A broad view of the stability characteristics is presented in figure 1. (With Pinaki Bhattacharya, Rama Govindarajan).

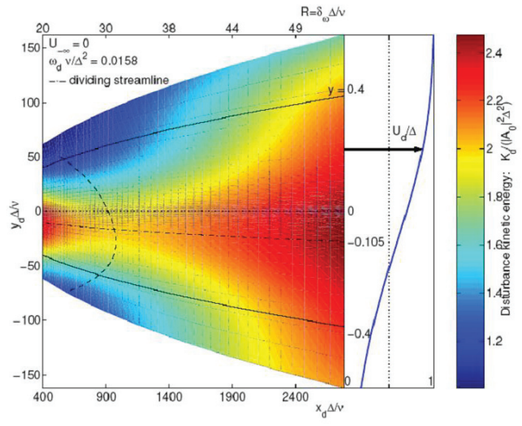

Figure 1: Variation of disturbance energy in a mixing layer flowing from left to right

3. An episodic description of turbulent flux events

Using data acquired at Jodhpur as part of a major atmospheric experiment known as MONTBLEX 90, a new stochastic description of turbulent flux processes is proposed. In this description the flux time series is replaced by a chronicle of flux events. Several statistical parameters characterizing these events, such as their inter-arrival times, intensities and widths have been derived from observations. A nearly-neutral atmospheric boundary layer is 'productive' (i.e. generates positive momentum flux) about 36% of the time, 'counter-productive' (i.e. generates negative flux) about 15% of the time, and 'idle' (i.e. generates no net flux) over the rest of the time. Such a description may have applications in flow control by manipulation of coherent structures.

4. Wavelet diagnostics for detection of coherent structures in flow imagery

Flow imagery acquired by the laser induced fluorescence technique has now been converted into wavelet movies. At appropriate wavelet scales coherent structures in turbulent flow can be identified from instantaneous images and the life cycle of the structure can be tracked. The picture is consistent with the idea that the base of a coherent structure in a turbulent jet is a vortex ring exhibiting the Widnall instability of a thin vortex ring.

Figure 2: Real clouds (left) and fake clouds in the laboratory (right). The latter are generated by dumping ohmic heat into a plume of electrically conducting fluid in a water tank of size 600 mm × 600 mm.

The data so analysed was acquired in an experiment whose objective was to reproduce cloud fluid dynamics in the laboratory. How successful this has been is shown in Figure 2 which compares clouds in nature with those produced in the laboratory by releasing heat into a turbulent plume, dynamically simulating the latent heat released on condensation of water vapour in the cloud. (With G S Bhat CAOS/IISc, Arun Srinivas)

5. Connections between solar activity and monsoon rainfall

Previous work by us (Geophys. Res. Lett. 2005, show-cased as editor's choice) has shown that rainfall all across India increases when solar activity is higher – in some regions at very high confidence levels (upto 99.99%). A detailed anlaysis of wavelet cross spectra between sun spot numbers and rainfall, using novel Monte Carlo methods for assessing statistical significance (due to appear in the Journal of Geophysical Research), confirms the earlier conclusion, but in addition enables us to propose a mechanism involving displacement of the two giant circulating systems that characterize the tropics, namely the Hadley and Walker cells. This displacement changes the location of convective systems, thus affecting local rainfall and explaining the spatial differentiation that characterises the effect. (With Subarna Bhattacharyya)

6. Cyclone track prediction

Following earlier work on a new scaling for convective boundary layers, a parameterization scheme for heat, momentum and moisture fluxes in convective conditions under low cross wind has been incorporated in the NAL Varsha model. Significant improvement in skill at cyclone track prediction has been demonstrated. (With U N Sinha, T N Venkatesh)

7. History of Science

An Encyclopaedia of Classical Indian Sciences, coedited with Helaine Selin of Hampshire College, Amherst, MA, was published in 2007 by Universities Press.

PhD Students

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MS Students

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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 improve current mathematical models. From late 2007, I have started developing a laboratory-facility to study granular matter and multi-phase flows.

Meheboob Alam received a PhD (1998) from the Indian Institute of Science and is a recipient of the Alexander von Humboldt Fellowship (2000) and the `Asian Young Fluid Dynamicist Award' (2007). He joined JNCASR in 2003. He is also the head of the `Max-Planck Partner Group' at JNCASR, supported by the Max Planck Society Germany.

Non-Newtonian rheology, fluctuations and microstructure in 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 well as a model for normal stress differences. Currently, we are probing the dense-phase rheology of granular matter, focusing on the normal stress behavior, the non-Gaussian velocity fluctuations, and the fluid-solid transition (shown in Figure 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 in dry granular flows and suspensions. One goal is to devise control strategies to manipulate microstructure formation in complex fluids according to process requirements.

In collaboration with a 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.

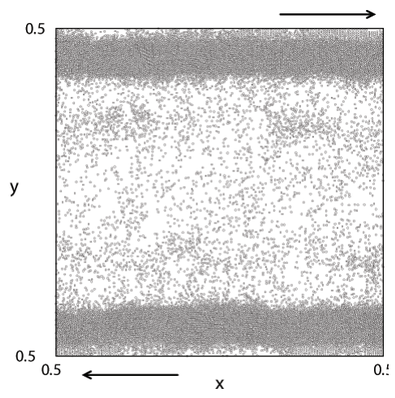

Figure 1: Phase separation and the coexistence of fluid and solid phases in a sheared granular material. For details, see Ref. 2.

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 which 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 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.

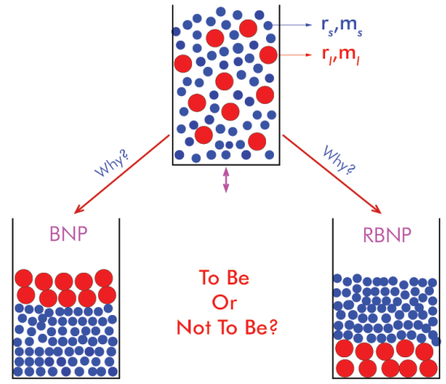

Figure 2: Segregation of granular mixtures under vertical vibration.

Geophysical convective flows

Recently we have started exploring the dynamics of large Prandtl number convective flows which are important in many geophysical contexts (magma, mantle plumes, etc.). We have discovered a new `buoyancy-driven' instability mode in a plane thermal plume. Our current focus is to investigate the related mixed convection phenomena with non-Newtonian rheology and non-Boussinesq approximation. Another project deals with exploring bubble-driven flows via laboratory experiments and theory.

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.

Recent Publications

1. Lakkaraju R, Alam M. Effects of Prandtl number and a new instability mode in a plane thermal plume. Journal of Fluid Mechanics, 592, 221-231, 2007.
2.Vijayakumar K, Alam M. Velocity distributions and the effect of wall roughness in granular Poiseuille flow. Physical Review E, 75, 051306, 2007.
3. Gayen B, Alam M. Algebraic and exponential instabilities in a sheared micropolar granular fluid. Journal of Fluid Mechanics, 567, 195-233, 2006.

PhD Students

Priyanka Shukla, M Malik (from IISc)

MS Students

Ashish Malik, Snehalatha B

Graduates

Bishakhdatta Gayen (MS), Rajaram Lakkaraju (MS), K Vijayakumar (MS)

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Flow instabilities and discontinuities, transition to turbulence

The main areas of interest of this group are (i) when and why a fluid flow becomes unstable, especially when the properties of the fluid, or of the flow, are not constant in space and time, (ii) the related question of the transition from order to chaos, with high emphasis on the laminar-turbulent transition, and (iii) flows at small length scales.

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 when and how a certain laminar flow becomes unstable and ultimately turbulent.

In this group we study instabilities and singular behaviour of various kinds. The people describe their work here.

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.

Harish Dixit

For several years now, our group has been interested in how stratification, for example of viscosity, can lead to interesting physical phenomena. My work centres around density stratified flows, which are frequently encountered in the atmosphere and in the ocean. A common example is the rise of a hot jet of smoke from a chimney, which flattens out upon reaching a particular height where its density is equal to that of the surrounding air. I am currently studying flow past bluff bodies both in a stratified and an unstratified system. I am interested in understanding the formation and evolution of the 'Benard-Karman street' in these systems. I carry out full numerical simulations and also study the stability aspects of these flows. I am also interested in understanding vortex dynamics in these situations.

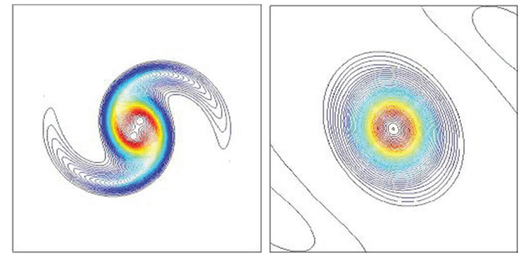

Figure 1: Vorticity plots showing the merger of two vortices in an unstratified and a stratified system at the same instant of time. Vortex merger is complete for a stratified system.

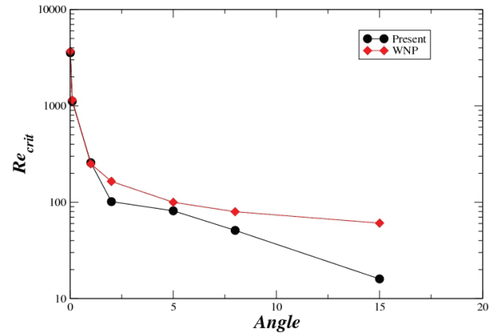

Figure 2: I show here the instability critical Reynolds numbers I calculated for channels with different angles of divergence, compared with those calculated using a quasi one-dimensional approach. The present approach predicts a significantly smaller critical Reynolds number.

Ratul DasGupta

The laminar hydraulic jump, very easily observable when water from a tap hits the kitchen sink (see picture), is a long studied problem. This phenomenon comprises a sudden discontinuity rather than an instability. A complete understanding of the complex mechanism at work which produces the jump has not been obtained so far. Through analytical work and numerical simulations, I hope to have a better understanding of the physical mechanism of the jump, and also of related flows such as through an axisymmetric cavity. Recent work in our group has shown a hydraulic jump can be produced by surface-tension at small length scales, in the absence of gravity. I am interested in understanding this flow well.

Gayathri Swaminathan

Non-parallel flows have been a long-standing interest of our group. We believe that some of them can follow a route to turbulence which is quite different from that in a channel or pipe. Our group, as well as others, have so far studied the instabilities in these flows using a one-dimensional or quasi one-dimensional approach. This approach is however not justified in a majority of such flows. My aim is to study the stability of non-parallel flows with a two-dimensional eigenvalue approach, which does not have this disadvantage. The first flow of interest to me is that in a diverging channel, where I am also interested in studying the effect of wall roughness and small scales. Using my approach I can study the stability of many other flows situations such as vortical flows, convergent-divergent pipes, wakes and separated flows.

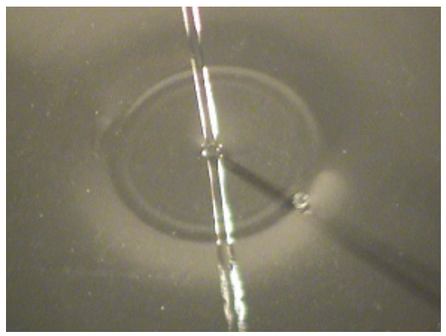

Figure 2

Sumesh PT, Vineetha Mukundan, Rahul Bale and Rakshith BR

New strengths are brought to the group by this group of students. Sumesh is deeply interested in small-scale flows, interfaces, droplet spreading and related things. Vineetha is studying instabilities in the flow of complex fluids like clays. Rahul is trying to understand the transient growth of instabilities in various flows. Rakshith is looking at the validity or otherwise of the no-slip boundary condition. Anubhab Roy is working jointly with Ganesh Subramanian, his work is described on Ganesh's page.

Recent Publications

1. The effect of wall heating on instability of channel flow. A Sameen & Rama Govindarajan, 2007, Journal of Fluid Mechanics, 577, 417-442.
2. The signature of laminar instabilities in the zone of transition to turbulence. N. Vinod & Rama Govindarajan, 2007, Journal of Turbulence, Vol. 8, pp1-17.
3. Stability of miscible core-annular flows with viscosity stratification. B. Selvam, S. Merk, Rama Govindarajan and E. Meiburg, Journal of Fluid Mechanics, 2007.
4. Gravity-free hydraulic jumps and metal femtolitre cups. Manikandan Mathur, Ratul DasGupta, Neena Susan John, N. R. Selvi, GU Kulkarni, & Rama Govindarajan, Physical Review Letters, 2007, 98, 164502.

Graduates

N Vinod (PhD), A Sameen (PhD), Kirti Chandra Sahu (PhD), Antina Ghosh (MS), Pinaki Bhattacharya (MS), Kaushik Srinivasan (MS), Rahul, Ratul, Harish, Gayathri, Vineetha, Rakshith and Sumesh

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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:
(a) Research on free-shear flows, which includes effects of axial acceleration, ambient viscosity and stratification on the entrainment process and dynamics of free-shear flows.
(b) Unsteady aerodynamics of insect flight, research in this area is aimed towards developing engineering guidelines needed for an optimum design of small mechanical objects that can use unsteady aerodynamics for propulsion and lift generation.
(c) Role of radiative heat transfer in the dynamics of nocturnal atmospheric boundary layer.
(d) Geofluid dynamics research in the group includes study of double diffusive fingerconvection, which plays an important role in determining salt and heat flux transported in oceans and the study of convection in the limit of high Prandtl and Rayleigh numbers, which is relevant to mantle convection.
(e) Other area of interest is on natural ventilation of buildings, using cooling towers, earthen-tunnels to reduce air-conditioning loads in buildings.

Few of these research topics have been described in detail in the following section. 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), high-speed imaging, hot-wire and thermocouple probes.

Sreenivas KR 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.

Experimental and numerical study of turbulent free shear flows

Under this research program, we study the effects of axial acceleration, ambient viscosity and stratification on the entrainment process and dynamics of free-shear flow. 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 group, 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.

Unsteady aerodynamics of insect flight

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.

Figure 1: Flow fields around a pair of wings executing asymmetric-flapping
(a) two-dimensional numerical simulation indicating velocity vectors and color-scheme indicating vorticity distribution
(b) experimental flow visualization using streak-photography.

Lifted Temperature Minimum (Ramdas Layer)

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 observed temperature profile is extremely stable even though the estimated Rayleigh number for the unstable Ramdas layer is about 105, 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. This problem has relevance in the retrieval of ground-surface temperatures from satellite, and in climate modeling and may be in coronal temperature distribution in stars.

Geo-fluid dynamics

(a) Convection in the limit of high Rayleigh and Prandtl numbers: Mantle convection is responsible for volcanism and plate-tectonics. Laboratory modeling of the mantle convection is challenging as one needs to address the effects of large variations in pressure, composition, temperature, density and viscosity and it corresponds to the large Rayleigh number convection in a medium with large Prandtl number. In our experiments, we simulate large Rayleigh number convection using concentration difference to drive the convection and also medium viscosity is enhanced using CMC to achieve high Prandtl numbers. We study the dynamics of convection and its structures under this limiting condition.

(b) Double diffusive convection: 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 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. Research on this topic is relevant to oceanography, mantle-convection, metallurgy and other engineering applications. In geology DDC may have a role in determining some of the basaltic rock structures.

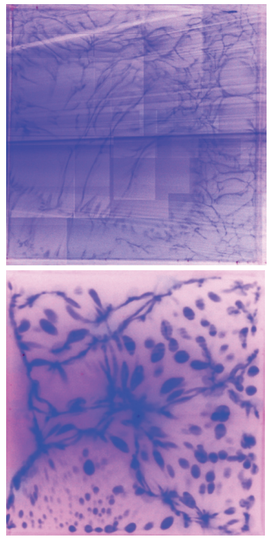

Figure 2: Plan views of plume structures in convection-system driven by concentration variation
(a) in a medium having no viscosity contrast between plume and medium (similar to standard Rayleigh-Be´nard convection)
(b) a medium of high viscosity in which plumes have lower viscosity (similar to buoyant mantle plume with high temperature and low viscosity)

PhD Students
Dhiraj Kumar Singh, Mukund Vasudevan, Subudhi S (IISc Student jointly with Prof. JH Arakeri)

MS (Engg.)
Aditya Konduri (Jointly with Prof. R. Narasimha), Devranjan Samanta Dinesh Kumar, Niranjan S. Ghaisas (IISc Student jointly with Prof. J. Srinivasan), Rajapandian A, Vivek Prakash N (Jointly with Prof. JH Arakeri)

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Dynamics and rheology of complex fluids, Hydrodynamic stability, Vortex dynamics

1. Dynamics, stability and rheology of complex fluids

A major theme relates to transport processes in complex fluids including suspensions of both active (bacteria) and passive particles, bubbly liquids, emulsions, and granular gases. In particular, we look at the effects of micro-scale inertia on transport processes and rheological properties of complex fluids. New physics accompanying the inclusion of even a small amount of inertia leads to results that differ profoundly from the inertialess case.

The essential idea is to examine the microstructural dynamics in an attempt to understand the resulting macroscopic flow behavior. This ranges from investigating the response of a single swimming bacterium, or a particle or a drop in an external flow, to simulating the collective dynamics of large interacting systems of such elements. Several ongoing projects under this broad heading are detailed below:

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 a dilute suspension, the rheological problem reduces to analyzing an isolated orientable particle in a shearing flow. An inertialess axisymmetric particle (e.g. a fibre) in simple shear flow rotates in Jeffery orbits, and the orientation dynamics, for all times, is determined by initial conditions. We have recently shown that inertia causes a fibre in simple shear flow 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 a spheroid to determine the critical aspect ratio at which the exchange of stability between the flow-gradient plane and the vorticity axis occurs, together with the rheological implications of this bifurcation in orientation dynamics. In a non-dilute suspension, hydrodynamic interactions play a crucial role in determining the single particle orientation distribution. It is therefore of interest to determine the steady orientation distribution that arises as a consequence of pair-interactions.

We also aim to study fibre motion in non-linear flows. An example is Poiseuille flow, wherein an inertialess fibre 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 laminar boundary layers.

Inertial pair-particle trajectories: application to aerosol/hydrosol coagulation and suspension rheology

Aerosol stability is vital to the shelf-life of paints, insecticides and pharmaceuticals, and is governed by several factors including Brownian motion, gravity, colloidal and hydrodynamic forces. For large particles, thermal effects are negligible, and the coagulation rate is 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.

We have shown that pair-particle trajectories in simple shear flow are dramatically altered with even a tiny amount of inertia. Simple shear is, however, a degenerate flow where extension and vorticity are in an exact 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 form structurally unstable configurations. Results will be relevant to turbulent coagulation of sub-Kolmogorov particles.

The above modifications also lead to a non-trivial microstructure and a non-Newtonian rheology; indeed, they help resolve a key indeterminacy arising in suspension rheology. Thus, even a tiny amount of inertia plays a crucial role in the rheology of non-Brownian suspensions.

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 has been initiated to verify the postulated regimes, including the predicted self-similar evolution of a planar cluster. The kinematic simulation uses a simplified representation of inertial interactions based on the single-particle velocity field, and offers an attractive alternative to full dynamic simulations. Applications include gravity currents, pollutants dispersion etc.

Particle motion and interactions in viscoelastic suspensions

The study of particle motion in non-Newtonian fluids is of interest. Many intriguing phenomena in this regard, including the formation of long chains in shearing flows, have been experimentally identified; most of these remain unexplained, however. It is our aim to try and account for these observations from a theoretical standpoint. For instance, one may try and explain the incipient stages of particle-chain formation in viscoelastic fluids by characterizing the nature of pair-hydrodynamic interactions.

Collective dynamics in 'active' particle suspensions

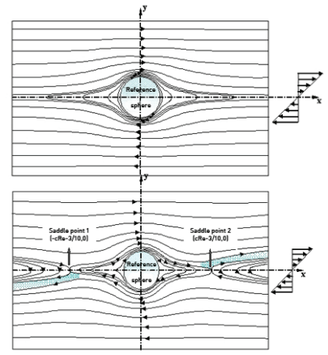
We have discovered a novel instability in a bacterial suspension that is expected to play an important role in determining the level of velocity fluctuations in such systems. The instability arises from the instrinsic stress associated with a swimming bacterium which, for long wavelengths, acts as a negative viscosity. We are also conducting a numerical investigation of pair-hydrodynamic interactions between swimming bacteria, which should lead to the prediction of the pair-distribution function in a dilute bacterial suspension. This will be a first step in understanding the role of hydrodynamic interactions in the collective dynamics of bacterial suspensions.

Heat and mass transfer from particles and drops in shearing flows

An ongoing analytical study examines the role of micro-scale inertia on the heat transfer from both particles and drops suspended in shearing flows. Heat transfer in these instances is crucially enhanced by inertia by destruction of a region of closed streamlines that persists around the particle or drop in inertialess conditions (see figure 1).

2. Vortex dynamics in polymeric turbulence

In collaboration with Dr. Rama Govindarajan, we are looking into the dynamics of high speed flows of dilute polymer solutions. This is in an attempt to understand the multi-scale structure of polymeric turbulence, and aspects in which it differs from turbulent flows of Newtonian fluids. The relevant fluid mechanical regime is characterized by high values of both the Reynolds number and the Weissenberg



number, and is therefore dominated by a balance of inertia and elastic forces, rather than an interplay of dominant inertial and weak viscous forces that characterizes Newtonian turbulence. The study is from a mechanistic viewpoint, and will try to understand the effects of small amounts of high molecular weight polymers on the canonical structures (for instance, vortices) that play a role in the dynamics of Newtonian turbulence. Turbulent drag reduction is an excellent example of the dramatic structural effects induced even at extremely small polymer concentrations.

In this regard, we have recently found that polymers modify the angular velocity profile in a Lamb-Oseen vortex in a manner as to concentrate the vorticity away from the axis. The resulting vortex is then susceptible to a Kelvin-Helmholz instability. The merging of Lamb-Oseen vortices governs the inverse cascade in two-dimensional Newtonian turbulence. The predicted instability should therefore play a crucial role in similar merger events occurring in dilute polymer solutions.

3. Radiation-induced stabilization and the Ramdas effect

We are interested in heat transfer processes influenced by radiation. An ongoing study examines the effect of radiation on the well known Rayleigh-Benard threshold for the onset of convective instability. This study is expected to yield insight into the apparent stability of the observed lifted temperature minimum (the 'Ramdas effect') at Rayleigh numbers well beyond the critical value predicted by conventional linear stability theory invoking a balance of conduction and convection. In an attempt to mimic the ingenious laboratory setup of my colleague, Dr. K.R.Sreenivas, the configuration comprises a fluid medium between two plates, maintained at fixed temperatures, and a third radiatively participating surface expected to stabilize the otherwise convectively unstable configuration.

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.

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Computational Fluid Dynamics

Our research primarily focuses on aerodynamics, aero-elasticity, computational fluid dynamics, and data assimilation for better weather forecast.

We are especially interested in the development of novel numerical methods in computational fluid dynamics (CFD). For example, we have developed kinetic methods and kinetic flux vector splitting (KFVS), KFVS on moving grids (KFMG), and least squares KFVS (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.

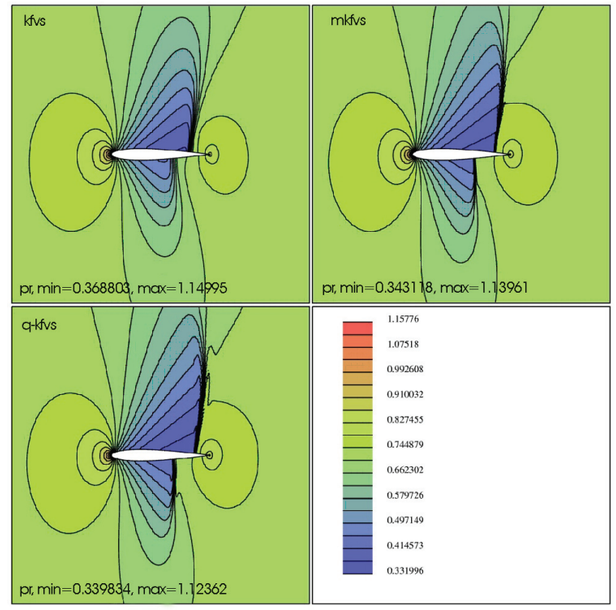


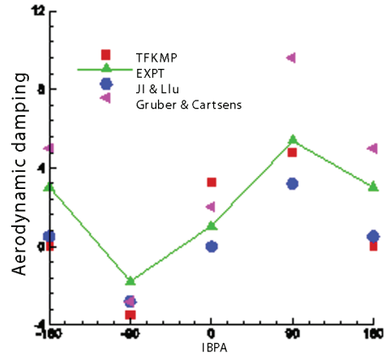
Figure 1: Pressure contours: Transonic flow past airfoil

Modified KFVS (mKFVS)

The dissipation inherent in the first order KFVS is reduced by developing modified KFVS (mKFVS). It gives a control on the dissipation present in the scheme. Adjoint based optimisation method has been used with φ as a control vector for minimising numerical entropy. TAPENADE has been used to obtain gradient vector of cost function. Very accurate results have been obtained through optimisation.

Multidimensional Upwind Algorithms

The violation of rotational invariance by LSKUM, like many other multidimensional solvers, has been addressed by developing KUMARI (Kinetic Upwind Method Avec Rotational Invariance). Subsequently the study revealed that LSKUM is not very much sensitive to the loss of rotational invariance.



Flutter prediction through aerodynamic damping

Weighted LSKUM (WLSKUM)

The robustness is an extremely important aspect in flow problems for complex geometries. The Weighted LSKUM (WLSKUM) precisely enhances the robustness of LSKUM by reducing the multidimensional least squares formulae for spatial derivatives to 1D formulae by appropriate choice of weights.

Turbomachinery unsteady flows

LSKUM has been extended to work on moving chimera clouds for computing unsteady flows normally encountered in turbomachinery. The LSKUM-MN (Least Squares Kinetic Upwind Method – Moving Nodes) has been applied to predict onset of flutter.

Publications

1. Ramesh V & SM Deshpande. "Unsteady Flow Computations for Flow Part Multiple Moving Boundaries using LSKUM". Computers & Fluids 2006, invited paper in the special issue of this Journal in honour of Prof. M. Napolitano.
2. K Anandhanarayanan, M Nagarathinam and SM Deshpande. "Parllelistion of Grid Free Kinetic Upwind Solver", AIAA 2005, Paper No: AIAA 2005–4628.
3. K Anandhanarayanan, M Nagarathinam and SM Deshpande. "Development and Application of a Grid Free Kinetic Upwind Solver to Multi-Body Configurations", AIAA 2005, Paper No: AIAA 2005-4846.
4. Flutter prediction through aerodynamic damping
R Krishnamurthy, BS Sarma and SM Deshpande. "Kinetic Schemes for Computational Aero elastic Analysis of 2D Airfoils in Transonic Flows". AIAA 2004, Paper No: AIAA 2004-2236.

PhD Student

(From IISc) N Anil

R&D Assistant

Keshav S Malagi

Evolutionary and Organismal Biology Unit

Chairman
Amitabh Joshi

Faculty
MK Chandrashekaran
Vijay Kumar Sharma
Kavita Jain (jointly with TSU)

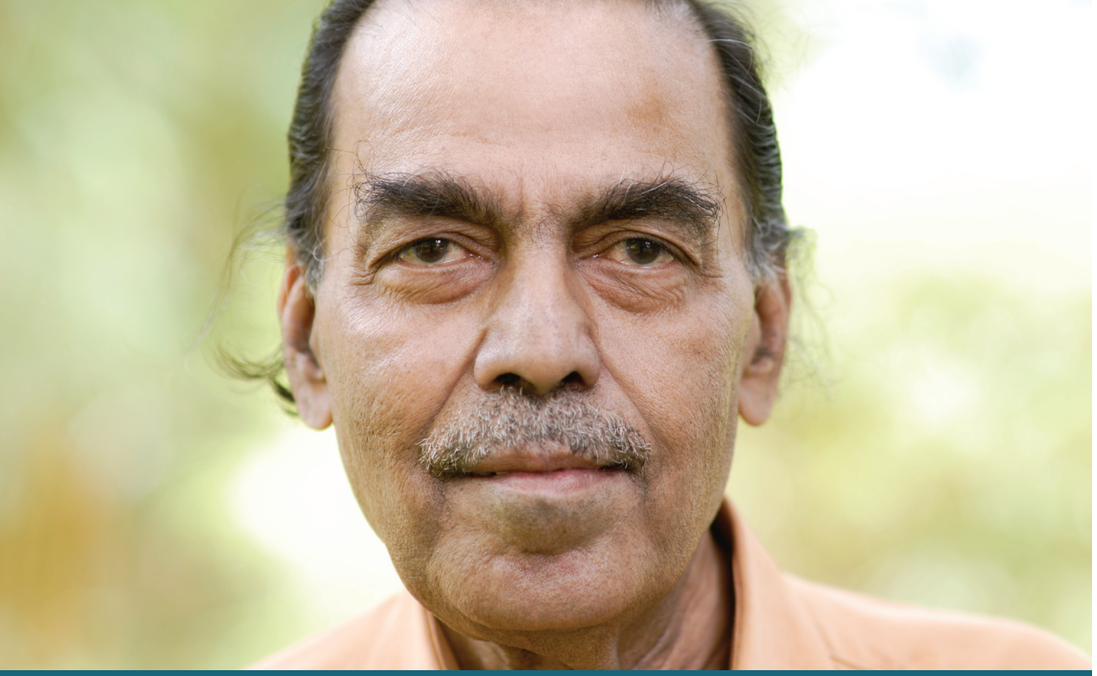
Biological systems are organized in an hierarchical manner structurally, and can be studied at levels ranging from molecules to ecosystems. Decades of narrowly focussed studies at one or the other level of structural complexity have greatly enhanced the body of information we possess about biological systems, leading to a state exemplified by TS 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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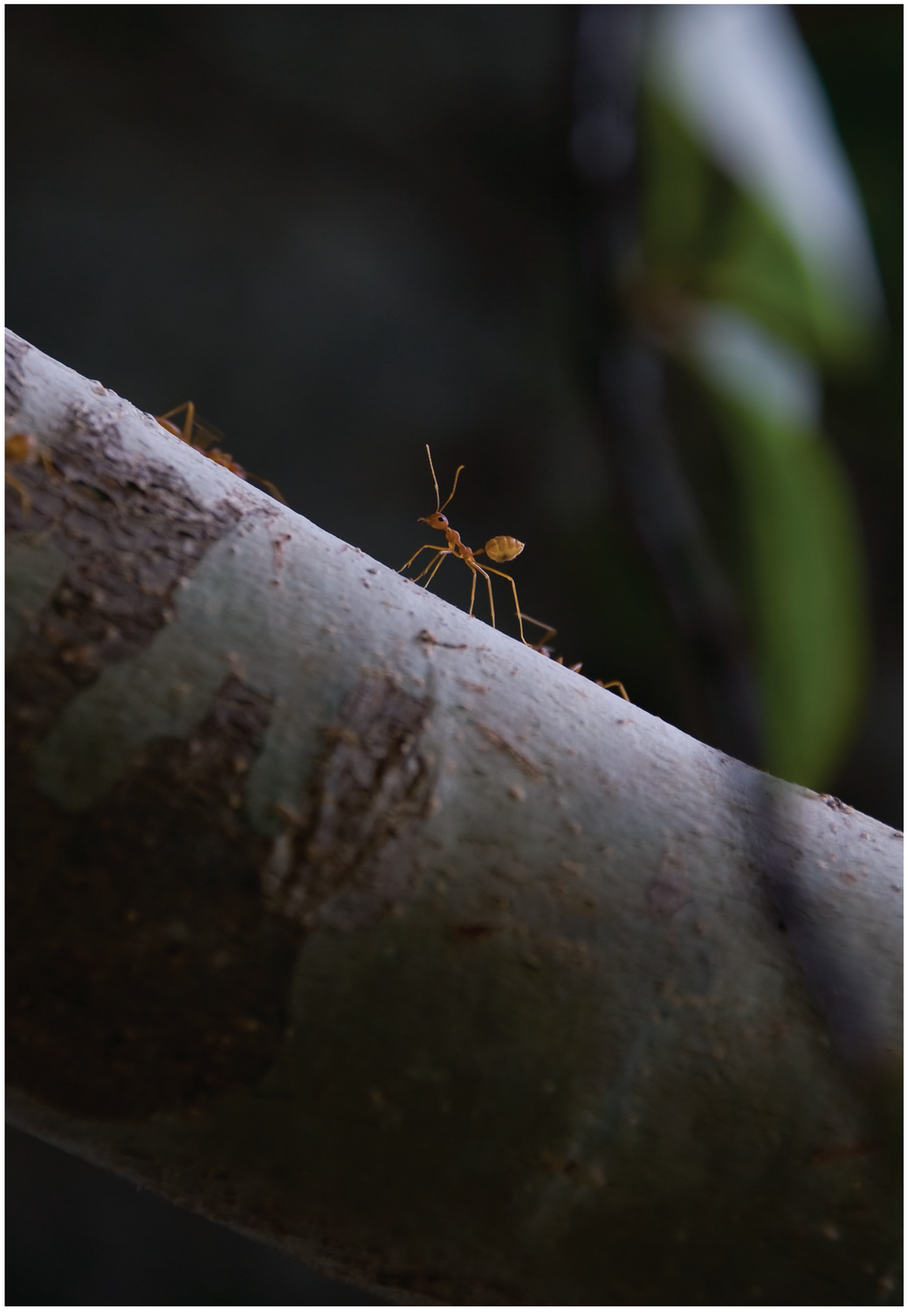
Chronobiology and Animal Behaviour

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.

M K 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 developmental biology as well as in many philosophical issues in evolution.

Amitabh Joshi did his Ph.D. in Genetics at Washington State University, Pullman, and was a post-doc at UC Irvine before joining JNC in 1996. Other than evolution and ecology, he has serious interests in philosophy, history, music, and poetry in English, Urdu and Persian.

Shampa Ghosh

I joined the lab in 2003, and have worked on characterizing life-history traits, and their phenotypic plasticity across multiple environmental axes, in *Drosophila melanogaster* populations selected for faster development and early reproduction for more than 350 generations. I am also interested to delve deeper into the issue of how variance in these traits is shaped by a combination of selection and plasticity. I also study whether long term selection for accelerated development has resulted in any reproductive divergence between these populations and their controls. The results from crosses performed between the two sets of populations indicate that the populations indeed have started showing some signs of divergence. In addition, I am examining direct and correlated responses to selection for faster preadult development in *D. annanassae* to examine whether the genetic architecture of fitness related traits in this species differs from that in *D. melanogaster*, an attempt to address the deeper issue of how conserved the genetic architecture of fitness is across closely related species.

N Archana

I joined the lab in 2004, and am working on adaptations to larval crowding in three different fruitfly species: *D. melanogaster*, *D. ananassae* and *D. nasuta nasuta*. I primarily study the different traits that evolve as populations of these species adapt to larval crowding, in order to assess how conserved the genetic architecture of fitness-related traits is across these species. I am also interested in the evolution of larval growth rates in these species. I have found that *D. ananassae* populations take a different evolutionary trajectory for adapting to larval crowding as compared to populations of the closely related species, *D. melanogaster*, that have extensively been studied earlier. The pattern of genetic correlations between development time, body weight, larval feeding rate and competitive ability is quite different in these two species.

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 350 generations. My major aim is to probe the 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. I have analyzed gene expression at different life-stages in these populations using microarrays, and have found that there are large difference in expression levels of many genes in the selected populations and their ancestral control. I now plan to study these genes and their expression in more detail in these populations.

Snigdhadip Dey

I joined the lab in 2006, and I study the dynamics of single populations and metapopulations, using a combination of simulations and experimental studies with fruitflies. One of my major focuses has been to study the interaction of migration, local dynamics, and various perturbations on the coherence and stability of metapopulations in order to understand the causes of out-of-phase local dynamics in metapopulations. In addition, I am also investigating demographic outcomes of selection on life-history related traits in *Drosophila* populations, as well as the dynamics of systems of competing species or strains in spatially structured habitats.

Rajdeep Bannerjee

I joined the lab in 2007, and my broad interest is in evolutionary genetics, especially life-history evolution. Currently, I am screening for possible inbreeding depression in laboratory populations of *Drosophila melanogaster* selected for faster development and also late reproduction.

BM Prakash

I joined the lab in 2007 and am studying the effects of parental age and parental rearing density on pre-adult survivorship and weight at eclosion in *Drosophila*, and how these effects evolve under selection for adaptation to high larval density or for different ages at reproduction. I also plan to explore the possible presence of *Wolbachia* endosymbionts in these laboratory populations of *Drosophila* and, if present, examine their effects on reproductive behaviour.

Punyatirtha Dey

I joined the lab in 2007 and am studying the underlying molecular bases of the difference in immunocompetence and body size of *Drosophila melanogaster* populations selected for faster development and early reproduction, compared to their ancestral controls. The study would help in understanding the molecular mechanisms mediating co-evolution of these important life history traits in *Drosophila*.

Key Publications

1. Mueller, LD and A Joshi. 2000. Stability in Model Populations. Monographs in Population Biology 31, Princeton University Press, Princeton, NJ, USA.
2. Joshi, A. 2001. Interspecific Competition. In Encyclopaedia of Life Sciences, Nature Publishing Group, MacMillan, London, UK (www.els.net).
3. Prasad, NG, Shakarad, M, Anitha, D, Rajamani, M and A Joshi. 2001. Correlated responses to selection for faster development and early reproduction in *Drosophila*: the evolution of larval traits. Evolution 55: 1363-1372.
4. Prasad, NG, Dey, S, Shakarad, M and A Joshi. 2003. The 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.
5. Shakarad, M, Prasad, NG, Gokhale, K, Gadagkar, V, Rajamani, M and A Joshi. 2005. Faster development does not lead to correlated evolution of greater pre-adult competitive ability in *Drosophila* melanogaster. Biology Letters 1: 91-94.
6. Dey, S and A Joshi. 2006. Stability via asynchrony in *Drosophila* metapopulations with low migration rates. Science 312: 434-436.
7. Dey, S and A Joshi. 2007. Local perturbations do not affect stability of laboratory fruitfly metapopulations. PloS ONE 2(2): e233.

PhD Students

Shampa Ghosh, N Archana, KM Satish, Snigdhadip Dey, Rajdeep Bannerjee

Post-doc Fellows

BM Prakash, Punyatirtha Dey

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Circadian rhythms in fruit flies and ants

In my laboratory we take an integrated approach to understanding circadian timing mechanisms, using behavioural, evolutionary, sociobiological, physiological, and molecular 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 studies on *Drosophila* populations selected for different circadian phenotypes. In future, we plan to search for new rhythm variants using various screening methods and investigate underlying molecular mechanisms. In recent years we have raised early and late populations of fruit flies which show morning and evening preference for behaviour. We have shown that circadian clocks evolve as a correlated response to selection on timing of emergence. Preliminary studies show that molecular clock of early flies is phase advanced, and those of late flies are phase delayed compared to controls. We have also initiated laboratory selection experiments to study the effect of selection for gated emergence on the circadian clocks and its precision. We have also generated selection lines wherein light/dark cycles alone are used as selection force. We have also been able to demonstrate the role of circadian clocks in the reputation of life history traits such as development and life span.

Another area of investigation that we are pursuing is understanding the circadian consequence of social organization. We maintain colonies of two ant species *Camponotus compressus* and *Camponotus paria* which comprise of two sexually active castes, queens and males, and three worker castes, namely major, media and minor workers. In a series of preliminary studies we have shown that these ants use circadian plasticity to manage challenges arising due to division of labor. Recently we have also been able to show that pre-adult development of these ants is accelerated by about 40% under constant light. We are planning to conduct extensive studies on these ant species to understand the molecular and physiological basis of circadian plasticity.

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

Koustaubh 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 circadian clocks. I am interested in understanding the molecular basis of early and late circadian phenotypes.

Pankaj Yadav

I joined the lab in 2006 and I am working on a project entitled "Evolution of Circadian clocks under periodic and constant environmental conditions." I am investigating the extent to which constant and light/dark cycles are effective in shaping up circadian clocks in fruit flies *D. melanogaster*. Previous studies from our lab have shown that circadian clocks play a crucial role in determining life history traits and rearing fruit flies in different light/dark environment modifies photic-response of circadian clocks.

Shahnaz Rahman Lone

I joined the lab in 2007 and I am interested in understanding the role of circadian clocks in social organization, aggression and speciation in eusocial insects. My studies have shown that there is wide diversity in overt rhythm of different castes in two species of ants. Interestingly, the circadian behaviors of these castes correlate well to the jobs assigned to them in the colony. These ants have seasonal clocks which times their pre-adult development. Currently I am studying how foraging ants are able to communicate information about local time to their nest mates who remain inside the soil. In a separate study, I have also shown that temporal partitioning of activity is vital in mating and in the act of avoiding interference between two sympatric species of social ants.

Manjunatha Thondamal

I joined the lab in 2007 and I am working on the neurogenetics of egg-laying rhythm in *D. melanogaster*. Previous studies from our laboratory suggest that egg-laying rhythm in *Drosophila* does not require some of the known core-clock genes such as *per* and *tim*, and the circadian neurotransmitter, *Pigment Dispersing Factor (PDF)*. Studies from our lab also suggest that egg-laying rhythm persist even in absence of the circadian pacemaker neurons. I have been able to show that temperature cycle is a stronger Zeitgeber for egg-laying rhythm than light/dark cycle. I am interested in understanding the neural and hormonal basis of egg-laying rhythm in *D. melanogaster*.

M Muzafar Beigh

I joined the lab in 2007. I am working on six wild species of Drosophilidae family that are being maintained in our lab. These wild species include *D. melanogaster*, *D. ananassae*, and *D. malerkotliana*, *D. nasuta*, *D. neonasuta*, and *Zaprionus indianus* which were collected from the vicinity of JNCASR Campus in Bangalore. My project includes studying the role of circadian clocks in sympatric speciation. My study will also include carrying ant behavioral as well as molecular studies to identify allelic polymorphism in core clock genes.

Key Publications

1. Sharma, VK, Lone, SR, and A Goel. 2004. Clocks for sex: Loss of circadian rhythms in ants after mating? Naturwissenschaften 91:334-337.
2. Howlader, G, Paranjpe, DA, VK Sharma. 2006. Non-ventral lateral neuron based non-PDF mediated clocks control circadian egg-laying rhythm in *Drosophila* melanogaster. Journal of Biological Rhythms 21:13-20
3. Howlader, G, VK Sharma. 2006. Circadian regulation of egg-laying behavior in fruit flies *Drosophila* melanogaster. Journal of Insect Physiology 52: 779-785.
4. Kumar, S, Vaze, KM, Kumar, D, VK Sharma. 2006. Selection for early and late adult emergence alters the rate of pre-adult development in *Drosophila* melanogaster. BMC Developmental Biology 6: 57.
5. Kumar, S, Kumar, D, Paranjpe, DA, Akarsh, CR, VK Sharma. 2007. Selection on the timing of adult emergence results in altered circadian clocks in fruit flies *Drosophila* melanogaster. Journal of Experimental Biology 210:906-918.
6. Kumar, S, Kumar, D, Harish, VS, Divya, S, and VK Sharma. 2007. Possible evidence for morning and evening oscillators in *Drosophila* melanogaster populations selected for early and late adult emergence. Journal of Insect Physiology 53: 332-342.

PhD Students

Koustubh M Vaze, Pankaj Kumar Yadav, Shahnaz Rahman Lone

MS Students

Manjunath T, Muzafar Baig

Geodynamics Unit

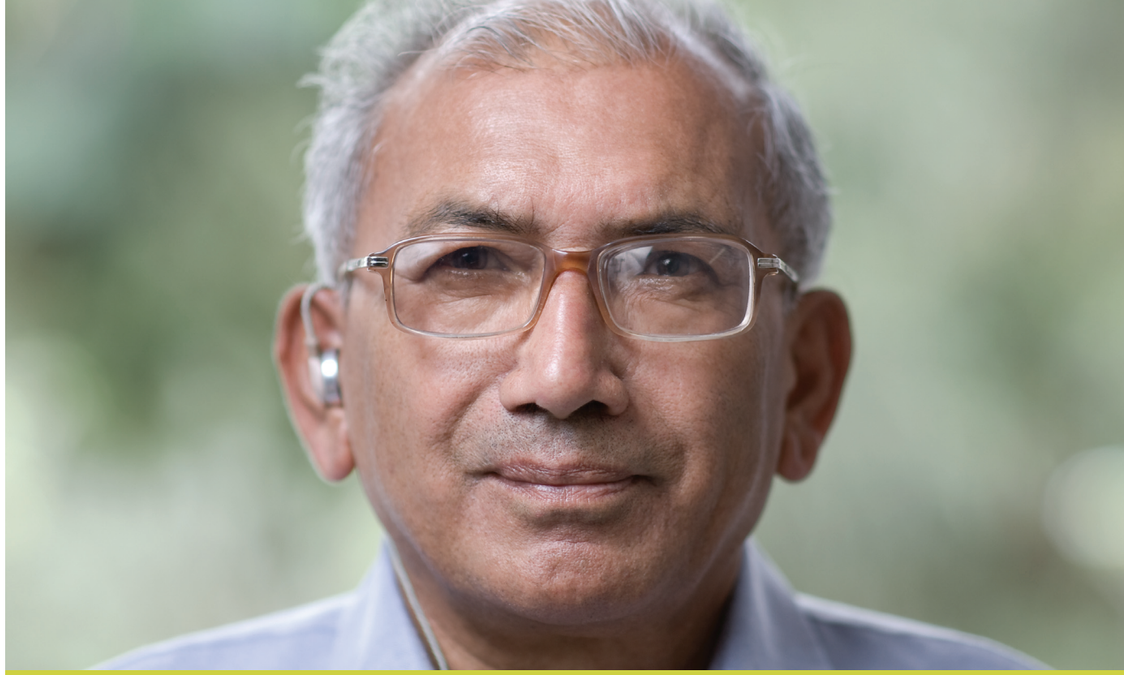
Chairman
KS Valdiya

Selected Research Papers

1. Valdiya KS. Trans-Himadri fault: Tectonics of a detachment system in central sector of Himalaya. *Jour. Geol. Soc. India, 65, 537-552*, 2005.
2. Valdiya KS. Tectonic resurgence of the Mysore plateau and surrounding regions in cratonic southern India. *Current Science*, 81, 1068-1089, 2001.
3. Valdiya KS. River response to continuing movements and the scarp development in central Sahyadri and adjoining coastal belt. *Jour. Geol. Soc. India*, 57, 13-30, 2001.

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

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Neotectonic 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 the 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.

KS Valdiya is an INSA Golden Jubilee Research Professor

Chairman
MRS Rao

Professor
Namita Surolia

Associate Professor
Anuranjan Anand
Hemalatha Balaram
Maneesha S Inamdar
Tapas K Kundu
Udaykumar Ranga

Faculty Fellow
Kaustuv Sanyal

Molecular Biology and Genetics Unit

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; Stem cells and Developmental Biology; Inherited human genetic disorders and Centromere function in yeast. 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 houses specialized equipment such as a multi-photon confocal microscope, spectropolarimeter, mass-spectrometer, a microarray facility and many more. An animal facility is available for routine experiments. The Unit presents a vibrant and highly interactive research atmosphere. Students at MBGU find themselves immersed in regular academic activities, including work presentations, journal club discussions, guest lectures and many more.

The pathogenic agents for AIDS and Malaria, two infectious diseases that are 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 discovered the type II fatty acid synthesis pathway in Plasmodium and was the first to demonstrate the antimalarial effect of the common antibacterial 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.

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 has worked extensively on 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. She has, more recently derived new human embryonic stem cell lines. Kaustav Sanyal's group studies regulations in cell cycle with special emphasis on the genetic and epigenetic controlling the mechanism of chromosome segregation using several pathogenic and non-pathogenic yeasts as model systems. Using genomics and genetics, this group has recently discovered that the centromeres are probably the most rapidly evolving loci in related yeast species. This group also studies the molecular architecture of centromeres/kinetochores in pathogenic yeasts to identify proteins that are species-specific and thus can be used as targets to develop anti-fungal drugs.

The Molecular Biology and Genetics Unit (MBGU) at JNCASR is internationally recognized for its innovative research programs in the biomedical and biological sciences. With eight laboratories conducting cutting-edge research, MBGU attracts the brightest students from all over India. Research in the laboratories spans diverse areas of biology bound by the common thread of biomedical application. The current areas of research are categorized as: infectious diseases; chromatin organization and transcription regulation; stem cells and cardiovascular development; inherited human genetic disorders and mechanism of chromosome segregation. MBGU is rapidly growing, not only in terms of facilities, personnel and research support, but in terms of national and international reputation as well. Research programs at MBGU are supported by grants from several national and international funding agencies and also from biotechnology companies.

The modest size of our Unit and the Centre is helpful in promoting active exchange of ideas and facilities not only within the department but also with fellow physicists, chemists and engineers at JNCASR as well as at other national and international laboratories. This is reflected in the inter-disciplinary nature of our publications. Research in the department is supported by state-of-the-art facilities that include a multi-photon confocal microscope, spectropolarimeter, mass-spectrometer, microarray facility, a core sequencing facility and a central animal facility. In addition, a specialized set of equipments caters to the needs of individual laboratories. A central computer centre provides high speed internet access and excellent technical support.

Students for the PhD program at MBGU are selected through a highly competitive national-level selection process. Our interactive PhD program provides training in a wide range of molecular-genetic, biochemical, cell- and developmental biology approaches for both basic and translational research and focuses heavily on the molecular models. The essence of the PhD program is to provide the student with greater flexibility and wider opportunities for choosing cutting edge research theme and provide him/her with a solid, broad-based training in multidisciplinary biomedical research. MBGU presents a vibrant and highly interactive research atmosphere for the students who find themselves immersed in several academic activities, including research presentations, journal club discussions, training workshops, conferences and guest lectures. Students are actively encouraged and financially supported to present their results at international meetings. Students who graduate from the department have a wider scope of career options be it academia or industry.

Our faculty members are always accessible and can be contacted through our website www.jncasr.ac.in/mbgu.

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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. Our laboratory is also working on Glioma to identify key genes that are essential for progression of low grade to high grade Glioma and also to identify key biomarkers for clinical management.

MRS Rao obtained his Ph D at the Indian Institute of Science. He was then a Research Associate 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 now the President of JNCASR.

We have recently studied the nuclear import machinery involved in transport of transition proteins to spermatid nucleus and identified importin 4 as the karyophilin recognizing the NLS of TP2 and facilitating its transport into the haploid nucleus (Figure1). We have recently discovered that transition protein TP2 undergoes acetylation by p300 and PCAF, TP2 also get methylated by CARM1. We would like to understand the significance of these modifications in the global chromatin remodeling process that takes place during the late stages of spermiogenesis. We would also be identifying the interacting protein partners that recognize the acetylated and methylated TP2.

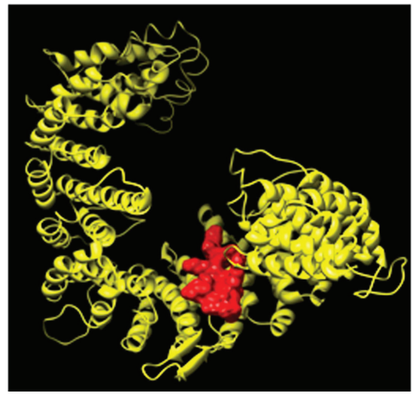

Figure 1

In continuation of our studies on the process of chromatin remodeling during mammalian spermiogenesis, especially during the replacement of histones by transition proteins and finally by protamines, we have observed histone H4-hyperacetylation as a plausible signal for histone replacement as it is seen to occur during early- to mid- elongating stages of spermiogenesis and ceases at the late-elongating stages. This signal in the elongating spermatids is not linked to transcriptional activity as is seen by our immunocytochemistry data (Figure 2). By RT-PCR and Real-time PCR analysis we have also observed that four ATP-dependent chromatin remodeling factors are over-expressed during the round spermatid stages. Two of these factors contain bromodomain, a domain known to recognize acetylated lysine residues. Only one among these four remodeling factors, continues to be present in elongating spermatids. We are now addressing the role of this remodeling factor in spermiogenesis. We would also want to study the functional significance of Cdyl, a histone acetyl transferase enzyme, which is expressed during the elongating stages of mouse spermiogenesis.

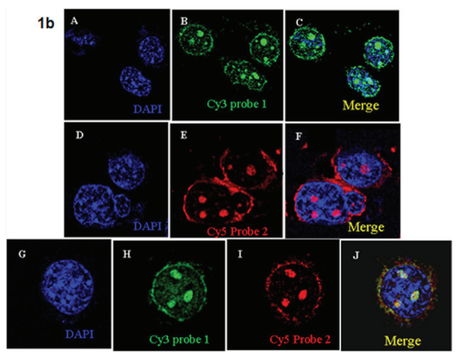

Figure 2

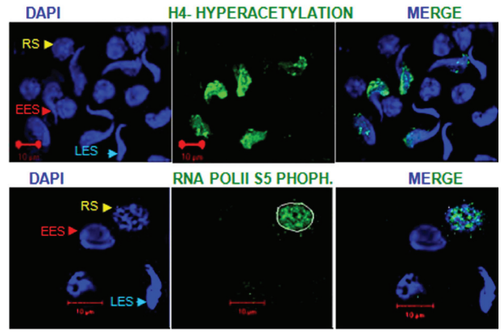

Figure 3

One of the important features of male germ cell differentiation is meiotic division in which recombination between the homologous chromosomes is one of the hallmarks. Recombination is not random but occurs at defined loci, which are called as hotspots. Recent evidences are accumulating to demonstrate that chromatin structure plays an important role in initiating the recombination process at these hotspots. We have recently identified and discovered a meiotic recombination hotspot in the mouse genome (Nishant *et al* 2004). We would like to understand the molecular features particularly at the chromatin structure that influences the recombination at this locus. We would also be identifying the role of chromatin remodeling factors and the histone variants and their posttranslational modifications at this chromatin domain.

We have also discovered that the mouse recombination hotspot locus that we have identified also encodes a noncoding polymerase II transcript. We have now characterized the properties of this transcript. We have observed that the 2.4 kb non coding RNA gets processed by the Drosha complex and both the processed and the precursor RNA are nuclear restricted showing a distinct localization pattern (Figure 3). We would like to understand the function of this noncoding RNA and its possible chromatin target(s).

With the aim of identifying gene signatures or markers differentiating between types of astrocytoma grades, we performed microarray analysis from the astrocytoma patient samples of various grades ranging from grade II to highly aggressive grade IV or GBM. The analysis resulted into identification of several genes that have been short-listed. We have shown that ASCL1 is a progressive or secondary GBM specific marker and that ASCL1 upregulation is accompanied by inhibition of Notch signalling as observed by uninduced levels of HES1 and increased levels of HES6. AEBP1 is another such gene, which we have found to be specifically upregulated in primary GBM as opposed to secondary GBM. This gene product is a transcriptional repressor. Understanding its biology and gaining insights into its role in the context of glioma is being pursued using techniques like RNA interference, microarray and ChIP on chip experiments. Initial experiments using Si RNA mediated down regulation have identified many genes whose expression are perturbed under these conditions.

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Molecular and Cellular Mechanisms of Human Genetic Disorders

The main focus of research in our laboratory is molecular genetics and cell biology of human genetic disorders. For a number of disorders that occur in the human populations, there is strong evidence that genes play major roles in their causation but nothing is known regarding many such genes. We are currently studying two human genetic disorders. These are: deafness (sensorineural, non-syndromic, severe-to-profound hearing disability) and epilepsy syndromes (a group of heterogenous neurological disorders). Major emphasis of our work involves: (i) whole genome-based studies to discover novel genes for deafness, (ii) whole genome-based studies to find novel genes for common forms of epilepsy syndromes and (iii) functional characterization of certain new disease genes belonging to the families of G-protein-coupled receptors and transcription factors to delineate the molecular genetic pathways these genes are a part of. A number of specific research projects exploring functional aspects of the disease genes mentioned above are presently underway in the laboratory. We are using techniques of gene expresssion, advanced microscopy, immunocytochemistry, immunohistochemistry, cell biology and expression microarrays and SNP microarrays, to address the questions we are asking. Knowledge generated from these studies is very useful, as it helps create the foundation for development of enhanced therapeutics as well as device effective early-detection/intervention strategies for the brain disorders. Much of our work is carried out in collaboration with medical institutions in the country. 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 a few other specialty hospitals. Ali Yavar Jung National Institute of Hearing Handicapped, Mumbai and Maulana Azad Medical College, New Delhi are our collaborators in the area of deafness genetics.

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

G-protein coupled receptors (GPCRs) and Transcription factors (TFs) in epilepsy disorders

Epilepsy is a neurological disorder that results from abnormal, excessive and synchronous activity of neuronal cells. Genetic factors are involved almost exclusively in susceptibility to certain forms of human epilepsies. Finding genes causing various forms of epilepsies and examining their functions is proving to be one of the best ways to understand biological mechanisms underlying these brain disorders. Genetics of epilepsy disorders has emerged as one of the most useful paradigms to understand biological basis of complex genetic disorders. Recent advances in human genetics are accelerating research in the area with the hope that a number of novel genes related to epilepsy will be identified, and the field of mouse genetics is providing additional boost to such studies.

We have recently identified three novel epilepsy-causing genetic genes, *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 causing epilepsy. *Seizure-1* encodes a protein belonging to a family of G-protein coupled receptors (Figure1). *Seizure-2* belongs to a family of transcription factors widely known to play role in neuronal cell fate specification and developmental regulation of gene expression.

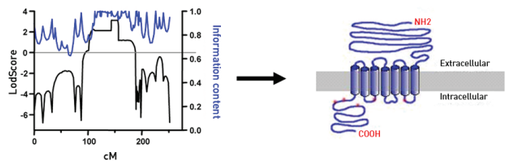

Figure 1

These findings are quite interesting as they are helping us to move on to investigate molecular genetic pathways functioning in the human brain cells which when disrupted can predispose to epilepsies and perhaps other brain disorders.

We are conducting experiments to examine role of *Seizure-1* and *Seizure-2* in context of the disease pathophysiology. We are studying expression of these genes in human 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 find targets of *Seizure 1* and *Seizure 2*, to try to understand the biochemical and developmental pathways these genes are capable of regulating. A detailed mutational characterization of *Seizure-3*, (5q12-14 JME; Figure 2a,b) is being conducted to identify pathogenic mutations in the crucial genetic interval.

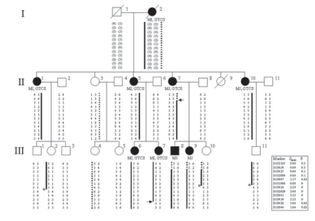

Figure 2a

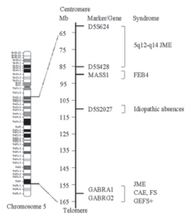

Figure 2b

Genes and mutations for deafness

Hearing impairment is the most frequent sensory defect in humans. About 80% of the hereditary deafness is non-syndromic and it occurs due to defects in the genes expressed and functioning in the cochlea which is auditory signal transduction apparatus in mammals. Genetic complexities of the deafness-causing genes in India are not well explored. One line of research in our lab focuses on 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. Second line of research is aimed at characterization of novel genetic loci responsible for severe-to-profound, non-syndromic, prelingual, sensorineural hearing loss.

Recent work from the laboratory has shown that about 22% of hereditary deafness in India is caused due to mutations at a single gene, *Connexin26 (Cx26)* (Figure 3). *Cx26* encodes gap junction molecules postulated to be involved in recycling of potassium ions and additional small molecules essential for initiation of action potentials in seosory cells in the cochlea.

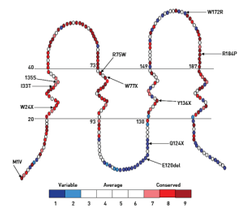

Figure 3

High prevalence of the *Cx26* mutations in the country is apparently due to an 8000-year old founder effect in the 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 4).

Additional deafness genes being studied at 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.*

Towards identification of novel deafness-causing genes, we are using strategies of genome-wide molecular mapping in multi-generational families with multiple affected members. These studies are leading to identification of novel genetic loci, which will be investigated in detail in the coming years at a detailed mutational and functional level.

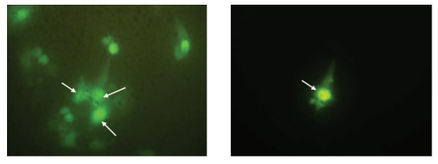

Figure 4

Lab members

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Protein Engineering and Molecular Parasitology

Plasmodium falciparum, the causative agent of malaria, is one of the most pathogenic microbes. Being an intra-erythrocytic parasite, *P. falciparum* 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 are focused on the characterization of the purine salvage enzymes, hypoxanthine guanine phosphoribosyltransferase, adenylosuccinate synthetase, adenylosuccinate lyase, GMP synthetase and 5' purine nucleotidases. Comparative studies on the human homologs have permitted the identification of structural and functional characteristics specific to the enzymes from the two species. We also study the homologs of these enzymes from the thermophilic archea *Methanocaldococcus jannaschii* with the aim of understanding the effect of temperature on catalysis and structural stability. Apart from the purine salvage enzymes we have also been involved in understanding the function and modulation of *P. falciparum* Sir2 (a NAD specific protein decetylase) activity. Tools of molecular biology, enzymology (steady state and burst phase kinetics, simulation of kinetic mechanisms using appropriate models), protein chemistry (chemical modification, mass spectrometric analysis) and biophysics (fluorescence, circular dichroism, dynamic light scattering, X-ray crystallography) are used to address different issues of protein structure and function.

Hema Balaram has a Ph D 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.

Purine nucleotide metabolism in *P. falciparum* infected human erythrocyte

P. falciparum lacks the ability to de novo synthesize purine nucleotides. Enzymes of both human and parasite origin contribute to purine nucleotide metabolism in the parasite-infected erythrocyte. Our aim is to elucidate the flux through this pathway by monitoring the fate of radiolabeled metabolites, effect of specific inhibitors and pseudosubstrates on parasite growth and, also by the biochemical analysis of the individual enzymes of this pathway.

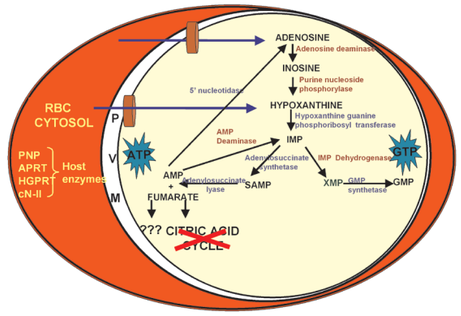

Figure 1: Purine nucleotide metabolism in *P. falciparum* infected erythrocyte

Protein dynamics and catalysis: Studies with *Methanocaldococcus jannaschii* adenylosuccinate synthetase (MJADSS)

Adenylosuccinate synthetase (AdSS) catalyzes the formation of succinyl-AMP from IMP and aspartate with the simultaneous conversion of GTP to GDP and inorganic phosphate. AdSS from the archaeon, *M. jannaschii* has been used to study two important attributes of enzymes from thermophilic organisms, namely thermophilicity and structural stability.

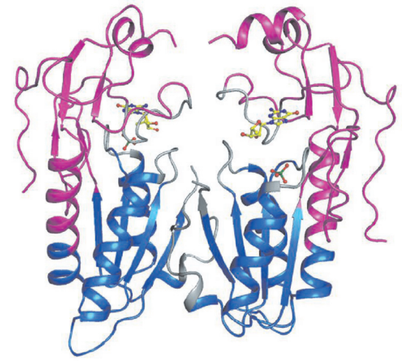

Figure 3: Altered subunit association in chimeric HGPRT

P. falciparum GMP synthetase (PfGMPS)

PfGMPS catalyses the conversion of XMP to GMP with the reaction occurring in two domains, the glutamine amidotransferase (GAT) and ATP pyrophosphatase (ATPPase). Coordination of activity across the two domains, achieved through channeling of ammonia from GAT to the ATPPase domain is the hallmark of amidotransferases. The mechanism of catalysis by PfGMPS, deduced in this laboratory is shown in Figure 2.

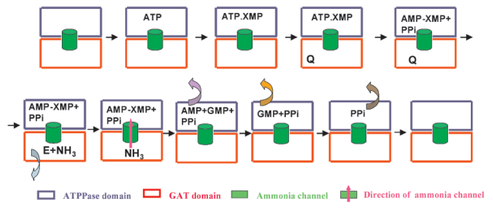

Figure 2: Proposed model for catalysis by *P. falciparum* GMP synthetase: A two domain, two catalytic site enzyme. Reaction involves channeling of NH_3 and coordination of activity across the two active sites.

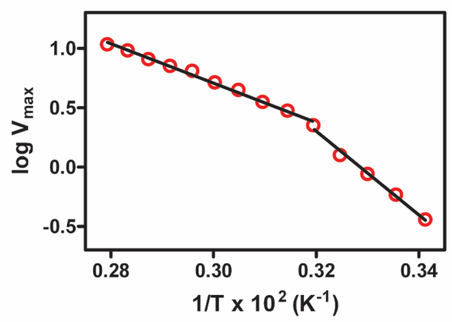

Figure 4: Temperature dependence of MjADSS catalysis. Plot of 1/T vs log V_{max} shows biphasic behaviour.

Hypoxanthine guanine phosphoribosyltransferase (HGPRT)

In an attempt to elucidate the structural basis of substrate specificity in HGPRTs, chimeric enzymes consisting of segments from the parasite and human proteins were constructed. The crystal structure of one of the chimeras, solved in collaboration with Prof. MRN. Murthy, MBU, IISc, shows altered subunit association with 180° flip of the subunits at the dimer interface. This laboratory is also probing the alterations in the structure of the purine bases and their nucleotides on liganding with HGPRT using resonance Raman spectroscopy in collaboration with Dr. Mrinalini Puranik, NCBS, Bangalore.

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Molecular, genetic and developmental analysis of the cardiovascular system

Cardiovascular disease and cancer are two major global health problems. Understanding cardiovascular development and angiogenesis are imperative to devising stem cell-based therapies for combating cardiac and ischemic diseases or tumor progression. A better understanding of the mechanistic and gene expression changes that occur in normal and pathological conditions as well as the ability to control stem cell differentiation will allow development of specific treatments and therapies.

While many conserved genes involved in heart, blood and blood- vessel formation have been studied in detail, several questions remain to be answered, particularly regarding early developmental stages. Our approach is to use vertebrate as well as invertebrate models to elucidate cell lineage specification, gene expression and function in circulatory systems. Our primary focus is on embryonic stem cells (ESCs) and their cardiovascular derivatives. Pivotal to our analysis are novel genes identified using ESCs and that have conserved gene expression and function in the circulatory system. Using this approach we investigate the mechanisms that control cardiovascular pathways of differentiation from ESC's as well as in animal models.

Maneesha Inamdar has a Ph.D. (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

Analysis of early mammalian vascularization is hindered, as development occurs in utero. This problem is overcome to some extent by using embryonic stem cells (ESCs) and in vitro differentiation models. ESCs are derived from the pluripotent cells of the inner cell mass and can differentiate to form almost all lineages including a functional cardiovasculature. 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 engineered gene constructs into ESCs, generate transgenic and knockout mice and thereby analyze gene function. We use human and murine embryonic stem cell models for our analysis.

Human Embryonic Stem Cell Laboratory

Recently we have set up a Human Stem Cell Laboratory at JNCASR funded by the Department of Biotechnology, Govt. of India. We are successfully growing and characterizing established human embryonic stem cell (hES) and embryonic carcinoma (hEC) cell lines. We have shown that genes of our interest (asrij and rudhira) are also expressed in hES and hEC cells and in human embryoid bodies used as a model for early human cardiovascular development. We have derived new hES cell lines. The laboratory is also involved in conducting international training courses in stem cell derivation, culture and differentiation.

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

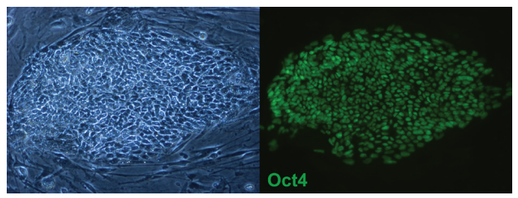

Figure 1: Human ES cell line BJN hem19 derived in our laboratory showing expression of the pluripotency marker Oct4

The OCIA domain family: A novel family of proteins expressed in ES cells and 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, namely, asrij and padosan. Both genes express in human and mouse ES cells and the developing vascular system. The Asrij and Padosan proteins have a novel conserved hydrophobic motif called the OCIA domain and localize to endocytic vesicles. 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 WD40 protein expressed in embryonic stem cells, erythropoiesis, angiogenesis and tumors

Using a functional genomics approach we identified a novel murine gene rudhira that is expressed at high levels in human and mouse embryonic stem cells and is restricted to blood islands and the erythroid lineage during embryonic development. Rudhira is also expressed in angiogenic precursors but is excluded from the differentiated endothelium. Rudhira is a 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 CardioVascular Biology

Transport of oxygen, nutrient and waste products is a fundamental requirement of all multicellular organisms. 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.

Our analysis and comparison of mammalian as well as *Drosophila* circulatory systems has given useful insight into gene function as well as ontogeny of the heart, blood and blood vessels. We have also undertaken analysis of these genes in the context of human development as well as in clinical studies with a focus on tumor angiogenesis and progression. These investigations will be valuable for understanding ES cell pluripotency, cardiovascular development, cell fate specification and regulation of function.

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Transcription regulation in humans by histone chaperones, epigenetic modifications, altered chromatin dynamics (by nonhistone chromatin proteins) and small molecule modulators of chromatin modifying enzymes

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 chaperones in the regulation of chromatin transcription and in the gene expression in response to stress. 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. We have synthesized nontoxic, p300 specific HAT inhibitors from the nonspecific and toxic inhibitor garcinol, which potently repress the HIV replication. Screening for specific modulators of Histone Methyl Transferases (HMTase) and Aurora kinases are 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. Recently, we have also extended this area of research in the field of nanotechnology in collaboration with Prof. C. Narayana and Dr. Eswaramoorthy of Chemistry and Physics of Materials Unit of our centre.

PhD, Department of Biochemistry, Indian Institute of Science, Bangalore (Mentor: Prof. MRS Rao), Post Doctoral Research, National Institute of Genetics, Mishima, Japan (Supervisor: Prof. Akira Ishihama) and The Rockefeller University, New York (Supervisor: Prof. Robert G Roeder).

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 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 dependent as well as independent DNA repair.

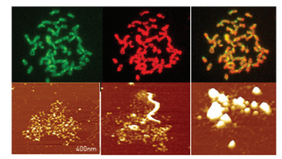
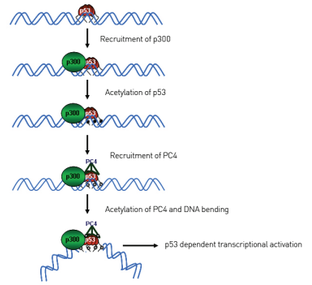


Fig. A: Distribution of PC4 on mitotic chromosomes. The condensed mitotic metaphase chromosomes from mouse L cells were spread on a slide and stained with Hoechst for DNA (I). The chromosomes probed with purified polyclonal antibody against PC4, followed by secondary antibody conjugated to rhodamine (II). The third panel (III) shows a merge of the antibody and DNA stained images.

Figure 1: Human Transcriptional Coactivator PC4 is a bonafied chromatin component

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.



Mol cell Biol. (2007) In press

PC4 activate p53 function through post translational modification and DNA bending: Transcriptional regulator p53 recruits p300, Which acetylates p53. Further PC4 is recruited to the complex by p53 through its interaction, which is followed by acetylation of PC by p300. Acetylated PC4 by providing better substrate for p53 binding activates p53 mediated transcription.

Figure 2: PC4 activate p53 function through post translational modification and DNA bending

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.

Nonotechnology and chromatin dynamics

By employing silver/ silver-gold nanoparticle and Raman Spectroscopy, we have reported the Surface-Enhanced Raman Scattering studies of histone acetyltranscferase (HAT) p300 and its mode of interactions with different small molecule modulators of the HAT. These work may provide an ideal tool to study the drug-protein interactions in therapeutics using SERS. We have also been able to find the nontoxic and cell permeable carbon nanoparticle, which could be highly useful both for basic (to understand chromatin dynamics) and applied (drug delivery/diagnosis) research

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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 infections in India. Subtype-C viruses have also been identified from Brazil and other South American countries; China, the UK and the African continent.

Are subtype-C viruses endowed with unique biological properties that make them successful as compared to other viral subtypes? 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. Some researchers believe that subtype-C virus has already taken one step in this direction and become relatively less pathogenic to the host.

Diverse research themes in our laboratory are directed essentially to find an answer to this elusive and challenging question. Are subtype-C viruses of HIV-1 attenuated to a greater degree?

Udaykumar Ranga is a PhD in Life Sciences (1990) from SLS, JNU. He worked as a Post-doctoral fellow at FDA and University of Michigan 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

The B/C recombinant viruses of HIV-1 identified by our laboratory in India are molecularly different from those of China and Thailand. Is a new recombinant viral epidemic emerging in India? Are there many more and diverse recombinant viruses in circulation in India? If the answer to these questions is in affirmative, we may have to rethink our disease management and intervention strategies including vaccine design. Blending HIV molecular biology and nano-technology, we are developing a micro-chip that should permit a large scale molecular analysis of the viral isolates in India. Once optimized, the micro-chip should have universal application and be able to identify diverse strains of recombinants.

3. Subtype-C strains of HIV-1 are probably incapable of causing neuron death in the brain

Infection of brain by HIV leads to neuron death that is clinically known as dementia. Incidence of dementia in the USA and Europe, where subtype-B viruses of HIV-1 are common, is as high as 35%. In contrast, incidence of dementia in India appears to be significantly low at 1-2%. To answer this puzzle, we identified a single amino acid natural variation in an important viral protein Tat of subtype-C, a cysteine to serine variation at position 31. We experimentally demonstrated and hypothesized that because of this important difference, subtype-C strains of HIV-1 can not cause death of neurons and trigger dementia. This work (Ranga U et al, 2004) is a landmark publication in HIV-1 neuro-pathogenesis because for the first time there was experimental evidence that viral subtypes can have different pathogenic properties. Following this publication, several laboratories in India, USA and other countries initiated programs to evaluate this hypothesis. Importantly, in May 2007, National Institutes of Health, USA dedicated nearly 10 million dollars and announced two major research programs to study subtype differences in HIV neuro-pathogenesis following the lead given by our laboratory. We and our collaborators have been extending these studies further. We isolated infectious molecular clones from a demented patient that demonstrated several interesting molecular properties. These are the first HIV-1 subtype-C molecular clones that can use any and several coreceptors to enter the target cell. Furthermore, although T-lymphocytes are the natural target cells for HIV, these viral clones appear to have some restriction in proliferating in T-cells whereas subtype-B viruses do not seem to have such problems (see the figure). Is there some subtype-specific restriction factor present in T-cells that controls subtype-C replication in these cells? If yes, this will be an important and interesting finding. We are presently pursuing this lead.

4. Optimization of DNA vaccines through engineering molecular adjuvants

Like viruses, DNA vaccines offer the greatest technical advantage that the encoded antigens are introduced directly 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 HIV-1 Tat as a model antigen, we have been engineering molecular components into expression vectors with an objective to improve the performance of DNA vaccines. We engineer T-cell epitopes, optimize transcript splicing, develop novel promoters, and many other strategies all to make DNA vaccines more efficient and powerful.

5. A human clinical trial to evaluate a Siddha medicine for HIV/AIDS

Limitations of the standard anti-retroviral medicine are many including being expensive, causing drug resistance, lack of viral eradication and limited immune reconstitution. In active collaboration with several organizations, including an NGO, a clinic, DST and a pharmaceutical company, our laboratory is evaluating the efficacy of a *Siddha* medication in a clinical trial. We are testing this medicine in a single-blinded study in 30 seropositive volunteers. As a control, 30 other volunteers are under standard anti-retroviral therapy. The results of this trial, the first study of this nature in India, will be known in August 2009.

6. Development of novel molecular diagnostic techniques for HIV

For optimal disease management of HIV/AIDS, availability of efficient and affordable diagnostic tests is as important as access to chemotherapy. In collaboration with other laboratories and several biotechnology companies, our laboratory is actively engaged in developing conventional and novel molecular diagnostic techniques for HIV. Our main thematic objective is to avoid PCR for clinical diagnosis. Although powerful and popular, PCR is practically unsuitable for a resource poor country like India. Is it possible to replace PCR as a molecular diagnostic technique? We believe so. By harnessing the potential of the Surface-enhanced Raman Spectroscopic technique and nano-technology, it should be possible to develop alternative technologies that should be cheaper and technologically simpler. Preliminary data from our laboratory are quite encouraging.

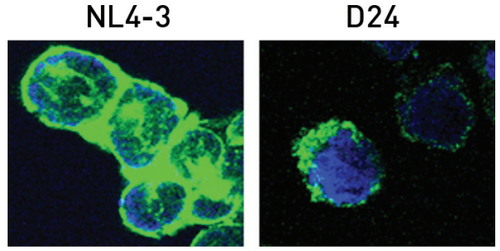

Figure 1: HIV proliferates on a target cell. A T-cell line SupT1 was infected with two different viral strains NL4-3 (left panel, American virus) and 03In94_D24 (right panel, virus isolated in our laboratory). After 7 days, the cells were stained for the viral protein p24 (green in color) and the images were captured using confocal microscopy. The nuclei are stained in blue color. Interestingly, the Indian virus doesn't seem to grow efficiently in the target cells. This quite puzzling finding is an active theme of investigation in our laboratory.

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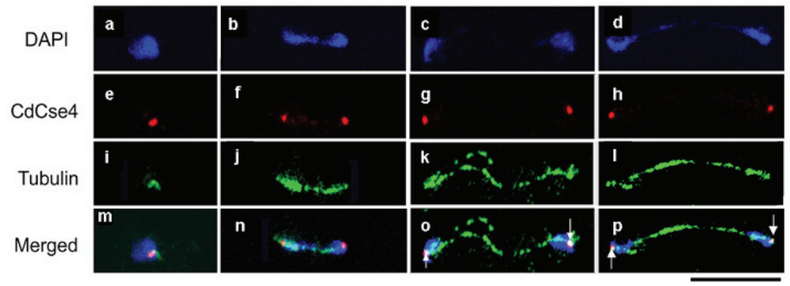
Mechanism of Chromosome Segregation: A Molecular Approach

Centromeres are 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 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 has a PhD in Yeast Genetics (1994 -1999) from Bose Institute (Jadavpur University) and did his postdoctoral work at University of California, Santa Barbara (1999 – 2005) before joining JNCASR in October, 2005



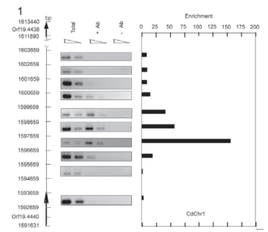


Figure 1: Identification of centromeres in C. dubliniensis. **(A)** Subcellular localization of CenH3 (red) in the nucleus (blue). **(B)** CenH3 is localized close to SPBs on kinetochore micotubules (green). **(C)** Chromatin immunoprecipitation using anti-CenH3 antibodies to localize and map centromeric chromatin on chromosome 1.

1. Epigenetic mechanism of centromere formation in *Candida* species

How centromeres are recognized and propagated is a subject of much conjecture. Several lines of evidence suggest that establishment of centromeres is not entirely dependent on underlying DNA sequences. We have recently demonstrated that in *Candida albicans*, centromere formation is epigenetically regulated. One of the most intriguing observations from our work on *Candida dubliniensis*, a very closely-related species of *C. albicans*, suggests that in spite of lack of homology in DNA sequence, the chromosomal locations of the centromeres are conserved in these two species. This raises a possibility that non-DNA sequence determinants are important for centromere recognition. We are currently trying to identify such genetic and epigenetic factors by genomic and proteomic approaches.

2. Architecture of *C. albicans* kinetochore

It is apparent that centromere sequences are more divergent than kinetochore proteins in different organisms. Identification of kinetochore proteins of budding yeasts and other eukaryotes suggests that while some of the proteins are species-specific, several proteins/protein complexes are conserved in organisms with regional centromeres. We have cloned, characterized and epitope-tagged three kinetochore proteins of *C. albicans* present at the inner (CaCse4p), central (CaMtw1p) and outer (CaDad2p) kinetochore. Using affinity chromatography and mass-spectrometric analysis, we are trying to identify interacting partners of these three proteins to understand the architecture and molecular mechanism of kinetochore function in *C. albicans*.

3. Does RNA interference exist in *Candida albicans*?

RNA interference (RNAi) has been shown to be important for transcriptional and post-transcriptional gene silencing. The centromeric heterochromatin formation by RNA interference in *S. pombe* has also been demonstrated. We have identified a homolog of argonaute (CaAgo1p) in *C. albicans* but other two important proteins of the RNAi machinery are apparently missing in *C. albicans* genome. Therefore, it will be interesting to find out the role of argonaute in regulation of gene expression in *C. albicans*.

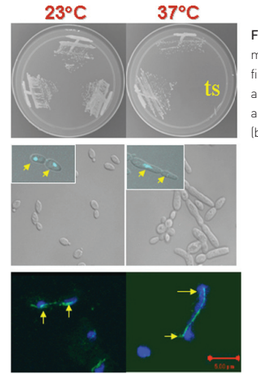


Figure 2: A *Candida albicans* kinetochore mutant (temperature-sensitive/ts) showing filamentous growth (middle panels), aberrant chromosome segregation (inset) and abnormally long spindle microtubules (bottom panels).

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*Plasmodiumfalciparum:*Functionalgenomics 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 Ph D in Biochemistry. 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.

Figure 1: Ribbon diagram of Pf FabI (the target of triclosan with NADH)

1. 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.

2. 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.

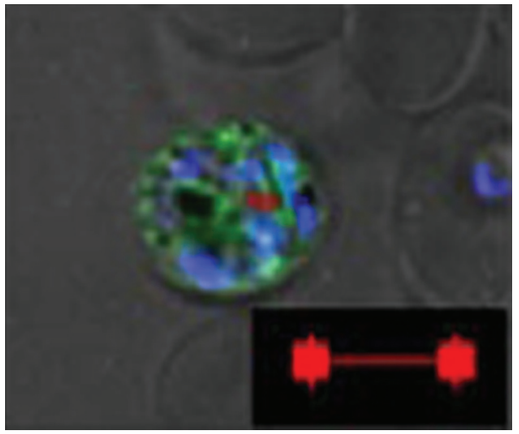

Figure 2: Targeting the trafficking of apicoplast proteins.

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Theoretical Sciences Unit

Chairman
Rahul Pandit

CSIR Bhatnagar Fellow
KB Sinha

Associate Professors
Shobhana Narasimhan
Swapan K Pati
Srikanth Sastry
Umesh V Waghmare

Faculty Fellows
NS Vidhyadhiraja
Subir Das
Kavita Jain (jointly with EOBU)

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, piezoelectricity, organic optoelectronics, generalized transport in organic devices and the external efficiency of organic photovoltaics.

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 various central computational facilities of JNCASR.

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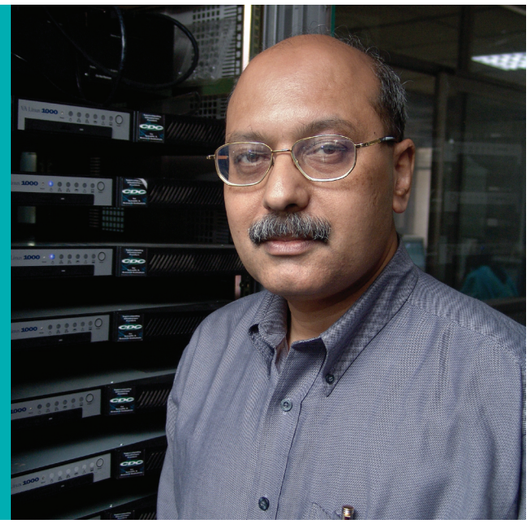

Equilibrium and Nonequilibrium Statistical Mechanics of Condensed-Matter Systems

I am interested in problems in condensed-matter theory, phase transitions, statistical mechanics, nonlinear dynamics, and turbulence. A list of my research interests is given below:

1. Spatiotemporal chaos in extended, deterministic dynamical systems such as the Kuramoto-Sivashinsky and Complex-Ginzburg-Landau equations, models for cardiac arrhythmias, and fluid, magnetohydrodynamic, and passive-scalar turbulence.
2. Complex Fluids: Microemulsion, micellar, lamellar, and sponge phases in oil-water-surfactant mixtures and bilayer systems, living polymers, and drag redcution by polymer additives in turbulent flows.
3. Non-equilibrium statistical steady states in driven, many-body systems.
4. The theory of interacting bosons in optical lattices and disordered environments.
5. The statistical mechanics of systems with surfaces, interfaces, and membranes.
6. Correlated electron systems such as the colossal magnetoresistance manganites.

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

1. The systematization of the multiscaling of time-dependent structure functions in fluid and passive-scalar turbulence.
2. 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.
3. 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.

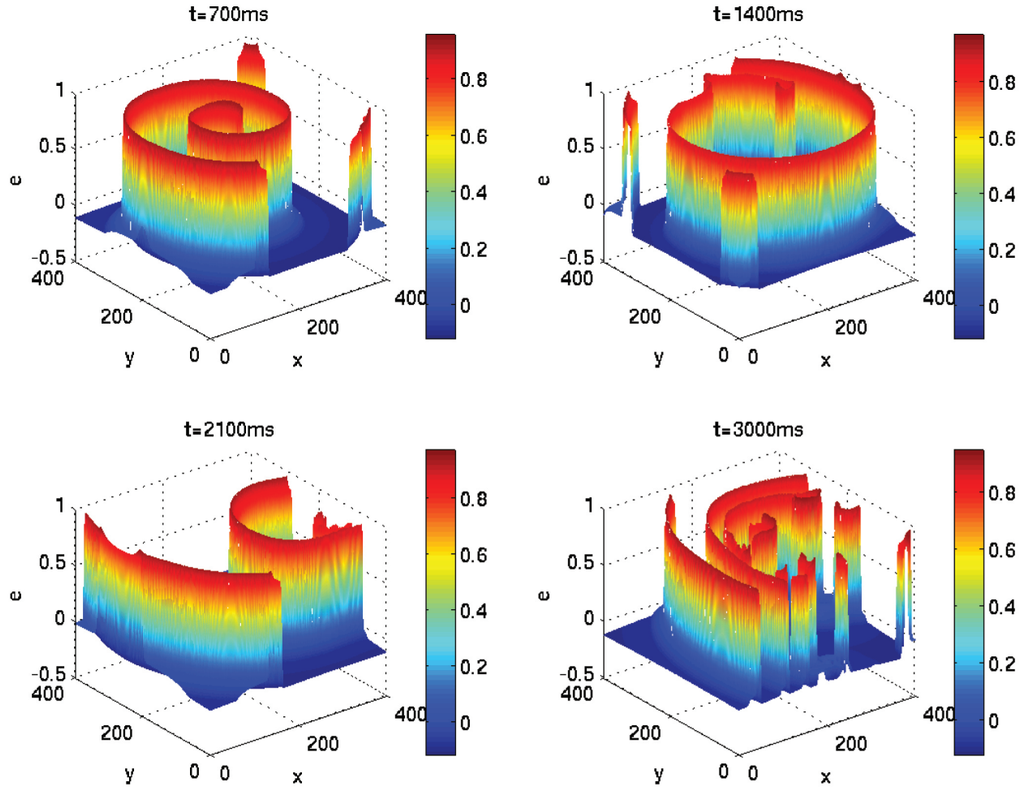

Figure 1: "Pseudocolour mesh plots for the voltage V as a function of the spatial coordinates x and y at different times $t=700$ ms, $t=1400$ ms, $t=2100$ ms, and $t=3000$ ms for $\epsilon_1=0.01$ illustrating formation and break up of spiral waves in the Panfilov model. A broken-wave initial condition is used at $t=0$. This leads to the creation of a spiral wave which breaks down as time increases leading to spiral turbulence with spatiotemporal chaos."

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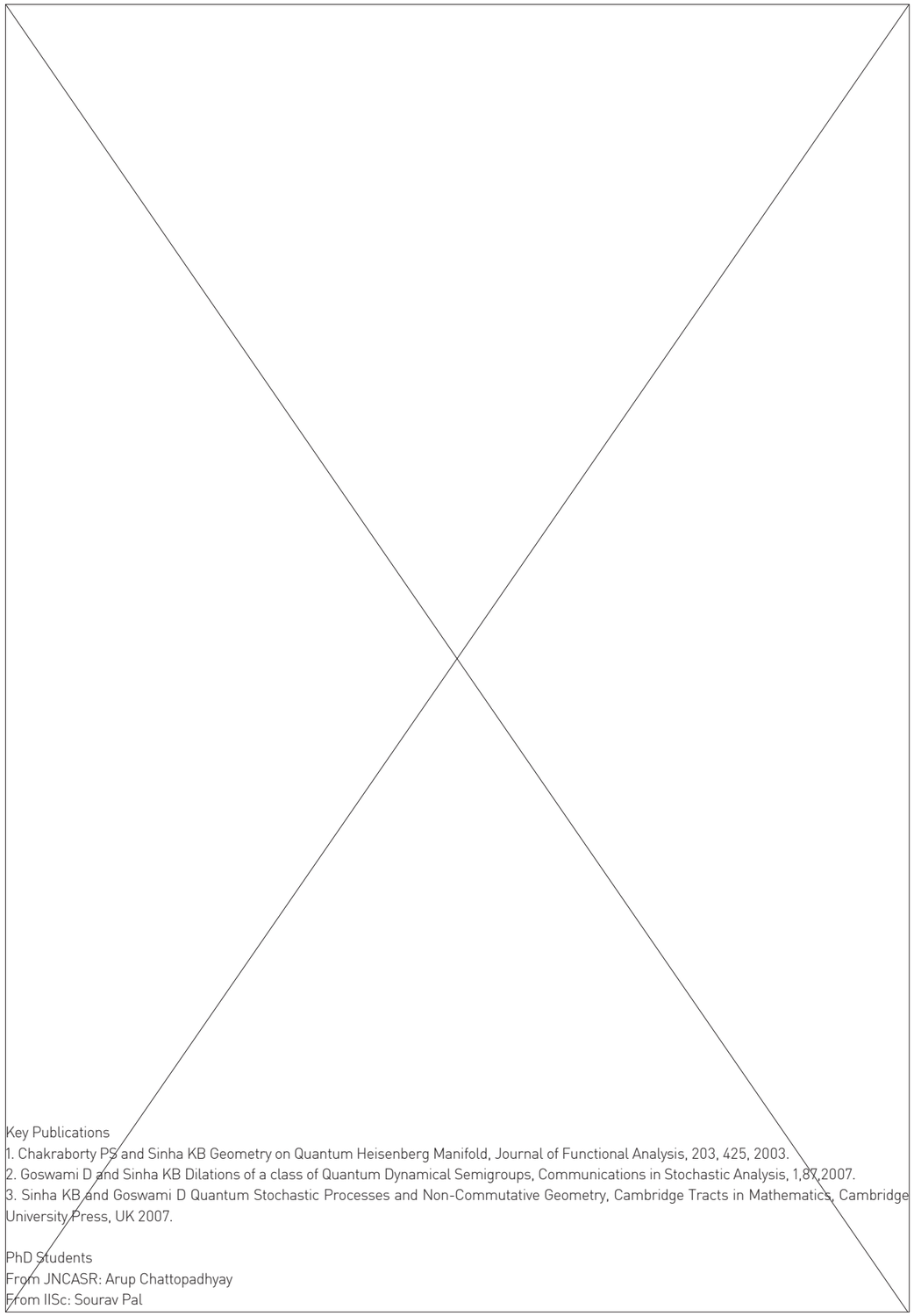
Non Commutative Probability and Geometry: Mathematics of Quantum Mechanics

The foundations of Quantum Mechanics brought up many new challenges to the community of Mathematicians – a whole new way of looking at spaces and functions on them as well as of assigning probabilities to hitherto non-compatible events (a truly non-Kolmogoroffian scenario).

One model of Non Commutative (or Quantum) Prabability theory was largely developed in the Delhi Centre of the Indian Statistical Institute during the last two and a half decades and aside from being a new non-classical theory of Probability and Stochastic Processes, it provides a possible non-Hamiltonian model of Quantum mechanical non-equilibrium systems. In this theory, the study of the structure of a semigroup of completely positive maps on the algebra of quantum observables and their stochastic dilations play a crucial role.

Taking the hints from the fact that many topological and geometric properties of a classical space can be encoded into specific properties of the Commutative algebra of (continuous or measurable) functions on the space, one studies just these properties on a more general class of abstract topological or von Neumann algebras. Here also intuition from Quantum Mechanics or Quantum Field Theory plays a crucial role.

Kalyan B Sinha has a PhD from the University of Rochester (USA), taught at the Universities of Geneva (Switzerland) and of Texas at Austin (USA) and was the Ulam Visiting Professor in the University of Boulder, Colarado. For nearly three decades, he was with the Indian Statistical Institute in which he was the Director till 2005. At present, he is at the JNCASR with the Bhatnagar Fellowship of CSIR.



Key Publications
1. Chakraborty PS and Sinha KB Geometry on Quantum Heisenberg Manifold, Journal of Functional Analysis, 203, 425, 2003.
2. Goswami D and Sinha KB Dilations of a class of Quantum Dynamical Semigroups, Communications in Stochastic Analysis, 1,87,2007.
3. Sinha KB and Goswami D Quantum Stochastic Processes and Non-Commutative Geometry, Cambridge Tracts in Mathematics, Cambridge University Press, UK 2007.

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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.

Size-dependent Properties of Nanosystems

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. We have also discovered some surprising scaling relations in the size- dependence of the mechanical properties of nanosystems.

Nanocatalysis

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. Most recently, we have studied the reduction of nitrogen monoxide on rhodium surfaces and clusters. Rhodium also possesses the interesting property that though it is not magnetic in its bulk form, it has a tendency to become magnetic when the coordination is reduced. Our studies show that small rhodium clusters may be good catalysts for this process; we have also observed an interesting interplay between magnetic effects and chemical bonding (see figure).

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. 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.

Coordination Number and Scaling Relations

We are interested in discovering and exploring scaling relations that describe how a variety of properties vary with coordination number. We have found some unexpected scaling laws relating bond lengths, bond stiffness and coordination number. Such work is of interest both because of its fundamental importance and because it can be used as a guide when developing interatomic potentials.

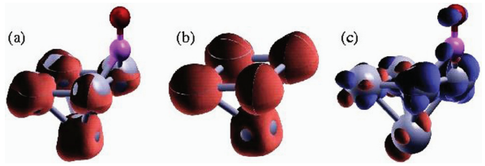

Figure 1: Spin polarized density for **(a)** NO adsorbed on a 5-atom Rh cluster and **(b)** the Rh cluster alone. The picture in **(c)** shows the difference between (a) and (b), i.e., it shows how the magnetization changes upon adsorbing NO. Red and blue regions indicate an increase/decrease in magnetization; these pictures show that the magnetization of the Rh atoms is quenched in the neighbourhood of NO. Magenta, red and grey spheres indicate N, O and Rh atoms respectively.

Novel Surface Alloys

It has been known from ancient times that alloying two metals can result in a new material that may possess, to an altered extent, the beneficial properties of its constituent elements. However, it has been realized only recently that some metals that are normally immiscible (i.e., they do not like to combine to make alloys) can form stable surface alloys. We are especially interested in studying the properties of magnetic surface alloys that are stabilized by strain due to the presence of a substrate; in particular, we want to see if alloying can enhance desirable magnetic properties such as magnetic moments and magnetic anisotropy, which would then make such materials ideal for magnetic memory storage. We are studying the stability and magnetic properties of such systems, and have shown that the trends we observe do not always follow earlier expectations. In this project, we are collaborating with experimentalists, who are being guided by our theoretical work in their search for new systems.

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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.

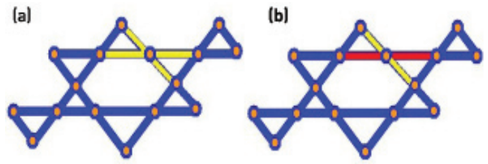

Figure 1: Spin-spin correlations of a kagome antiferromagnet with local lattice imperfections. (a) for spin-1/2 system (b) spin-1 system (Color Code represents correlation strength: Blue (regular), Red (strong) and yellow (weak)).

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.

Transport in Nanostructures and Bio-molecular systems

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 configuration interactions methods have been successfully applied through non-equilibrium Green function formalisms to understand various transport characteristics in a number of nanosystems.

We have also been actively involved in the field of bio inspired nanoelectronics. We have studied the effect on incorporating magnetic ions into the DNA helix for possible applications in spintronics. We find that the alignment of magnetic ions within the DNA helix creates a spin channel due to the efficient orbital interactions between the magnetic ions. This also gives rise to odd-even effects in the low frequency region of the optical spectra, which can be used as a signature to identify the spin-spin interactions.

We have also modeled molecular switches based on the reversible protonation and de-protonation profiles of the DNA basepairs under varying pH conditions. We find that the A:T basepair shows excellent rectification behavior which is absent for the G:C basepair. We also find that non-canonical A:A basepairs can be used as efficient pH dependent molecular switches. These pH dependent electronic properties of the DNA basepairs have been explained by chemical potential models, which are also complemented by the orbital interaction analysis.

Initial studies for understanding the mechanisms of light absorption and electron transport in photosynthetic centers is currently underway. The primary interest of the project is to understand the correlation between the active Magnesium-chlorin centers and various side chain functionalities of LHCs (Light harvesting complexes) present in photosynthetic centers.

Hydrogen Storage in organic molecular solids

The storage of molecular hydrogen in a safe and affordable manner is one of the most challenging problems of the current decade. The ever-increasing demand on energy, limited resources and polluting nature of fossil fuels has led to an interest in materials that are capable of storing molecular hydrogen. Our major goal has been to design the molecular solids of high hydrogen adsorption efficiency computationally. For this purpose we look into various organic systems with different structures like Sulflower, Sumanene crystals and new extended carbon systems like Nanotubes and Graphene layers. Whether such systems also could be used for effective field effect transistor actions is also being actively pursued.

Figure 2: Hydrogen adsorption in Sumanene.

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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 Ph D (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.

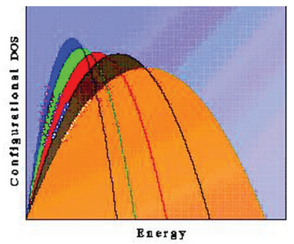

Figure 1: The distribution of local energy minima vs. their energy for a glass forming liquid, for different densities. The shape of the distribution is related to the fragility of the glass.

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.

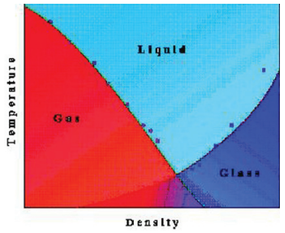

Figure 2: Schematic is the liquid-gas mechanical stability limit (spinodal) and the glass transition line, which intersect at a finite temperature.

Ongoing work also addresses the nature of the glass transition, the role of structure and configuration space geometry in determining glassy dynamics, and glass forming ability, and involves the development of new computational methods to analyse energy landscapes and structure, and improved simulation techniques. Ideas developed concerning good glass formers have recently been successfully applied in the experimental synthesis of a monoatomic metallic glass.

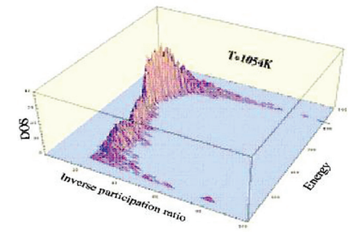

Figure 3: The electronic density of states of liquid silicon in the low temperature phase displaying localization of states near the Fermi energy.

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.

Nucleation

The kinetics of phase transformations, in particular the formation of crystals in supercooled liquids is of wide interest in materials science. Aspects of the kinetics of crystallization, including the role of surfaces in supercooled droplets, presence of metastable critical points, and the relation to good glass forming ability, are presently being studied.

Biomolecular systems

The ideas and methods developed in the above studies are also being applied recently to the study of biomolecular systems, with more complex molecular detail. Work along these lines includes the geometric analysis of protein structure and the application of statistical mechanical methods to understanding protein aggregation.

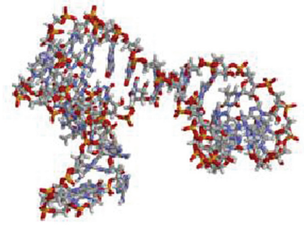

Figure 4: Three dimensional structure of an RNA molecule.

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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.

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.

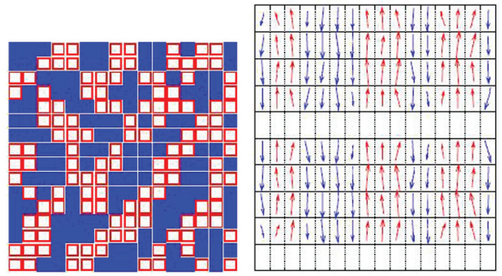

Figure 1: Formation of domains in a 2 nm thick film of $BaTiO_3$ sandwiched between electrodes with a long screening length.

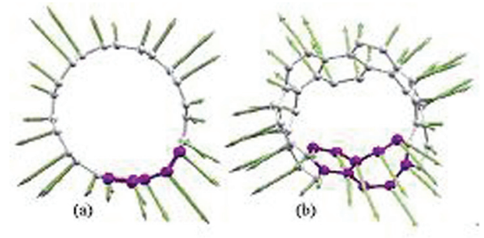

Figure 2: Radial breathing modes of a carbon nanotube with a line defect.

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.

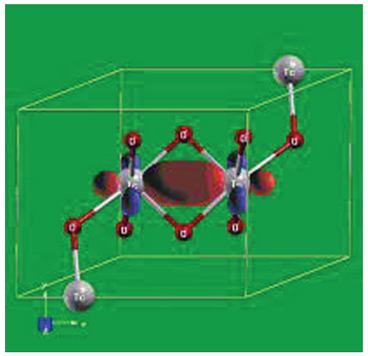

Figure 3: A Wannier function representing a Tc-Tc bond in TcO_2.

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.

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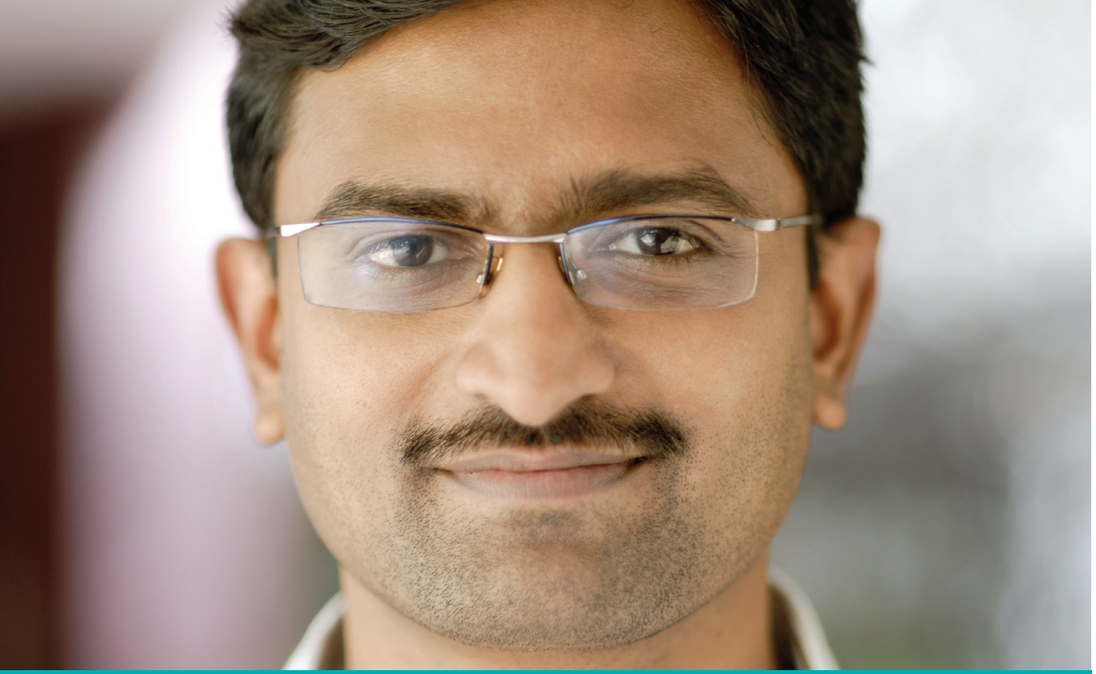

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Strongly correlated electron systems

The main focus of my work is the class of materials known as strongly correlated electron systems (SCES). This class comprises materials wherein inter-electron interactions play the dominant role in determining physical properties such as specific heat, susceptibility and resistivity. Compounds that exemplify SCES include transition metal oxides such as V_2O_3 and $YBa_2Cu_3O_{7-\delta}$, rare earth lanthanides and actinides such as $CeAl_3$, SmB_6 and $YbRh_2Si_2$, manganites such as $La_{1-x}Sr_xMnO_3$. These materials exhibit exotic phenomena, the most well-known of which are high temperature superconductivity in cuprates, heavy fermions in lanthanides and actinides and colossal magnetoresistance in manganites.Despite the decades of research in this area, huge challenges remain for theoreticians and experimentalists. Even the simplest theoretical models for SCES such as the Hubbard model have defied general solutions to this date. Our group employs the techniques of quantum many body theory to develop perturbative and non-perturbative approximations for these models; the aim being to address issues relating to transport and thermodynamics of heavy fermion systems and transition metal oxides.

Apart from SCES, I have been actively working on modeling organic optoelectronic and photovoltaic devices. In collaboration with the molecular electronics lab in JNCASR headed by Prof. KS Narayan, we have developed a circuit level description for organic Schottky junction based devices. The long term goal in this area is to develop a multiscale model that encompasses the multiple length scales such as the crystalline domain sizes and charge carrier diffusion lengths, that exist in organic devices.

NS Vidhyadhiraja has a PhD (2001) in Physics from the Indian Institute of Science. He was a post-doctoral fellow at the Physical and Theoretical Chemistry Laboratory, Oxford University, UK before joining JNCASR in 2005. He has held visiting professor positions at Motorola India Research Labs and the University of Cincinnati, USA.

Heavy fermions

The field of heavy fermion systems was born in 1975 with the discovery of a huge electronic contribution to specific heat at low temperatures ($\gamma \sim 10^3 mJK^{-1}mol^{-1}$) and a large coefficient of the T^2 term in resistivity of $CeAl_3$. Since then, a large number of intermetallic compounds, showing not only heavy fermion behaviour but also exotic magnetic ordering, superconductivity and small-gap insulating behaviour have been discovered. This class of materials comprises rare earth lanthanides and actinides such as $CeAl_3$, $CeCu_6$, $CeCu_2Si_2$, $YbRh_2Si_2$, SmB_6 and UPt_3. In the last decade, interest in heavy fermions has been renewed because of the finding that some of these systems can be tuned with external parameters like pressure, doping or magnetic field through a quantum phase transition. The open issues in this field include the origin of heavy fermion behaviour, the competition between the Kondo screening of local moments and the tendency of local moments to order magnetically (RKKY interaction) and the origin of superconductivity in heavy fermions.

The periodic Anderson model forms the general paradigm for the theoretical investigation of heavy fermion systems. We have developed a non-perturbative quantum many body approximation, namely the local moment approach (LMA) within the dynamical mean field theory (DMFT) to solve the model and understand transport and thermodynamics of heavy fermions within this framework. This technique is based on diagrammatic perturbation theory and builds up transverse spin fluctuations over the unrestricted Hartree-Fock approximation. We have found that the single particle dynamics and transport quantities exhibit universality in the strong coupling regime. Further, a direct quantitative comparison of theory to experiment for a variety of compounds, utilizing universality in strong coupling, yielded excellent agreement with minimal free parameters. Some of the projects that we are presently involved in are (i)understanding the effects of magnetic field, (ii) computing thermodynamic quantities, (iii) extending LMA beyond DMFT, (iv)including the effects of crystal field splitting , (v) integrating first-principles band-structure calculations with quantum many body techniques.

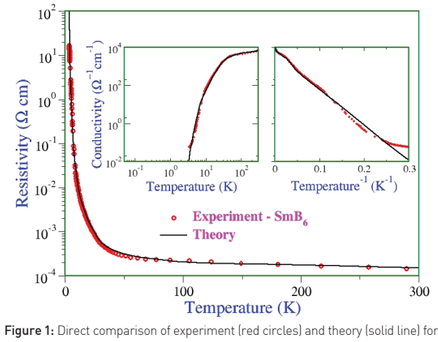

Figure 1: Direct comparison of experiment (red circles) and theory (solid line) for dc transport in the classic Kondo insulator SmB_6. The agreement is excellent over five orders of magnitude.

Mott metal-insulator transition

In the early seventies, McWhan et al, found that the transition metal oxide, V_2O_3 undergoes large jumps in resistivity as a function of temperature upon doping with Ti and Cr. This strong correlation induced Mott metal-insulator transition in V_2O_3 has since then been investigated extensively with a wide variety of experimental and theoretical probes. Important theoretical progress was made in the nineties with the advent of DMFT. It has now been established that the finite temperature transition belongs to the universality class of the liquid-gas transition. The Mott transition has been found to occur in a number of other transition metal oxides as well. The generic theoretical paradigm for investigating transition metal oxides has been the Hubbard model. We have been intensively working towards understanding transport and thermodynamics across the Mott transition using a diagrammatic perturbation theory based approximation known as iterated perturbation theory. We find that our results are in close agreement with experimental results such as the thermal hysteresis in resistivity, the critical exponents found in transport measurements on Cr-doped V_2O_3, etc.

Organic optoelectronics

Organic conductors/semiconductors have been projected as the most serious candidates for replacing silicon as the base component in the microelectronics industry.

However, theoretical investigations of devices based on organic polymers such as poly-(3-hexylthiophene) (P3HT) or poly-(2-methoxy, 5-(2-ethylhexoxy)-1,4-phenylene vinylene) (MEHPPV) have been hampered due to the highly disordered nature of these polymers, complex charge transport processes, trap states and many such details that have little or no correspondence in their inorganic-silicon based counterparts. We have developed a model in collaboration with Prof. K.S.Narayan and his group in the Chemistry and Physics of Materials Unit, JNCASR for studying the lateral photovoltaic effect in organic position-sensing devices based on Schottky junctions between organic semiconductors and metals. Our approach is based on a discrete circuit model interconnected through a spreading impedance network. We have obtained excellent agreement between our model calculations and measurements made on devices fabricated in Prof.Narayan's laboratory. We are generalizing the model further to include finite bias effects, transient processes and complex geometries. Attempts to relate the macroscopic features of the model to the microscopic charge transport processes are also underway.

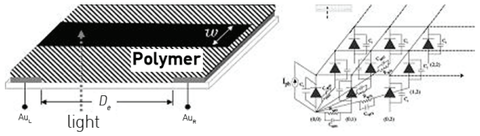

Figure 2: A typical organic position sensing device fabricated in the molecular optoelectronics laboratory in JNCASR. The right figure shows the discrete circuit network model incorporating a spreading impedance approach.

Selected Publications

1. *Charge carrier dynamics in organic semiconductors by position dependent optical probing.* Authors: D Kabra, S Shriram, NS Vidhyadhiraja and KS Narayan. Journal of Applied Physics 101 (2007), 064510.
2. *On the specific heat of heavy fermion systems using the periodic Anderson model.* Author: NS Vidhyadhiraja Europhysics Letters 77 (2007), 36001.
3. *Optical and transport properties of heavy fermions: theory compared to experiment.* Authors: NS Vidhyadhiraja and David E Logan Journal of Physics: Condensed Matter 17 (2005), 2959.
4. *Dynamics and transport properties of Kondo insulators.* Authors: NS Vidhyadhiraja, Victoria E Smith, David E Logan and HR Krishnamurthy Journal of Physics: Condensed Matter 15 (2003), 4045-3087.

PhD Students

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Statistical Physics of Equilibrium and Nonequilibrium Condensed-Matter Systems

My primary research involvement has been in the statistical mechanics of phase transitions and areas related to that. I am interested in investigation of condensed-matter systems both at and away from equilibrium, for which I use Monte Carlo, Molecular Dynamics and Field Theoretic Continuum Dynamical Models.

In this broad field, following topics have been my focus in recent years:
a) Static and Dynamic Critical Phenomena.
b) Kinetics of Phase Separation in Multicomponent Mixtures.
c) Structure and Dynamics in Confined Systems.
d) Structure and Dynamics in Supercooled Liquids.
e) Pattern Formation in Granular, Chemical, and Biological Systems.

Subir K. Das obtained his Ph.D. From Jawaharlal Nehru University in 2002 which was followed by postdoctoral positions in Johannes-Gutenberg Universitaet Mainz and University of Maryland (College Park). He joined JNCASR in 2007.

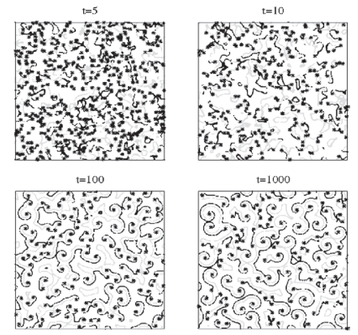

Figure 1: Pattern formation during the nonequilibrium evolution of the complex Ginzburg-Landau equation in two dimensions. The lines (black and grey) represent constant phases of the 2-component order parameter and the asterisks mark the locations of the cores of the spiral defects.

Recently, there has been revival of interest in the area of critical phenomena that occurs in the vicinity of continuous or second order phase transition (e.g., paramagnetic to ferromagnetic transition at the Curie point), particularly, after the recent development of finite-size scaling techniques and increasing computer power. While there has been substantial understanding of the behavior of various thermodynamic properties in the vicinity of the critical point, transport properties received much less attention both theoretically and computationally, because of some obvious difficulties. Even though there are mode-coupling and dynamic renormalization-group theoretical calculations for a class of systems, simulation in this area is extremely demanding due to the critical slowing down and strong finite-size effect near T_c. Nevertheless, in one of our recent works, it has been successfully demonstrated that molecular dynamics (MD) simulations have advanced enough to look at the dynamic properties at criticality, if finite-size effects are appropriately accounted for.

While studying various systems at criticality, it is of obvious interest to quench the system below the critical point. Once these systems are suddenly quenched below the critical point from a high temperature random phase, they become thermodynamically unstable and starts phase-separating. This phase-separation or phase-ordering is a highly nonlinear process where the domains of different components (e.g., domains of up and down spins for a para to ferromagnetic transition, low density and high density regions for a gas-liquid transition) grow with time obeying certain power laws. In the case of simple two-component systems, there have been lot of approximate analytical, numerical and experimental works, when the growth is purely diffusion driven. However, current interest of my group is to study the fluid systems where hydrodynamics play very important role, thus posing more challenge both theoretically and numerically.

Both in the critical dynamics and phase ordering dynamics, it is also very interesting to look at the effects of confinement (e.g. thin film) since these systems are very important in nano-science and technology. It's a problem of substantial theoretical challenge when there is interplay between surface effects and finite-size effects (in the direction normal to the surface) with the bulk behavior of these systems that leads to complex phenomena such as wetting, prewetting, layering transition, etc.

We have been looking at these problems in detail via appropriate analytical modeling and devising efficient simulation techniques. One major draw back of MD simulation is that because of the lack of computer power, one cannot consider very large systems -- thus finite-size effects become very important and so getting the asymptotic behavior becomes very difficult. To avoid this problem, we want to combine the microscopic MD simulations with coarse-grained models through appropriate bridging (Multiscale Modeling).

Another area of interest to me is the study of pattern formation in nonequilibrium systems (phase ordering dynamics is already an example of it). Pattern formation is a ubiquitous phenomena in nature and occurs when certain system becomes unstable to fluctuations in certain region of parameter space (e.g., temperature and density). Starting from astrophysical dimension to microscopic objects, beautiful patterns are observed almost everywhere in nature. Currently I am interested in understanding pattern formation in granular matter and biological systems

Selected Publications

1. Subir K Das, Sanjay Puri, and Michael C Cross, Nonequilibrium Dynamics in the Complex Ginzburg-Landau Equation: Analytical Results, Physical Review E 64, 046206 (2001).
2. Subir K Das and Sanjay Puri, Pattern Formation in the Inhomogeneous Cooling State of Granular Fluids, Europhysics Letters 61, 749 (2003).
3. Subir K Das, Juergen Horbach, MM Koza, Suresh M Chatoth, and Andreas Meyer, Influence of Chemical Short--Range Order on Atomic Diffusion in Al--Ni Melts, Applied Physics Letters 86, 011918 (2005).
4. Subir K Das, Sanjay Puri, Juergen Horbach, and Kurt Binder, Molecular Dynamics Study of Phase Separation Kinetics in Thin Films, Physical Review Letters 96, 016107 (2006).
5. Subir K Das, Michael E Fisher, Jan V Sengers, Juergen Horbach, and Kurt Binder, Critical Dynamics in a Binary Fluid: Simulations and Finite-size Scaling, Physical Review Letters 97, 025702 (2006).
6. Subir K Das, Juergen Horbach, Kurt Binder, Michael E Fisher, and Jan V Sengers, Static and Dynamic Critical Behavior of a Symmetrical Binary Fluid: A Computer Simulation, Journal of Chemical Physics 125, 024506 (2006).
7. Subir K Das, Jan V Sengers, and Michael E Fisher, Simulating critical dynamics in a liquid mixture: short-range and long-range contributions, Journal of Chemical Physics, 127, 144506 (2007).
8. Juergen Horbach, Subir K Das, Axel Griesche, MP Macht, G Frohberg, and Andres Meyer, Selfdiffusion and Interdiffusion in Al80--Ni20 Melts: Simulation and Experiment, Physical Review B, 75, 174304 (2007).

PhD Student

Suman Majumder

Collaborations

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Nonequilibrium Statistical Mechanics

I work in the broad area of nonequilibrium statistical mechanics. In recent years, I have applied statistical mechanics methods to problems in biology (see I below). Besides I retain an active interest in traditional problems in statistical physics concerning phase transitions and their universality classes (see II below).

I. Biological Physics: In this field, my main interest lies in the evolutionary dynamics of simple biological organisms. The basic question regards how the genetic composition of a population changes in time under the influence of various evolutionary forces such as selection, mutation and genetic drift. Using numerical simulations and statistical mechanics ideas (scaling theory, extreme value statistics), we study deterministic [1,2] and stochastic [3] models of biological evolution.

II. Statistical Physics: While the systems with equilibrium steady states are well studied, much less is known about nonequilibrium systems which are characterised by a nonzero current. I am interested in systems driven far-from-equilibrium due to some external current and out-of-equilibrium systems relaxing towards a steady state. We study models that are paradigms of phase transitions and phenomena which do not have equilibrium analogue. Examples include condensation transitions [4], absorbing-state transitions [5] and pumping in classical systems [6].

Kavita Jain has a PhD [2003] in Physics from TIFR, Mumbai. She was a postdoctoral fellow at Cologne University, Germany and Weizmann Institute, Israel before joining JNCASR in 2007.

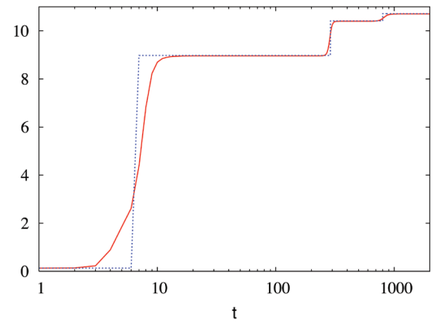


Figure 1: Punctuated change in the population fitness (solid line) and the fitness of the most populated genotype (dotted line) in a single realization of a maximally rugged fitness landscape.

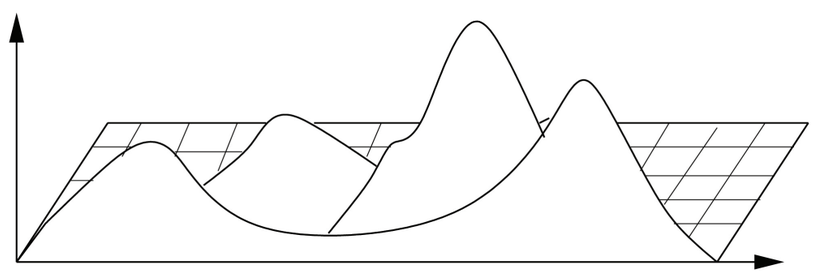


Figure 2: Schematic representation of a rugged fitness landscape defined over a two dimensional genotype space.

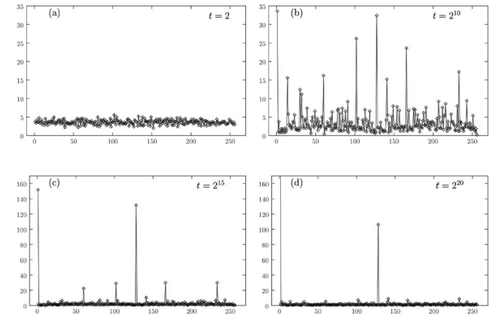


Figure 3: Density profile in the condensate phase of disordered zero range process at (a) t=2 (b) t=2^10 (c) t=2^15 (d) t=2^20. The site with the lowest hopping rate is located at k=1 and the second lowest at k=128.

MS Student
Gayatri Das.

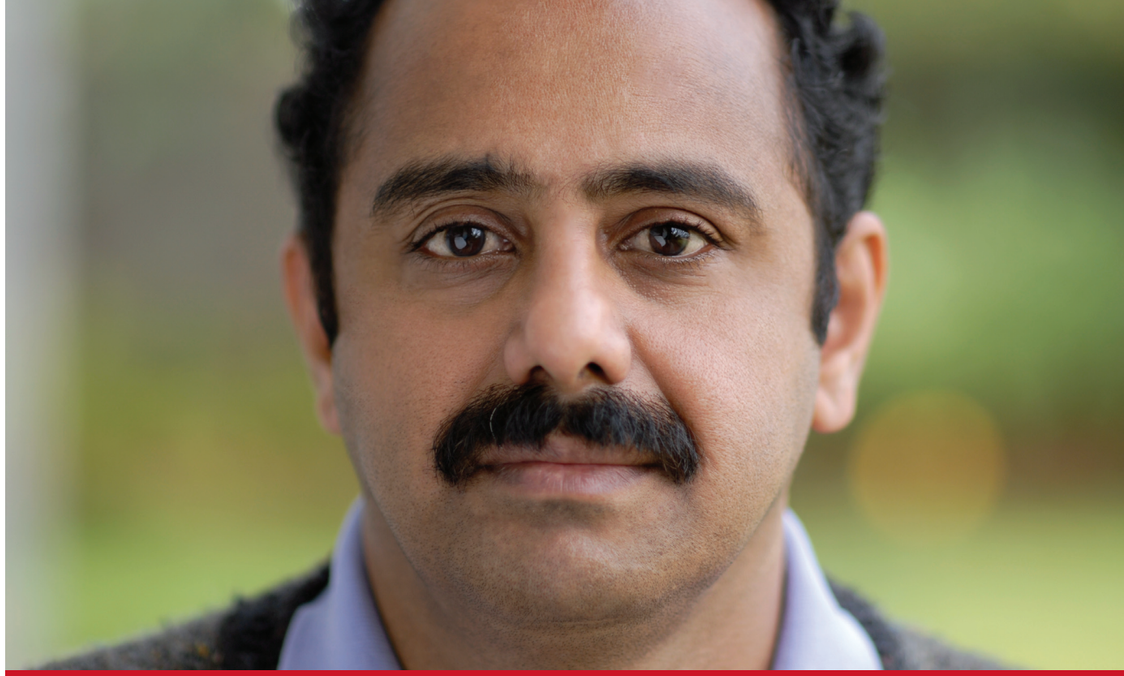
Selected Publications

1. Evolutionary trajectories in rugged fitness landscapes. K Jain and J Krug, J. Stat. Mech. P04008 (2005)
2. Evolutionary dynamics of the most populated genotype on rugged fitness landscapes. K Jain, Phys. Rev. E 76, 031922 (2007)
3. Deterministic and stochastic regimes of asexual evolution on rugged fitness landscapes. K Jain and J Krug, Genetics 175, 1275 (2007)
4. Dynamics of a disordered, driven zero range process in one dimension. K Jain and M Barma, Phys. Rev. Lett. 91, 135701 (2003)
5. Nonuniversal exponents in sandpiles with stochastic particle number transfer. K Jain, Europhys. Lett. 71, 8 (2005)
6. Driving particle current through narrow channels using a classical pump. K Jain, R Marathe, A Chaudhuri and A Dhar, Phys. Rev. Lett. 99, 190601 (2007)

CSIR Centre of Excellence in Chemistry

Head
CNR Rao

Honorary Faculty Fellow
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.

1. 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.
2. 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.
3. Synthesis, characterization and properties of nanotubes and nanowires of various inorganic materials including elements, metal oxides, nitrides, carbides and chalcogenides using new synthetic strategies.
4. Synthesis of composites of nanotubes and nanowires with various polymers to enhance their properties for potential applications in mechanical, electronic, sensor and other devices.
5. The study mainly in phenomena and properties exhibited by transition metal oxide systems, including high temperature superconductivity, colossal magnetoresistance, metal-insulation transition and multifunctionality.
6. 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.

A Govindaraj has a PhD (1996) in Chemistry from University of Mysore. He was a visiting scientist of Tokyo University, Tokyo Metropolitan University (Tokyo), University of Witwatersrand (South Africa) and University of Paul Sabatier (France).

Chemical Biology Unit

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Uday Maitra

Honorary Faculty
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Santanu Bhattacharya
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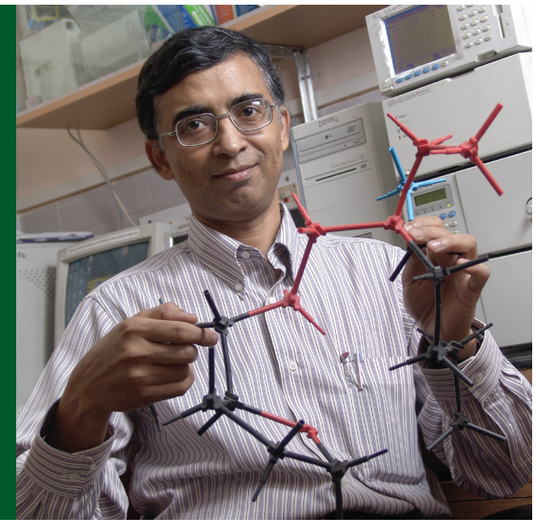

The Chemical Biology Unit is located on the campus of the Indian Institute of Science. The work carried out in this unit by the Honorary Faculty Members of JNCASR covers many of the emerging areas of chemical biology.

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 has 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 has 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 chemistry

The study of novel analogs of bile acids has 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. A bile acid derived polymer bound K^+ sensitive fluorescent sensor has been designed.

Condensed Matter Theory Unit

Chairman
HR Krishnamurthy

Faculty
G Ananthakrishna
B Bagchi
BJ Cherayil
C Dasgupta
S Jain
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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.

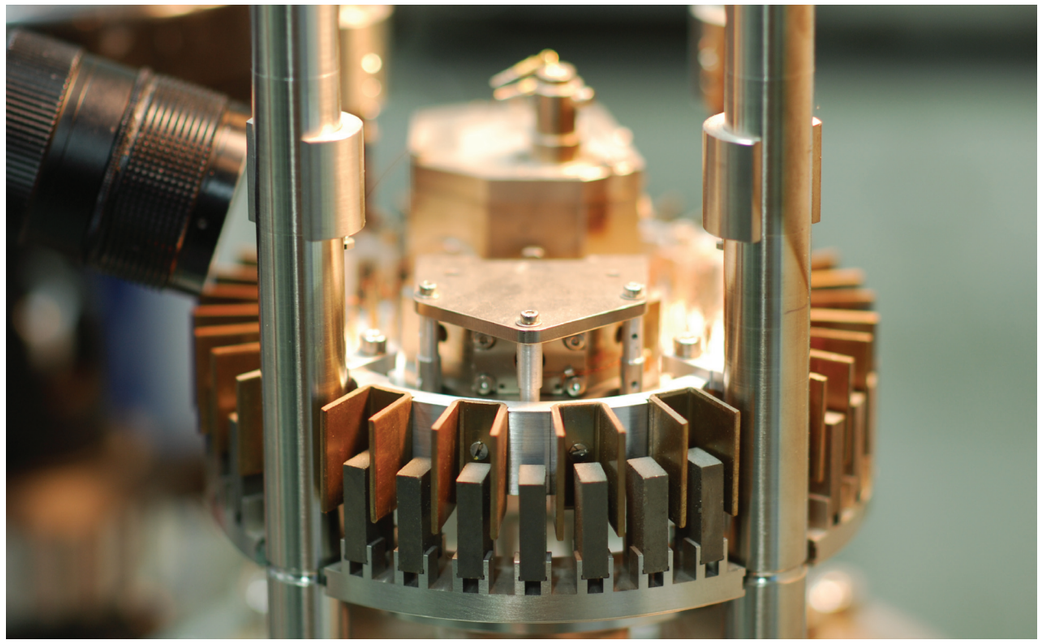
Research Facilities

Network of workstations, personal computers and peripherals.

Members
CNR Rao
GU Kulkarni
SK Pati
KS Narayan
A Sundaresan
A Govindaraj
M Eswaramoorthy
KS Kini

Technical Assistance
NR Selvi (FESEM)

DST Unit on Nanoscience



The Nanoscience Initiative in India from the Department of Science and Technology (DST) has established Research Units at various places including JNCASR, since April 2005. Besides creating new laboratory site, the Unit hosts a number of research facilities for Nanoscience research. Nanoscience being an interdisciplinary topic, calls for a multi-faceted approach. The members of the Unit with varied expertise have formed a group to pursue research activities on different aspects of Nanoscience. In order to boost research interest in nanoscience, many academic activities such as courses in nanoscience, discussion meetings and symposia are being conducted.

Main activities are stated below:

- Developing new strategies for the synthesis and purification of nanowires and nanotubes; multiwalled and single walled carbon nanotubes, junction nanotubes, nanowires and nanotubes of transition metal oxides, nitrides, carbides and chalcogenides, new precursor routes to metal and semiconductor elemental nanowires, aligned nanotubes
- Synthesis of metal and semiconductor nanocrystals in colloidal sols as well as at liquid-liquid interfaces, ligand shell modification, core-shell nanocrystals, magic nuclearity nanocrystals, mesoscalar assemblies
- Patterned nanomaterials, Electron beam and AFM based high resolution nanolithography
- Thin films of novel functional oxides, transition metal oxides of interest in high T_c superconductivity, synthesis using RF magnetron sputtering, characterization and processing.
- Characterization of nanoobjects using electron and scanning probe microscopy techniques, UV-Vis spectroscopy, X-ray photoelectron spectroscopy
- Characterization of nanomaterials using high-resolution powder X-ray diffraction, RDF from Rietveld analysis, Reflectivity studies on films
- Electrical and magnetic properties of the oxide films as well as on nanocrystalline metal and semiconductor films
- Direct measurement of electrical properties of nanowires and nanotubes coupled to nanoelectrodes drawn using e-beam lithography, Nanocrystals anchored to conducting organic molecules
- Theoretical calculations of conductance, capacitance and current as a function of the external bias, temperature and magnetic field, Effect of the dimensionality and the geometry of the contacts, modeling advanced materials showing rectification and those of interest in spintronics.

Centre for Computational Materials Science

www.jncasr.ac.in/ccms

The Centre for Computational Materials Science (CCMS) was established in 2006 and is supported through a grant provided by the Nanoscience and Technology Initiative of the Department of Science and Technology, Government of India. The Coordinator of CCMS is Balasubramanian Sundaram, and the other faculty members associated with this Centre are Shobhana Narasimhan, Swapan K Pati, Srikanth Sastry and Umesh V Waghmare. The Centre also has Associate Members drawn from institutions across India.

Members of CCMS carry out research in the broad area of computational materials science, using a variety of analytical and computational tools. The list of topics studied in recent years is rich and diverse, including: the electronic structure of nanomaterials, charge transport and catalysis in nanosystems, novel magnetic materials and their properties, non-linear optical materials, disordered systems, biomimetic systems and biomaterials. The techniques employed include ab initio calculations, molecular dynamics simulations and many body theory. Research is also carried out on developing various techniques, such as free energy methods to study phase transitions, novel ways of using geometric phases to get information about material properties, and new formulations of configuration interaction methods.

The Centre has recently acquired a High Performance Computing Facility, which was inaugurated in February 2007 by Profs. Mike Klein and Michele Parrinello. This facility is a HP XC Cluster, comprised of 128 nodes of dual core, dual CPU Xeon Woodcrest CPUs over a low latency network. The theoretical peak performance of this configuration is estimated at 6 TFLOPS, which makes it one of the most powerful academic computing resources in the country.

Along with supporting the research programmes of its members, CCMS carries out a number of outreach activities: in addition to an active Visitors' programme, several schools and conferences are conducted every year. The schools consist of theoretical and practical sessions. An Instructional Computing Laboratory, containing 30 computers enables the students attending workshops to acquire hands-on experience in writing and running sophisticated codes. Topics that have been covered in these schools include electronic structure methods, molecular simulations, numerical many-body methods in physics and chemistry, and biomolecular simulations. The first of these schools was marked by a unique feature: all the lecturers and students worked together on a research problem, which has resulted in a paper with 64 authors!

Academic Activities

Academic Programmes

Graduate Student Programmes

JNCASR has a bright and diverse student body. At present, there are 138 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 (Engg.) 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 2007, 650 students applied, 400 were called for interviews, and finally 50 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 California, Canada, Dhaka, England, France, Germany, Greece, Ireland, Japan, Malaysia, Poland, Singapore and USA.

We generally expect students to take less than five years to complete a regular 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 three 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 communication. 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, 89 degrees have been awarded; these include 58 PhD's, 17 MS degrees, 13 MS (Engg.) and 1 MSc (by research) (Biological Sciences). Students who are alumni of the Centre have gone on to enjoy successful academic and R&D careers in leading international laboratories, 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.* 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. There is also provision for outstanding students who have not cleared any of these exams to face the interview committee of the Centre.

Integrated PhD Programme in Materials Science

The Chemistry and Physics of Materials Unit has initiated an Integrated PhD Programme in Materials Science starting from August 2007. Ten students who have majored either in Chemistry or Physics in their undergraduation (BSc) have joined this programme. They were selected out of about 250 candidates who appeared for a national level entrance examination and a subsequent interview.

The programme consists of three parts:
(i) course work spanning little more than three semesters,
(ii) research over another three semesters culminating in a thesis towards a MS degree in Materials Science, and
(iii) doctoral research leading towards a PhD degree to be pursued in the succeeding two to four years.

The programme draws support from the faculty members of the Theoretical Sciences Unit and Engineering Mechanics Unit, especially in the conduct of the courses.

Scholarships/Fellowships/Assistantships

All Integrated PhD students receive a stipend of Rs.8,000 in their first two years; this is raised to Rs.12,000–14,000 in subsequent years. All PhD and MS/MS (Engg.) students receive scholarships of Rs.12,000–14,000. [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:
1. The Babu Matru Prasad Scholarship is available for an Integrated PhD student.
2. The Smt & Sri Bapu Narayanaswamy Prize is given to the best MS thesis of an Integrated PhD student.
3. The Prof CNR Rao Medal is 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 202	3:0	Experimental Techniques for Materials
JC 205	3:0	Seminar Course
JC 206	3:0	Physical Chemistry
JC 208	0:4	Organic and Inorganic Chemistry Lab.
JC 209	3:0	Basics in Nanoscience
JC 210	3:0	Group Theory & Molecular Spectroscopy
JC 213	3:0	Inorganic Chemistry
JC 214	0:3	Laboratory – I
JC 215	3:0	Electromagnetism
JC 217	3:0	Organic Chemistry
JC 304	3:0	Chemistry of Materials
JE 201	3:0	Population and Quantitative Genetics
JE 202	3:0	Basic Chronobiology
JE 203	3:0	Introduction to Population Dynamics
JE 204	3:0	Basic Quantitative Tools in Biology
JE 301	3:0	Evolutionary Genetics of Fitness
JE 302	3:0	Chronobiology: Advanced Aspects
JF 201	3:0	Applied Mathematics
JF 202	3:0	Nonlinear Dynamics: Applications to Fluid Dynamics
JF 203	3:0	Introductory Fluid Dynamics

JF 301	3:0	Advanced Topics in Fluid Dynamics
JF 302	3:0	Multiphase Flow
JF 303	3:0	Microhydrodynamics- With applications to multi-phase flow
JM 201	3:0	Human Molecular Genetics
JM 202	3:0	Basic Biological Chemistry
JM 203	3:0	Advanced Molecular Biology & Genetics
JM 204	3:0	Basics in Immunology
JM 205	3:0	Cell and Molecular Biology
JM 206	3:0	Gene Expression and Development
JM 207	3:0	Advanced Course in Regulation of Gene Expression
JM 208	3:0	Signal Transduction in Biological Systems
JN 202	1:0	Scientific Communication-I
JT 201	3:0	Solid State Physics
JT 202	3:0	A first course in Computational Methods
JT 205	3:0	Quantum Mechanics I
JT 301	3:0	Computational Methods for Electronic Structure
JT 302	3:0	Topics in Condensed Matter Theory
JT 303	3:0	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, 89 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.

We list all the students who have been awarded degrees during 1997 to 2007.

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)
• T Bhuvana, An Investigation of the Nanogranular Au films Electrolessly deposited on Sit Surfaces (Advisor: GU Kulkarni)
• Kumar Ramanatha Datta K, Synthesis and Characterization of nano-particles Stabilized in aminoclay, agarose and plant virus matrices (Advisor: Dr M Eswaramoorthy)

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)
• Manikandan MS, Effects of Ambient Viscosity on the Entrainment and Dynamics of a Buoyant Jet (Advisor: KR Sreenivas)
• Shreyas JV, Experiments and Numerical Simulations of Flapping-wing Flight (Advisor: KR Sreenivas)
• Gomati A, Urea Root to the Synthesis of Metal Nitrides and to Coat One-dimensional Nanostructures by Boron Nitride (Advisor: CNR Rao)
• Punit Tiwari, Laboratory Simulation of Lifted Temperature Minimum (Advisor: Prof KR Sreenivas)
• Tiju Thomas, Polytypes and Stacking Faults in C, Si, Ge and SiC (Advisor: Prof Umesh V Waghmare)
• Rajaram Lakkaraju, Studies on Buoyancy-Induced Open Flows: Plane Thermal Plume (Advisor: Dr Meheboob Alam)
• Kaushik Srinivasan, Direct numerical simulation of transition in unstably stratified Poiseuille flow (Advisor: Prof Rama Govindarajan)
• Pinaki Bhattacharya, A Linear stability analysis of the spatially-developing incompressible plane laminar mixing layer using minimal composite theory (Advisor: Prof. Roddam Narasimha and Prof. Rama Govindarajan)
• Bishakhdatta Gayen, Velocity Fluctuation, Correlation and Rheology in Frictional Granular Shear Flow(Advisor : Prof Meheboob Alam)

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)
• Sandeep Chakrabarti, Hydrothermal Investigations on Arsenates and Arsenate–Oxalates (Advisor : S Natarajan)
• Leonard Deepak F, Investigations of Inorganic Nanowires, Carbon Nanotubes and Co/Mn Doped ZnO (Advisor: CNR Rao)
• Soumya Dutta, Polymer Field-effect Transistors: Electrical Transport Properties and Studies of Photoinduced Charge Generation and relaxation Processes (Advisor: KS Narayan)
• Asish K Kundu, Electronic phase separation and related aspects of rare earth manganates and cobaltates of the type, Ln1-xAxMO3 (Ln= trivalent rare earth, A = divalent alkaline earth and M = Mn or Co) (Advisor: CNR Rao)
• Ayan Datta, Theoretical investigations of optical polarizations in chromophoric aggregates and nonlocal charge distributions in clusters (Advisor : Swapan K Pati)
• Vinod N, Stability and Transition in Boundary Layers: Effect of Transverse Curvature and Pressure Gradient (Advisor: Rama Govindarajan)
• Subarna Bhattacharyya, A wavelet analysis of possible connections between solar processes, Indian monsoon rainfall and ENSO indices (Advisor: R Narasimha)
• Dhanashree A Paranjape, Phenotypic and evolutionary effects of light on circadian clocks and related life history traits in Drosophila melonogaster, (Advisor: Vijay Kumar Sharma)
• N Sharmila Bharathi, Variation and covariation in life-history related traits in some species of Drosophila (Advisor: Amitabh Joshi)
• Shailesh Kumar, Behavioral and molecular analyses of laboratory populations of Drosophila melanogaster selected for early and late adult emergence (Advisor: Vijay Kumar Sharma)
• Venkatesh Swaminathan, Regulation of Acetylation-Dependent Chromatin Transcription by Human Nucleophosmin, a Histone Chaperone, (Advisor: Tapas Kumar Kundu)
• Arpita Mukhopadhyay, Characterization of asrij Expression, Function and Regulation in Embryonic Stem Cells and the Developing Cardiovascular System, (Advisor: Maneesha S Inamdar)
• Ragani Pushpa N, Structural and Vibrational Consequences of Reduced Coordination (Advisor: Shobhana Narasimhan)
• Ashwin S Sampangiraj, Topics in Dynamics, Thermodynamics and Electronic Structure of Supercooled Liquids (Advisor: Srikanth Sastry)
• Joydeep Bhattacharjee, Geometric phases, localized orbitals and distribution of electron charge centres (Advisor: Umesh V Waghmare)
• Kirti Chandra Sahu, Novel Stability Problems in Pipe Flows (Advisor: Prof Rama Govindarajan)
• Chandrima Das, Functional Mechanisms of human transcriptional coactivator PC4, a bona fide nonhistone

component of chromatin (Advisor: Prof Tapas Kumar Kundu)
• M Ram Shankar, Molecular genetic aspects of non-syndromic hearing loss in India (Advisor: Prof Anuranjan Anand)
• Kavitha Siva, Rudhira – A Novel WD40 Protein Expressed in Embryonic Stem Cells, Erythropoiesis, Angiogenesis and Tumors (Advisor: Prof Maneesha S Inamdar)
• Neena Susan John, Investigations of Metal and Metal-Organic Bilayer Nanostructures Employing Atomic Force Microscopy and Related Techniques (Advisor: Prof GU Kulkarni)
• Sutirth Dey, Experimental and Theoretical Investigation of the Dynamics and Stability of Single Populations and Metapopulations of Drosophila melanogaster in the Laboratory (Prof Amitabh Joshi)
• Ashish Kapoor, Studies on molecular genetic aspects of idiopathic generalized epilepsies, (Advisor: Prof Anuranjan Anand)
• Dinesh Kabra, Studies of Length Scales in Semiconducting Polymers using Scanning Photocurrent Contrast Microscopy (Advisor: Prof KS Narayan)
• S Lakshmi, Theoretical modeling of electron transport through molecular bridges (Advisor: Prof Swapan K Pati)
• Moumita Saharay, Computer Simulation Studies on Supercritical Carbon Dioxide (Advisor: Prof S Balasubramanian)
• Prasanta Kumar Dash, Isolation and biological characterization of infectious molecular clones of HIV–1 subtype – C with expanded coreceptor usage from an Indian demented subject (Advisor: Prof Ranga Uday Kumar)
• Mousumi Upadhyay Kahaly, First-principles Studies of One-dimensional Nano-structures (Advisor: Prof Umesh V Waghmare)
• Prasenjit Ghosh, Theoretical Investigations of Properties of Low Dimensional Systems and Nanomaterials (Advisors: Prof Umesh V Waghmare and Prof Shobhana Narasimhan)
• Kiran Batta, Functional cooperativity of Tumor suppressor p53 and Transcriptional coactivator PC4: Transcription to Repair (Advisor: Prof. Tapas Kumar Kundu)
• Debjani Das, Macromolecular uptake in Drosophila pericardial cells requires Rudhira function(Advisor : Prof. Maneesha Inamdar)
• Gargi Dutta, Theoretical Study of Metal Ion Substituted CeO2 for Environmental Catalysis: Origin of Oxygen Storage Capacity, Hydrogen Spillover and Carbon Monoxide Oxidation (Advisor: Prof Swapan K Pati)
• Bhargava BL, Room Temperature Ionic Liquids: Classical and Ab initio Molecular Dynamics Simulation Studies (Advisor: Prof S Balasubramanian)
• Pavan Kumar GV, Utilization of Surface enhanced Raman Scattering in Biomolecular detection and Characterization (Advisor: Prof N Chandrabhas)

Student Life

At JNCASR, an aptitude for learning and growth is well reflected through a vibrant student life, both in and outside the laboratory. The students are accommodated in a modern, spacious and architecturally striking hostel. Inside the hostel, one can find students in a well-catered mess, watching the latest programs in TV rooms, or enjoying a game of table tennis. A book club, having a diverse and rapidly growing collection, helps the students unwind amidst their research schedule. Moreover, the sports facilities—volleyball, badminton and basketball courts and a well-equipped gymnasium— add to the richness of student life.

This engagement is fostered through the multifarious expressions of students' voices. For example, the student's movie committee arranges the screening of a new or popular movie every Saturday night. Inputs from the students to decide the monthly mess menu is taken care by the mess committee. The sports committee arranges several sports activities and provides improvements to the existing ones. The Hostel Day celebration, held during the third week of January, provides a platform for the students to showcase their talents in fine arts, music and sports. Regular events like 'Dhwani' and 'Point-to-Point' draw rousing discussions on anything from philosophy to current pressing issues from the world over, coupled with occasional brainstorming on ongoing research problems. Abhilekh, the student magazine, lets students express views on a plethora of academic and non-academic issues. 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

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 carried out in the host institution 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 Rs.18,000 as honorarium. The timing of the visit may be decided according to mutual convenience. Research scientists/engineers (preferably with a PhD), who have permanent positions in educational institutions, R&D laboratories etc. are invited to apply. So far sixty-eight scientists have visited the Centre under this programme from various parts of India.

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 **www.jncasr.ac.in/extn_prog/vf** or obtained by writing to the Assistant Coordinator, JNCASR, Jakkur, Bangalore 560 064. The deadline for applying is 31st August every year.

Short-Term Courses

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-four 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; Photophysics of Organic Systems: Theory and applications, Bharathiyar University, Coimbatore.

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. **www.jncasr.ac.in/extn_prog/stc**

Summer Research Fellowships Programme

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 6000 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.5000. Selected students get the opportunity to participate in cutting-edge research, and several summer projects have led to publications in leading journals. 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 **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

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.5000.

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. Some of them have published research papers in reputed international journals.

The announcement appears in the newspapers and on our website around December each year. At the appropriate time, application forms may be downloaded from 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

As part of Science Outreach, the Centre has initiated the Project Oriented Biological Education programme (POBE) for undergraduate students. The programme is being 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 are paid a monthly scholarship of Rs. 5000.

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, the focus is on equipping students with the conceptual, experimental and inferential tools that will help them in subsequent research work. The students are introduced 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 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 is being 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)
- Richard N Zare, All that glitters is not gold (2006)

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)
- David Gross, Nobel Laureate, String theory and the coming revolutions of fundamental physics (2006)

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)
- Ramachandra Guha, Adivasis, Naxalites, and Indian Democracy (2006)
- K Ullas Karanth, Practicing Conservation Science in the Tiger's World (2007)

DAE-Raja Ramanna Lecture Series in Physics
The Department of Atomic Energy has instituted this lecture series in 1999.

Foundation Lectures
- 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)
- AK Raychaudhuri, Noise as a probe of the condensed matter: adding new dimensions (2006)
- SM Chitre, The inconstant sun (2007)

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)
- Sriram Ramaswamy, Bugs, molecular motors, Brownian inchworms and copper rods (2006)
- Rahul Pandit, The mathematical modelling of cardiac arrhythmias (2007)

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

Foundation Lectures
- 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)
- S Chandrasekaran, Studies on the synthesis of Thiasugars (2006)
- KN Ganesh, Editing PNA structures for DNA/RNA Binding selectivity (2007)
- Satyamurthy, Atomic and molecular clusters: Designer materials for the nanoworld(2008)

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)
- DD Sarma, Understanding the growth process of semiconducting nanoparticles (2006)
- Uday Maitra, A decade of tinkering with bile acids (2007)
- Suresh Das, Photoresponsive soft materials (2008)

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)
- NK Ganguly, Quality and challenges for stem cell therapy in Indian and International scenario (2006)
- Partha P Majumdar, Our footprints in the sands of time: a statistical-genetic traceback (2007)

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)
• GU Kulkarni, How many atoms maketh a metal(2006)
• Shobhana Narasimhan, Does one size fit all (2007)

IPR Lectures
• A Damodaran, Economics of IP Protection in Hi Tech Sectors: The case of IT andBiotech (2007)
• Chandran Iyer, Patenting Nanotechnology (2008)

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 2005, 2006 and 2007 are listed below:
• 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)
• S Dattagupta, From coherence todecoherence (2006)
• Senthil Todadri, (De)Constructing matter (2006)
• Rajesh Gokhale, How metabolite diversity could be generated from limited number of genes (2006)
• M Eswaramoorthy, Making materials at different length scales (2006)
• Ganesh Subramanian, Using hydrodynamic irreversibility to enhance transport process in multi-phase systems (2006)
• EV Sampathkumaran, Surprising Transport and Magnetotransport Anomalies in some Rare-earth Intermetallic compounds (2007)
• George Thomas Hierarchical Integration of Molecules and Nanomaterials(2007)
• Tapas Kumar Maji, Novel Functional Materials Based on Metal-Organic Hybrid Framework (2007)
• Kaustuv Sanyal, Staying Together or Getting Separated : A Tale of Two Sisters (2007)
• LS Sashidhara, Downstream of Hox Genes (2007)

JNCASR Colloquia
• CNR Rao, Some recent results in the Chemistry of Nanomaterials (2008).
• James Langer, The Mysterious Glass Transition (2008).
• MRS Rao, Genomic approaches to understand the biology and clinical management of Glioma (2008).
• Aruna Roy, Democracy as Common Sense: Can the "Right to Information" bring Rationality and Ethics into Democratic Decision Making", Mazdoor Kisan Shakti Sanghatan, National Campaign for People's Right to Information (NCPRI), April 22, 2008.
• SM Shivaprasad, An atomistic view of the initial stages of interface formation (2008)

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 495t meetings have been held.

The meetings held at Bangalore during 2006, 2007 and 2008 are listed below:

1. High School Science Teachers programme, January 3-12, 2006 at Kolar District, Prof Arun M Umarji (IISc)
2. International symposium on 'Organic Chemistry – today and tomorrow", January 5 – 7, 2006, Prof Uday Maitra and Prof Santanu Bhattacharya (IISc)
3. Mahabaleswar Seminar on "From molecules to networks and behaviour", January 7 – 14, 2006, Prof KS Krishnan (TIFR,Mumbai)
4. Recent developments in metal oxides and related materials, January 9 – 11, 2006, Prof S Natarajan (IISc)
5. Symposium on Recent trends in research on spectroscopy and related fields, January 18-20, 2006, at IACS, Kolkata, Prof T Ganguly and Prof Rai Dastidar (IACS)
6. School on "Computational methods for materials science", January 18 – 21, 2006, Prof S Balasubramanian and Prof Umesh V Waghmare (JNCASR)
7. Workshop for college chemistry post-graduate students and teachers, January 23-25, 2006, Prof S Chandrasekaran (IISc) and Dr Suresh Das (RRL, Trivandrum)
8. 17th AGM of the Materials Research Society of India (MRSI), February 13-16, 2006 at Lucknow, Dr Poonam Tandon (Lucknow University)
9. Flow control and diagnostics, February 19-22, 2006, Dr Sajeer Ahmed (NAL)
10. Workshop on "Molecular characterization of glycoproteins and glycolipids and their interactions with lectins and receptors" and International symposium on "Glycans on proteins and lipids: Implications in cellular functions and evolution", February 22-26, 2006, Prof A Surolia (IISc)
11. Conference and Workshop on Analyses & Applications, March 14-23, 2006, Prof G Rangarajan (IISc)
12. International symposium on "Non-oxide and new optical glasses", April 10-14, 2006, Prof KS Sangunni (IISc)
13. Indo-Israel Conference – 2006, May 4-8, 2006, Prof C N R Rao and Prof Umesh V Waghmare (JNCASR) and Prof DD Sarma (IISc)
14. Eleventh Asian Congress of Fluid Mechanics (XI ACFM), May 22-25, 2006, at Kualalumpur, Malaysia, Dr PR Viswanath (NAL)
15. Geometric methods in topology, June 8 – 29, 2006, Dr Harish Seshadri (IISc)
16. Summer School on Computational Materials Theory, July 10-22, 2006, Prof Shobhana Narasimhan and Prof Umesh V Waghmare (JNCASR)
17. International Workshop on Strongly Correlated Systems, July 16-20, 2006, Prof DD Sarma and Prof Senthil Todari (IISc)
18. Harvard – JNC – NCBS Symposium, August 1-13, 2006, Prof Srikanth Sastry (JNCASR)
19. 9th Annual CFD Symposium, August 11-12, 2006, Dr Sekhar Majumdar (NAL)
20. Consortium of Students in Management Research (COSMAR) – 2006 – An International Seminar, September 21-23, 2006, Prof KR Yogendra Simha (IISc)
21. National Conference in Chemistry – 2006, September 27-29, 2006, Dr VV Suresh Babu and Prof V Vishnu Kamath, Bangalore University.
22. Workshop on "Issues of Higher Mathematics", October 24-25, 2006, Dr BV Sreeekantan (NIAS).
23. "Genes, Development and Disease", October 27-28, 2006, Prof H Sharat Chandra, Centre for Human Genetics (IISc)
24. JNC Conference on Chemistry of Materials, October 29-31, 2006 at Kollam, Kerala (JNCASR)
25. National Conference on "Challenges and Vision 2026 in Science Communication", November 26, 2006, Prof JV Narlikar and Mr AP Deshpande (NCSC)
26. Workshop in Chemistry for Postgraduate Students, November 27-29, 2006 at Trivandrum, Prof S Chandrasekaran (IISc)
27. Workshop on "Level Set Methods and its Application", December 4-15, 2006, Prof Phoolan Prasad (IISc) and Mr Vanninathan and G D Veerappa Gowda (TIFR)
28. Course for University & College Teachers on "Current Frontiers of Research in Natural Sciences, Social Sciences and Humanities", December 6 – 26, 2006, Dr K Kasturirengan (NIAS)
29. Symposium: Chromosome; Functional Thread of Life, December 11 - 13, 2006 Prof Tapas Kumar Kundu (JNCASR)
30. National Symposium on "Theoretical Chemistry" (TCS 2006), December 11-13, 2006, Dr P Venuvanalingam (Bharathidasan University, Thiruchirappalli)
31. Tenth Transcription Assembly, December 14-16, 2006, Prof Siddhartha Roy (IICCB Kolkata)
32. International Winter School on Chemistry of Materials, December 14 – 20, 2006, Prof AK Cheetam, and Prof CNR Rao, Prof SK Pati and Dr A Sundaresan (JNCASR)
33. Workshop on Cancer: Epidemics, Cause and Remedy for High School Students, December 18-20, 2006, Dr Ramendu Ghosh, Prayash Atreyee, West Bengal.
34. High School Science Teachers Programme, December 22-31, 2006, at Gadag, Prof Arun M Umarji and Prof S Ramkumar (IISc)
35. 32nd Mahabaleshwar Seminar on "Parasite Immunology and Immunologenetics" January 7-11, 2007, Prof Shobhona Sharma (TIFR, Mumbai)
36. Conference on "Recent Trends in Many Body Methods for Electronic Structure and Properties of Atoms and Molecules", January 11- 13, 2007, Prof Debashis Mukherjee (IACS, Kolkata)
37. Molecular & Cellular Biology and Therapeutics of HV and Associated Viral Infections, January 12-14, 2007, Dr Anand K Kondapi (University of Hyderabad)
38. International School on "Understanding Molecular Simulation" January 22-27, and International Conference on "Nucleation, Aggregation and Growth", January 29-31, 2007, Prof Srikanth Sastry (JNCASR)
39. Asian Spectroscopy and Asian Biospectroscopy Conference, January 29 to February 3, 2007, Prof S Umapathy and Prof E Arunan (IISc).
40. Symposium on Nanomaterials and Soft Matters, February 8-9, 2007, Prof CNR Rao and Dr A Sundaresan (JNCASR)
41. Symposium on Trends in Computational Materials Science, February 15-17, 2007, Prof S Balasubramanian and Prof Shobhana Narasimhan (JNCASR)
42. Annual Meeting of the Molecular Immunology Forum-2007, March 1-3, 2007, Prof R Manjunath and Prof Anjali Anoop Karande (IISc)
43. 31st Annual Conference of the Society along with a National Symposium on Women in Agriculture, April 10-12, 2007, Dr Shakunthala Sridhara (University of Agricultural Sciences, Bangalore)
44. National Conference on 'Parasitic Diseases- Emerging parasitic diseases and their control in new millennium', April 13-15, 2007, Prof NJ Shetty (Janardhana Foundation, Bangalore)
45. Symposium-cum-Workshop on AIDS/HIV, July 8-13, 2007, Prof Ranga Uday Kumar (JNCASR).
46. International Conference Stochastic Processes and Application, July 16-21, 2007, Prof G Rangarajan (IISc)
47. National Symposium on Electrochemical Science & Technology, NSEST-2007, July 20-21, 2007, Dr JR Mudakavi (IISc)
48. 9th Annual CFD Symposium, August 11-12, 2007, Dr Sekhar Majumdar, (NAL)
49. International Symposium on "Earthern Structures (SES-2007), August 22-24, 2007, Prof PP Mujumdar (IISc)
50. National Conference "Millennium Energy Summit-2007", September 27 – 29, 2007, Dr RN Basu, CGCRI, Kolkata.
51. National Seminar on Geotechnics for Infrastructure (GEO INFRA – 07), September 28-29, 2007, Prof PV Sivapullaiah, IISc., Bangalore.
52. JNC Research Conference on Chemistry of Materials, September 28 – October 1st, 2007, Dr M Eswaramoorthy (JNCASR)
53. India-NIMS Workshop on Nano-materials, October 6-7, 2007, Prof CNR Rao (JNCASR) and Prof Terno Keshu NIMS, Japan.

54. IUMRS International Conference on Advanced Materials (IUMRS-ICAM 2007), October 8 – 13, 2007, CSIR/JNCASR.
55. Frontier Lectures in Chemistry, October 24 – 26, 2007, Prof V Krishnan, JNCASR
56. CCMS School on "Numerical Quantum Many-body methods in Physics & Chemistry (NQM 2007 school), October 29-November 4, 2007, Prof Swapan K Pati and Dr NS Vidyadhiraja, JNCASR
57. School on Biomolecular Simulation, November 6 -16, 2007, Prof S Balasubramanian, JNCASR.
58. Symposium on Applied Aerodynamics and Design of Aerospace Vehicles(SAROD-2007) , November 22-23, 2007, Dr BN Suresh, Director, Vikram Sarabhai Space Centre, Trivandrum.
59. 7th Asian CFD Conference (ACFD-7), November 26-30, Dr Sekhar Majumdar, NAL, Bangalore.
60. JNC Biomedical Sciences Meeting , November 29-30, 2007, Prof Namita Surolia, JNCASR.
61. JNCASR-FCBS Workshop for Postgraduate students in Trivandrum, December 3-5, 2007, Prof S Chandrasekaran, IISc.
62. International Winter School on Chemistry & Physics of Materials in collaboration with ICMR, Univ. of California, Santa Barabara, USA, December 6-13, 2007, Prof Swapan K Pati and Dr A Sundaresan, JNCASR
63. Consortium of Students in Management Research (COSMAR-2007), An International Seminar, December 12-13, 2007, Prof K B Akhilesh, IISc.
64. INDIA-NIMS Workshop on Advanced Materials, December 17-18, 2007, Dr A Sundaresan (JNCASR)
65. Discussion Meeting on the Theme of Phenotypic & Developmental Plasticity, December 17-21, 2007, Prof V Nanjundaiah, IISc.
66. High School Science Teachers Programme, December 21-30, 2007, Prof Arun M Umarji and Prof S Ramakumar, IISc.
67. International Symposium on 'Fluid Days", December 31, 2007 and January 1, 2008, Prof R Narasimha
68. Indo-US Advanced Study Institute on Nano Scale Science & Engineering, January 9-19, 2008, Convener: Dr. T. Pradeep, IIT Madras.
69. International Symposium on "Atomic, Molecular and Optical Sciences & High Performance Computing: A Seamless Frontier", January 10-12, 2008, Convener: Prof. D. Mukherjee, IACS, Kolkata.
70. Workshp on "Physics and Chemistry of Materials", January 11-12, 2008, Convener: Prof. N Chandrabhas, JNCASR.
71. Asian Conference on Transcription–X, January 13-16, 2008, Convener: Prof. Dipankar Chatterji, IISc.
72. UGC-Sponsored Orientation Course – "Frontier Areas of Research & Education: The Role of Universities", January 16-February 5, 2008, Convener: Dr. K Kasturirangan, NIAS.
73. 8th International Symposium on "Biochemical Roles of Eukaryotic Cell Surface Macromolecules, January 21-25, 2008, Convener: Dr. Amit Chattopadhyay, CCMB.
74. Mahabaleshwar Seminar 2007 in Modern Biology on "Laws of Intracellular Transport: Motors, Tracks & Traffic Jams", January 27 – February 2, 2008, Convener: Dr. Krishanu Ray, TIFR.
75. National Symposium in Chemistry (NSC – 10), February 1-3, 2008, Convener: Prof. AG Samuelson, IISc.
76. International Conference on Advanced Materials, February 18-21, Convener: Dr. Suresh Mathew, Mahatma Gandhi University, Kottayam.
77. 15th Annual Conference of Principals of Colleges, March 14-16, 2008, Principal, Poornaprajna College, Udupi.
78. Discussion meeting on "Futuristic Aspects & Directions in Advanced Materials (FADAM), April 16-19, 2008 at Shimla.
79. Frontier Lectures in Chemistry, April 12-13, 2008, at Mangalore University, Prof Uday Maitra, IISc.
80. Bangalore Area Statistical Mechanics Meeting – 2008, April 12-13, 2008, Dr Subir K Das, JNCASR

Publications:
Publications in Scientific Journals (2006-2008)

Chemistry and Physics of Material Units

1. Dan M, Rao CNR. Building up process and open-framework metal carboxylates, involving a progressive increase in dimensionality. Angew. Chem. Int. Ed. 45, 281, 2006.

2. Rao CNR, Behera JN, Dan M. Organically templated metal sulfates, selenites and selenates. Chem. Soc. Rev. 35, 375, 2006.

3. Thirumurugan A, Avinash MB, Rao CNR. 1,2-, 1,3- and 1,4-cyclohexane dicarboxylates of Cd and Mn with chain and layered structures, Dalton Trans, 221, 2006.

4. Lee C, Mcllot C, Slater B, Wu G, Harrison WTA, Rao CNR, Cheetham AK. Interplay of thermodynamic and kinetic factors in the hydrothermal synthesis of hybrid networks: Zinc 4-cyclohexane –1, 2-dicarboxylates. Chem. Commun. 2687, 2006.

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6. Kundu AK, Nordblad P, Rao CNR. Spin-glass behaviour in $Pr_{0.7}Ca_{0.3}CoO_3$ and $Nd_{0.7}Ca_{0.3}CoO_3$. J. Solid State Chem., 179, 923, 2006.

7. Kundu AK, Nordblad P, Rao CNR. Glassy magnetic behaviour in the rare earth manganates, $Ln_{0.7}Ba_{0.3}MnO_3$ (Ln = Nd or Gd). J. Phys: Condens. Matter., 18, 4809, 2006.

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9. Khan M, Sood AK, Deepak FL, Rao CNR. Nanomotors using asymmetric nanorods in an optical trap. Nanotechnology, 17, 5287, 2006.

10. Bhat SV, Govindaraj A, Rao CNR. Tuning the emission bands of nanophosphors through refractive index of the medium. Chem. Phys. Lett. 422, 323, 2006.

11. Biswas K, Rao CNR. Metallic ReO_3 nanoparticles. J. Phys. Chem., B110, 842, 2006.

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13. Agarwal W, Mahalakshmi P, Kulkarni GU, Rao CNR. Nanocrystalline films of Au-Ag, Au-Cu and Au-Ag-Cu alloys formed at the organic-aqueous interface. Langmuir, 22, 1846, 2006.

14. Rout CS, Govindaraj A, Rao CNR. Hydrogen sensors based on ZnO nanoparticles. Solid State Commun., 138, 136, 2006.

15. Ghosh M, Biswas K, Sundaresan A, Rao CNR. MnO and NiO nanoparticles: Synthesis and magnetic properties. J. Mater. Chem., 16, 106, 2006.

16. Kalyanikutty KP, Gautam UK, Rao CNR. Ultra-thin crystalline films of ZnS and PbS formed at the organic-aqueous interface. Solid State Sci.,8, 296, 2006.

17. Khan M, Sood AK, Mohanty SK, Gupta PK, Arabale GV, Vijayamohanan K, Rao CNR. Optical trapping and transportation of carbon nanotubes made easy by donation with palledium. Optics Express, 14, 424, 2006.

18. Gomati A, Rao CNR. Nanostructures of binary nitrides. BN_1TiN and NbN_1 prepared by the urea route. Mater. Res. Bull. 41, 941, 2006.

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20. Rao CNR et al. Soft chemical approaches to inorganic nanostructures, Pure. Appl. Chem. (IUPAC Plenary Lecture), 78, 1619, 2006.

21. Saharay M, Balasubramanian S. Electron Donor-Acceptor Interactions in Ethanol-CO2 Mixtures: An Ab Initio Molecular Dynamics Study of Supercritical Carbon dioxide. Journal of Physical Chemistry B, 110, 3782-3790, 2006. (Professor M.L. Klein Festschrift issue)

22. Bhargava BL, Balasubramanian S. Intermolecular structure and dynamics in an ionic liquid: A Car-Parrinello molecular dynamics simulation study of 1,3-dimethylimidazolium chloride. Chemical Physics Letters, 417, 486-491, 2006.

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31. Behera JN, Rao CNR. A Ni^{2+} (S = 1) kagome compound templated by 1, 4-diazacubane. J. Am. Chem. Soc., 128, 9334, 2006.

32. Cheetham AK, Rao CNR. Structural diversity and chemical trends in hybrid inorganic–organic framework materials. Chem. Commun. (Feature article), 4780, 2006.

33. Dan M, Cheetham AK, Rao CNR. Diverse structures and dimensionalities in hybrid frameworks of strontium and lanthanum with isomeric hydroxybenzoates. Inorg. Chem., 45, 8227, 2006.

34. Behera JN, Rao CNR. Synthesis and magnetic properties of an amine-templated Fe^{2+} (S=2) sulfate with a distorted kagome structure. Inorg. Chem., 45, 9475, 2006.

35. Behera JN, Rao CNR. Amine-templated metal sulfates with chain structures including a mixed-valent Fe compound with a half-kagome structure. Chem. Asian. J., 1, 742, 2006.

36. Shenoy VB, Sarma DD, Rao CNR. Electronic phase separation in correlated oxides: The phenomenon, its present status and future prospects. Chem. Phys. Chem. (Mini Review), 7, 2053, 2006.

37. Edwards PP, Rao CNR, Kumar N, Alexandrov S. Possibility of a liquid superconductor. Chem. Phys. Chem., 7, 2015, 2006.

38. Serrao CR, Krupanidhi SB, Waghmare U, Kundu A, Rao CNR. $InMnO_3$, a biferroic. J. Appl. Phys., 100, 076104, 2006.

39. Sharma RB, Late DJ, Joag DS, Govindaraj A, Rao CNR. Field emission properties of B- and N-doped carbon nanotubes. Chem. Phys. Lett., 428, 102, 2006.

40. Rout CS, Ganesh K, Govindaraj A, Rao CNR. Sensors for the nitrogen oxides, NO_2, NO and N_2O based on In_2O_3 and WO_3 nanowires. Appl. Phys. A., 85, 241, 2006.

41. Rout CS, Govindaraj A, Rao CNR. High-sensitivity hydrocarbon sensors based on tungsten oxide nanowires. J. Mater. Chem., 16, 3936, 2006.

42. Rout CS, Harikrishna S, Vivekchand SRC, Govindaraj A, Rao CNR. Hydrogen and ethanol sensors based on ZnO nanorods, nanowires and nanotubes. Chem. Phys. Lett., 418, 586, 2006.

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46. Kalyanikutty KP, Nikhila M, Maitra U, Rao CNR. Hydrogel-assisted synthesis of nanotubes and nanorods of CdS, ZnS and CuS showing some evidence for oriented attachment. Chem. Phys. Lett., 432, 190, 2006.

47. Kumaramangalam R V, Iyo A, Sundaresan A, Krupanidhi SB, Rao CNR. Ferroelectricity in $Bi_{26-x}M_xO_{40-\square}$ (M = Al and Ga) with the $\square$-Bi_2O_3 structure. Solid State Commun., 140, 42, 2006.

48. Sundaresan A, Bhargavi R, Rangarajan N, Rao CNR. Ferromagnetism as a universal feature of nanoparticles of the otherwise nonmagnetic oxides. Phys. Rev. B. 74, 16136R, 2006.

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56. Yamanaka S, Kubo A, Kini NS. An attempt to prepare carbon clathrate compounds using high pressure and high temperature conditions. Physica B, 383, 59-62, 2006.

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58. Bhat SV, Biswas K, Rao CNR. Synthesis and optical properties of In-doped GaN nanocrystals. Sol. Stat. Comm., 141, 325-328, 2007.

59. John NS, Kulkarni GU, Ayan Datta, Pati SK, Komori F, Kavitha G, Chandrabhas N, Sanyal MK. Magnetic Interactions in Nickel Alkanethiolates, Journal of Physical Chemistry C (Letter), 111, 1868-1870, 2007.

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64. Bhuvana T, Pavan Kumar GV, Chandrabhas N, Kulkarni GU. Nanogranular Au films deposited on carbon covered Si substrates for enhanced optical reflectivity and Raman scattering. Nanotechnology, 18, 145702, 2007.

65. Pavan Kumar GV, Shruthi S, Vibha B, Ashok Reddy BA, Kundu TK, Chandrabhas N. Hot Spots in Ag Core-Au Shell Nanoparticles Potent for Surface-Enhanced Raman Scattering Studies of Biomolecules. J. Phys. Chem. 111, 4388, 2007.

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Intellectual Property

JNCASR realizes the paradigm shift which has occurred due to globalisation of our economy that makes it imperative to protect the Intellectual Property (IP) generated at our Academic Institutions. The IP generated by our scientific community in the form of new knowledge, processes, products, designs, softwares, books, monographs, multimedia packages, etc. has great commercial value.

The Intellectual Property Management Committee of JNCASR fosters IPR culture and addresses all issues concerned with securing, maintaining, protecting and valorizing the IP. The Committee facilitates the scientific community in obtaining patents and also for post patent actions. To sensitize the scientific community on issues of IPR, experts are invited to deliver lectures from time to time.

The innovative research at the Centre has led to filing of 40 national and international patent applications. So far 8 patents have been granted and rest of the applications are at various stages of prosecution. Most of the inventions are available for licensing to potential Industries. A couple of inventions have been licensed to Industries in India, Switzerland and USA. Negotiations are on to license a few more inventions.

The Centre also holds copyright over a number of educational monographs and multimedia packages on interesting areas in science, technology and engineering.

Invention	Inventor/s
Process for Extraction of Superior Quality Plasmid DNA	Ranga U
A Novel Composition to be Used in the Field of Molecular Biology	Ranga U
Use of Hydroxydiphenyl Ether Class of Chemicals, as Exemplified by Triclosan, as an Antimalarial and Identification of Fatty Acid Synthesis at its Target Applicants: JNCASR and Indian Institute of Science	Surolia N Surolia A
Photo Responsive Organic Field Effect Transistor	Narayan KS
Modulators (Inhibitors/Activators) of Histone Acetyltransferases	Kundu TK Balasubramanyam K Swaminathan V
Polyisoprenyl Benzophenones as Inhibitors of Histone Acetyl Transferases and Uses Thereof	Kundu TK Balasubramanyam K Mantelingu M Mohammad A Swaminathan V Radhika AV
Use of Curcumanoids as Histone Acetyltransferases (HATs) Inhibitors	Kundu TK Balasubramanyam K Varier RA Altaf M Swaminathan V
Highly Specific Polyclonal Antibodies of Individual Core Histone and Uses Thereof	Kundu TK Kulangara FK Varier RA Das C
Derivatives of 3,6-Disubstituted 1,2,4-Triazolo-1,3,4-Thiadiazole, A Process And Uses Thereof Applicants: JNCASR and University of Mysore	Kundu TK Varier RA Shivananju N Basappa Rangappa KS

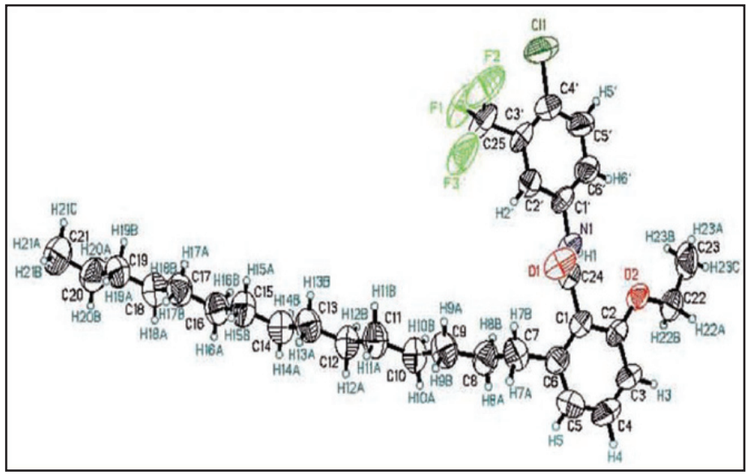


Figure 1: Based on the natural inhibitor of histone acetyltransferases (HATs), Anacardic acid, inventors have synthesized the first known small molecule activator of HAT that is specific to p300.

Invention	Inventor/s
A High Sensitivity Assay For Molecular Typing of Biological Sample Using Surface-Enhanced Raman Scattering Applicants: JNCASR and M/s Microtest Innovations Private Limited	Ranga U Chandrabhas N Jayasuryan N
Inherently Fluorescent Carbon Nanospheres and a Process Thereof	Kundu TK Eswaramoorthy M Ruthrotha Selvi B Dinesh Jagadeesan
A Metal Embedded Nanoparticles Composition and a Process Thereof	**Chandrabhas N**
A Mirror Adapted in Microscope to Perform Surface-Enhanced Raman Spectroscopy, A Microscope and Methods Thereof	**Chandrabhas N** **Pavan Kumar GV**
A Template Free Metal Nanosponge and a Process Thereof	**Eswarmoorthy M** **Saikrishna K**
A Tat Vaccine, A Process and an Expression Cassette	**Ranga U**

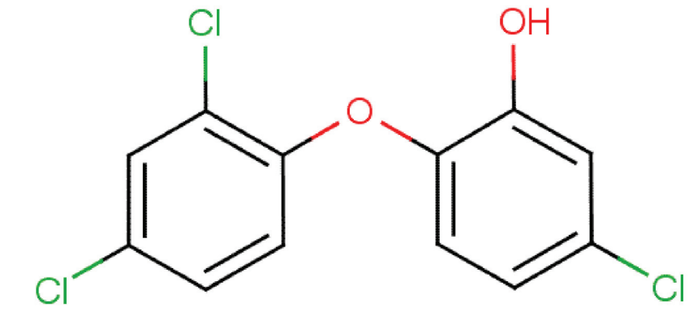


Figure 3: Triclosan

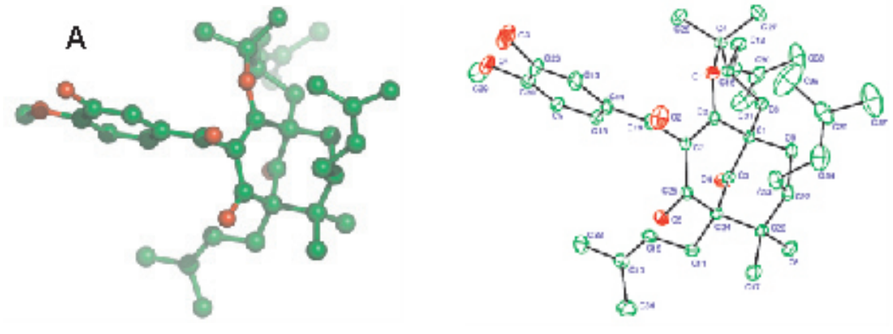


Figure 2: X-ray crystal structure of LTK-14. (A) Ball and Stick representation generated by Pymol (hydrogen atoms are not shown for clarity). (B) ORTEP diagrams showing the displacement Ellipsoids are at the 10% probability level. Color coding of the atoms; green represent carbon atoms and red represent oxygen.

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 aims to facilitate research through humane and efficient management of the laboratory animals in compliance with the CPCSEA guidelines. The facility is registered with the CPCSEA (Reg No.201/CPCSEA). The animal facility is responsible for the supply of laboratory animals used for various research at JNCASR. The animals are maintained under controlled environmental conditions to ensure minimum discomfort and distress. An Institutional Animal Ethics Committee has been constituted, which review the scientific projects involving laboratory animals before the initiation of the experiment by the investigators.

Member of the Facility: Dr. RG Prakash

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). To ensure maximum efficiency and reliability, an outside contractor also provides additional round-the-clock technical support. Both the high performance computing and network facilities are upgraded regularly to meet the growing IT needs at the Centre.

Members of the Computer Laboratory include Computer Laboratory Head Prof. Meheboob Alam (June 2008-), Prof. Umesh Waghmare (upto May 2008) and Staff Members Ravikumar, Dharmasena, Girish and Nishaj.

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. In order to share information resources, the library keeps good liaison with many of the related institutional libraries in the city or elsewhere in the country.

Steadily amassing books at the rate of several hundred per year, the library contains a comprehensive collection of documents synchronizing multidisciplinary research areas of the Centre. Currently, over 5000 documents — books, conference proceedings, monographs and theses — and over 120 journal subscriptions are housed in the library. In addition, the library holds collection of CDs of some important online databases, viz Elsevier, JASTOR, Nature Publications.

Of late, the library has moved towards a greater priority for electronic information sources rather than traditional hard copies. Consequently, the computer facilities available to users have been increased, and further improvements in this move towards a largely e-library are expected in coming years.

JNCASR Digital Repository (DR) is being contemplated showcasing entire research output of the institute and digitization of all papers since 1989 is in progress. 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. The library also joins consortia for subscription of journals like Nature, Scientific American Online Archive, etc.

Members of the Library include Nabonita Guha, Nagesh Hadimani, E Nandakumari, HL Jaiprakash, and J. Rajeev
Website: www.jncasr.ac.in/library
Email: library@jncasr.ac.in

Endowed Chairs and Honorary Faculty

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.

DS Kothari Chair

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

Hindustan Lever Chair

V Krishnan, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.

Linus Pauling Research Professor

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

CSIR Bhatnagar Research Professor

Kalyan B Sinha, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore.

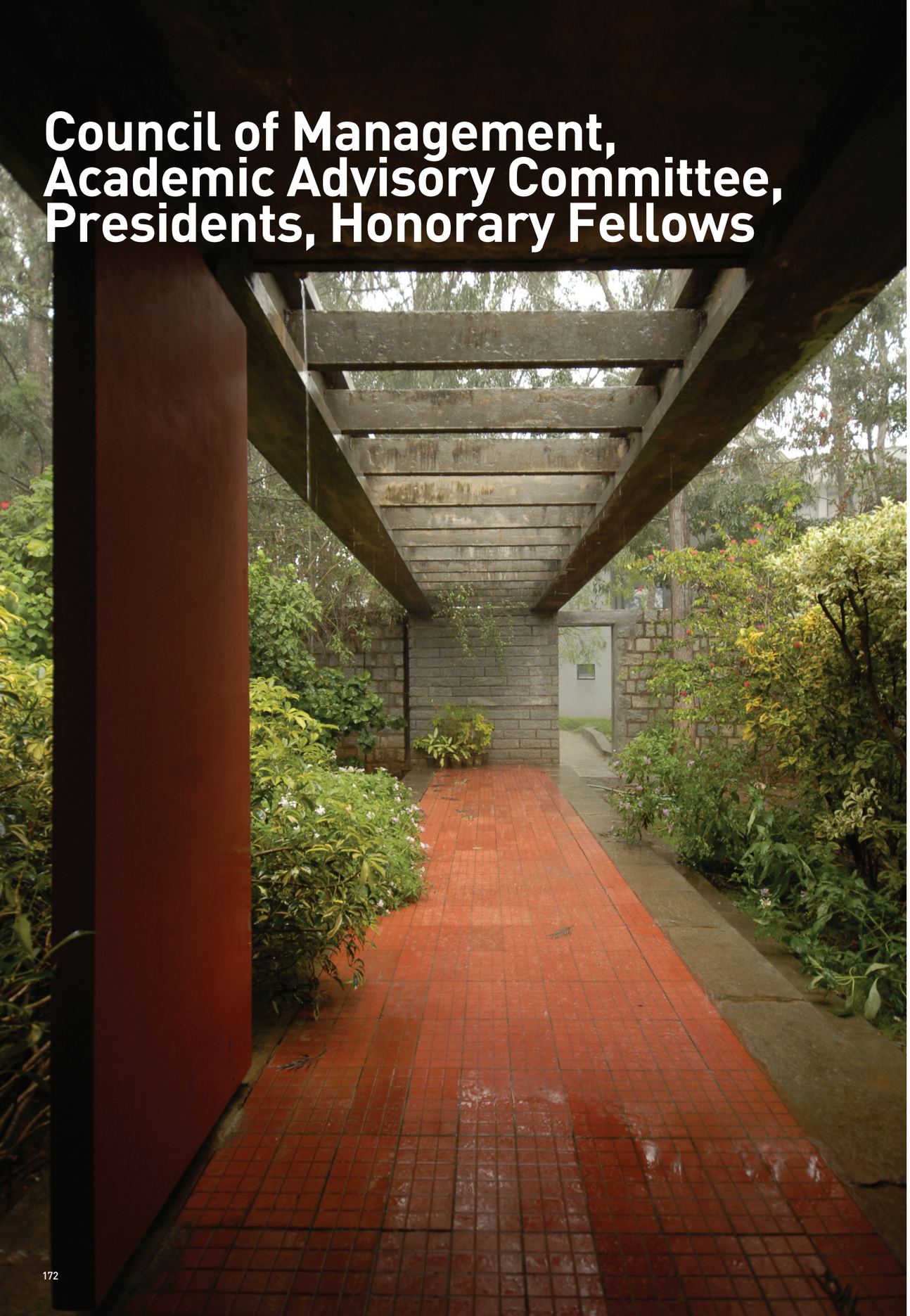
In additon, the Centre hosts AstraZeneca Chair, SS Bhatnagar Chair, Gharda Chair, IBM Information Technology Chair and Vikram Sarabhai Chair.

Honorary Faculty

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. In addition to the Honorary Faculty members mentioned under various Units, the following is the list of other Honorary Faculty Members and Senior Associate, associated with the Centre :

- N Balakrishnan, Indian Institute of Science, Bangalore.
- MK Bhan, Dept. of Biotechnology, New Delhi.
- S Bhattacharya, Tata Institute of Fundamental Research, Mumbai.
- A Chakravorty, Indian Association for Cultivation of Science, Kolkata.
- H Sharat Chandra, Indian Institute of Science, Bangalore.
- S Chandrasekaran, Indian Institute of Science, Bangalore.
- Dipankar Chatterji, Indian Institute of Science, Bangalore.
- Amitabha Chattopadhyay, Centre for Cellular and Molecular Biology, Hyderabad.
- S Dattagupta, Indian Institute of Science Education and Research, Kolkata.
- Raghavendra Gadagkar, Indian Institute of Science, Bangalore.
- KN Ganesh, Indian Institute of Science Education and Research, Pune.
- NK Ganguly, Indian Council for Medical Research, New Delhi.
- K George Thomas, Regional Research Laboratory, Trivandrum.
- MV George, Regional Research Laboratory, Trivandrum.
- Rajesh S Gokhale, National Institute of Immunology, New Delhi.
- J Gopalakrishnan, Indian Institute of Science, Bangalore.
- Seyed E Hasnain, University of Hyderabad, Hyderabad.
- ED Jemmis, Indian Institute of Science, Bangalore.
- SK Joshi, National Physical Laboratory, New Delhi.
- SB Krupanidhi, Indian Institute of Science, Bangalore.
- R Kumar, JNCASR, Bangalore.
- PT Manoharan, Indian Institute of Technology, Chennai.
- RA Mashelkar, National Chemical Laboratory, Pune.
- Satyajit Mayor, National Centre for Biological Sciences, Bangalore.
- Debashis Mukherjee, Indian Association for Cultivation of Science, Kolkata.
- N Mukunda, Indian Institute of Science, Bangalore.
- V Nagaraja, Indian Institute of Science, Bangalore.
- Vidyanand Nanjundiah, Indian Institute of Science, Bangalore.
- G Padmanaban, Indian Institute of Science, Bangalore.
- Gangan Prathap, CSIR Centre for Mathematical Modelling and Computer Simulation, Bangalore.
- S Ramakrishnan, Tata Institute of Fundamental Research, Mumbai.
- TV Ramakrishnan, Banaras Hindu University, Varanasi.
- VS Ramamurthy, Inter-University Accelerator Centre, New Delhi.
- P Rama Rao, International Advanced Research Centre for Powder Metallurgy and New Materials, Hyderabad.
- T Ramasami, Secretary, Dept. of Science and Technology, New Delhi.
- S Ranganathan, Indian Institute of Science, Bangalore.
- G Rangarajan, Indian Institute of Science, Bangalore.
- AK Raychaudhuri, SN Bose National Centre for Basic Sciences, Kolkata.
- EV Sampathkumaran, Tata Institute of Fundamental Research, Mumbai.
- LS Shashidhara, Centre for Cellular and Molecular Biology, Hyderabad.
- KB Sinha, Jawaharlal Nehru Centre for Advanced Scientific Research.
- AK Sood, Indian Institute of Science, Bangalore.
- J Srinivasan, Indian Institute of Science, Bangalore.
- A Surolia, Indian Institute of Science, Bangalore.
- Senthil Todadri, Institute of Science, Bangalore.
- M Vijayan, Indian Institute of Science, Bangalore.
- K VijayRaghavan, National Centre for Biological Sciences, Bangalore.
- G Vijay Nair, Regional Research Laboratory, Trivandrum (Senior Associate).

Council of Management, Academic Advisory Committee, Presidents, Honorary Fellows



Council of Management

- P Rama Rao, ARCI, Hyderabad—Chairman
- P Balaram, IISc, Bangalore
- S Chandrasekaran, IISc, Bangalore
- SK Joshi, NPL, New Delhi
- KP Pandian, DST, New Delhi
- T Ramasami, DST, New Delhi
- CNR Rao, JNCASR, Bangalore
- MRS Rao, JNCASR, Bangalore
- Bikash Sinha, VECC & SINP, Kolkata
- AN Jayachandra, JNCASR, Bangalore—Secretary

Academic Advisory Committee

- MRS Rao, JNCASR, Bangalore—Chairman
- MK Chandrashekaran, JNCASR, Bangalore (upto June 10, 2007)
- KB Sinha, JNCASR, Bangalore (from June 11, 2007)
- Dipankar Chatterji, IISc, Bangalore
- Rama Govindarajan, JNCASR, Bangalore
- KS Narayan, JNCASR, Bangalore
- Rahul Pandit, IISc, Bangalore
- P Ramachandra Rao, Hyderabad
- CNR Rao, JNCASR, Bangalore
- AK Raychaudhuri, SNB NCBS, Kolkata
- K VijayRaghavan, NCBS, Bangalore
- AN Jayachandra, JNCASR, Bangalore—Secretary

Presidents

• CNR Rao	1989–1999
• V Krishnan	2000–2003
• MRS Rao	2003–present

Honorary Fellows

• Ashok Ganguly	1995
• KR Narayanan, Former President of India	1995
• Raja Ramanna	1995
• C Subramaniam	1998
• NR Narayana Murthy	1999
• CNR Rao	2000
• MM Sharma	2003
• Arcot Ramachandran	2005
• S Varadarajan	2006

Administration

Administration Personnel

- **President:** MRS Rao
- **Head, Faculty Affairs:** MK Chandrashekaran (upto June 10, 2007) and KB Sinha (From June 11, 2007)
- **Head, Academic Affairs:** KS Narayan
- **Head, Fellowships and Extension Programmes:** Rama Govindarajan
- **Warden:** Hemalatha Balaram (upto 28.2.2007) and Umesh V Waghmare (from 1.3.2007)
- **Associate Warden:** S Balasubramanian (upto 28.2.2007) and Maneesh S Inamdar (from 1.3.2007)
- **Administrative Officer:** AN Jayachandra

- **Project Engineer:** S Chikkappa
- **Assistant Administrative Officer:** TN Vishwanath
- **Assistant Coordinator:** Princy Jaison Pereira
- **Accounts Officer:** RS Gururaj
- **Stores and Purchase Officer:** K Bhaskara Rao
- **Consultant:** G Jayaram
- **Library-cum-Information Officer:** Nabonita Guha
- **Senior PA to President:** A Srinivasan
- **Junior Engineer (Civil):** Nadiger Nagaraj
- **Junior Engineer (Elec.):** Sujeeth Kumar S
- **Technical Officers:** Jatinder Kaur, V Sreenath, S Srinivas, Usha G Tumkurkar
- **Chief Medical Officer:** BS Subba Rao
- **Consulting Medical Officers:** MLV Archana, Kavitha Sridhar
- **Honorary Medical Officers:** GR Nagabhushana, RK Nivedita, R Nirmala, PK Raghupathy, C Satish Rao, L Sharada
- **Honorary Security Officer:** MR Chandrashekar

Scientific, Technical, Secretarial and Support Staff

J Anil Kumar, R Bannaiah, G Basavaraju, D Basavaraj, D Chandraiah, CS Chitra, N Ganganna, Hanume Gowda, G Harisha, HR Jayaramaiah, G Keshava Murthy, M Krishna, TR Krishna Rao, MN Krishnaiah, BK Kumaraswamy, H Lingamurthy, KC Lokesh, Malathi K Rao, Mehaboob Peer, SN Murugeshwar, AV Nagarathnamma, Nandini Prakash, SR Narasimharaju, MB Narayanaraje Urs, M Narayanaswamy, M Rajkumar, MV Rajaprabagaran, J Rajeeva, Sachin Belvadi, S Samuel, N Sampangi, VR Satyendranath, HS Seetharama Sharma, NR Selvi (under DST Project), Shamsundar, Shashi Karthikeyan, M Shivanna, BS Sreedharamurthy, A Sreenivasa Rao, BM Srinivasa, R Srinivasa, VS Srinivasan, N Srinivasa Raju, S Subash, J Sudha, TV Sudheendra, G Sukanya, A Supriya, K Suresh, G Susheela, K Varadaiah, BS Vasudeva, Veena Maiya, V Venkataiah, B Venkatesulu.