

2013-2014

JNCASR



1989

Establishment of JNCASR
With mission to pursue and promote world-class scientific research and training at the frontiers of Science.



1991

Summer Research Fellowship
Institution of JNCASR flagship programme for undergraduates.



1994

Integrated Ph D
Introduction of Integrated Ph D programme in Chemical Science.



1995

Jakkur Campus
Inaugurated by Hon'ble Vice President of India, Shri KR Narayanan.

Ph D Programme
Commenced Ph D Programmes in Chemistry and Physics of Materials Unit; and Fluid Dynamics Unit (now Engineering Mechanics Unit).



2000

AMRL Inauguration
Inauguration of Advanced Materials Research Laboratory (AMRL) building.



2002

Deemed University
JNCASR becomes a deemed university.



2004

Outreach Programmes
Launch of project-oriented research programmes for undergraduates [Project-Oriented Chemical Education - POCE (2004) & Project Oriented Biological Education - POBE (2006)].



2010

ICMS and CNR Rao Hall of Science
Inauguration of International Centre for Materials Science (ICMS) and CNR Rao Hall of Science by then Prime Minister Dr Manmohan Singh.



2012

Institution with Highest Scientific Impact (CPP & RCI)

As per the publication data of 2000-01 and 2011-12, a study shows that JNCASR has the highest Citations Per Paper (CPP) as well as highest Relative Citation Impact (RCI) in India.



2013

The Titan Microscope

Installation of the most advanced ultra-high-resolution transmission electron microscope in the world. The microscope at JNCASR is one of just three in India.

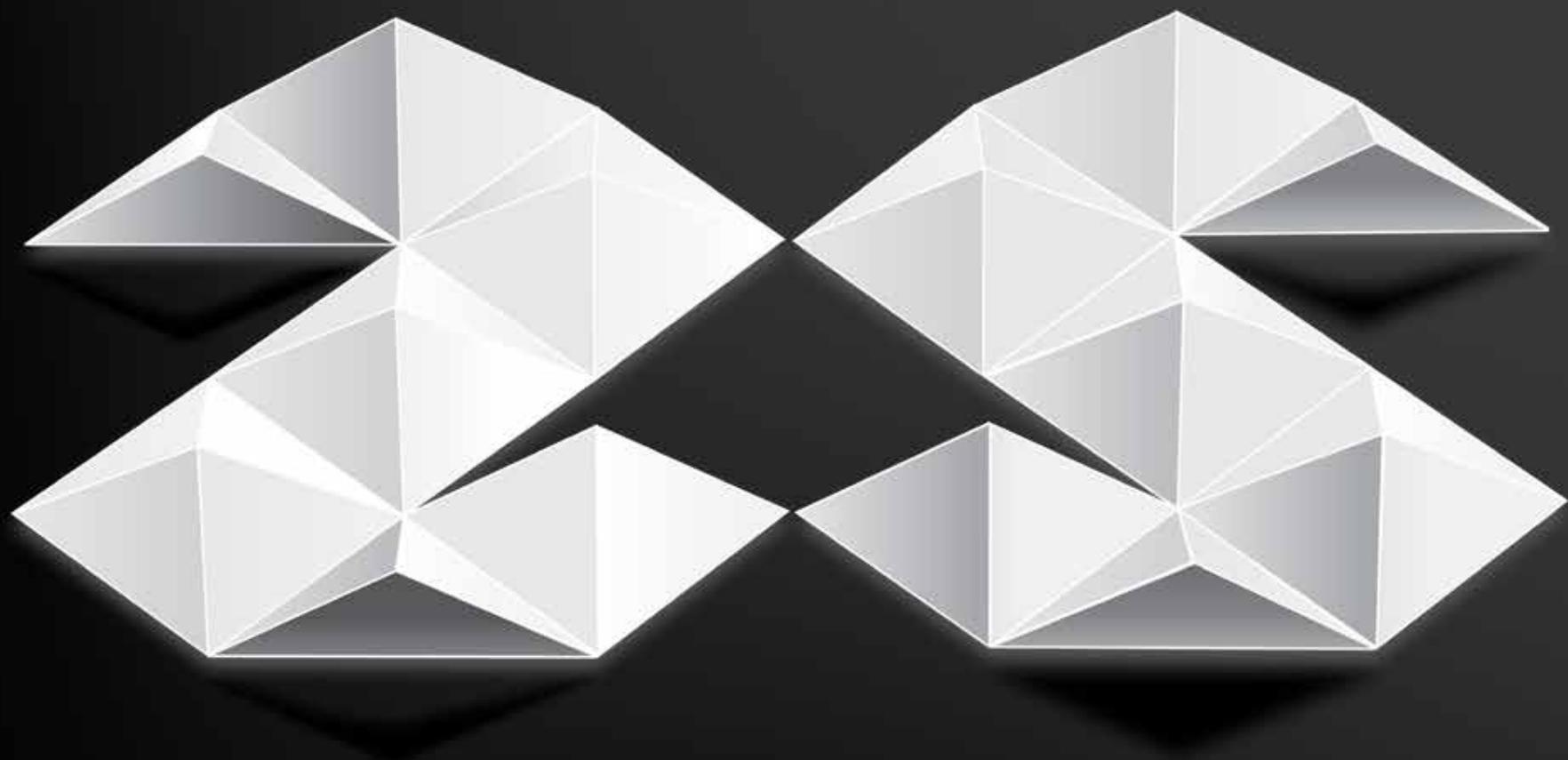


2014

Bharat Ratna for Prof CNR Rao

The Government of India confers the Bharat Ratna, the highest civilian award on eminent scientist Prof CNR Rao.

Celebrating science for 25 years



JNCASR

2013-2014



Foreword

The volume you hold in your hands has been, in a sense, 25 years in the making – decades spent at the very forefront of interdisciplinary scientific research. Focused on areas with the greatest possible relevance to society at large, and India in particular.

Since 1989, the Jawaharlal Nehru Centre for Advanced Scientific Research has worked to create new knowledge, and encourage its use in innovative applications. Its diverse research interests, unmatched ambience, and small size offer an ideal environment for scientific and academic pursuits.

The environment is one of effortless collaboration, driven by cross-discipline expertise, and state-of-the-art infrastructure. This has enabled a per-faculty output of publications that is among the highest in the country. It has also resulted in awards and recognition from some of India's, and the world's, best-known institutions.

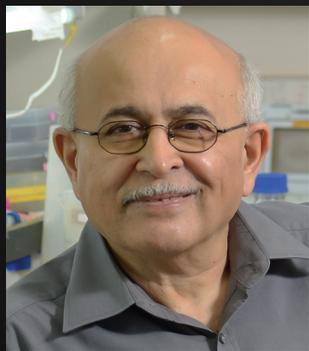
At the end of our Silver Jubilee year, we reflect on over quarter century of cutting-edge conceptual and technological research, engaging science outreach activities, and an exceptional array of seminars, workshops and conferences of international standards.

The unstinting support of the Department of Science and Technology (DST), as well as other governmental and private sources, has consistently enabled us to embark on new research activities.

As we introspect on the 25 years that have gone by, we cannot help but be enthused, and look forward to the years to come.

Narayan KS
Former In-charge President
Jawaharlal Nehru Centre for Advanced Scientific Research





From the President's desk

I have joined the Centre when this volume was at its final stage of production. Within is the depiction of the evolution of JNCASR to its present form with its diverse hues and colours. The myriad fauna and flora at display has facilitated the JNCians to achieve the current distinguished status within and outside India. The seamless blend of nature with the diverse research activities has provided opportunities for nurturing and furthering interdisciplinary areas of science. As a result, now the Centre is poised to leverage its research breakthroughs to be showcased and translated.

This brochure commemorates the completion of 25 glorious years of the Centre. The contents inside reveal insights into our journey. It also provides pointers for the directions to be taken in the immediate future and the next decade. While the research highlights and accomplishments of JNCians presented in the following pages is a testimony of the depth and strength of the Centre, interphase of various areas and the indicators of translational science, it is time now to gather momentum. With the strong foundation that we have, and the appetite for innovation, let us reinvent ourselves.

Nagaraja V

President

Jawaharlal Nehru Centre for Advanced Scientific Research

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introduc

There is a spirit of curiosity and fearlessness that permeates every aspect of the 25-year history of the Jawaharlal Nehru Centre for Advanced Scientific Research.

2014 was JNCASR's Silver Jubilee year, and celebrations were observed throughout the academic calendar. After all, it has been two and a half decades of fuelling the spirit of discovery, and combining research and innovation to create better, more efficient solutions to challenges, in fields as diverse as energy, healthcare, and engineering. 25 years of building a rich, glorious history, and a powerful reputation.

The first celebratory moment of the year came in the form of a stellar sarod performance by Ustad Amjad Ali Khan and his sons Ayaan, and Amaan. This was followed by an engaging and motivating inauguration lecture by Prof CNR Rao, as well as a faculty meet and in-house symposium that featured contemporary research of the highest quality in the form of talks and posters.

Special Silver Jubilee lectures were delivered by three of the world's finest researchers in

their fields. The first, Balancing the budget: What drives the global circulation of the oceans, was delivered by Prof Ross Griffiths of the Australian National University. The second, Brain stem cell progeny create functional units, was delivered by Prof Vijay Raghavan, Department of Bio-technology, Government of India. The final lecture, Spintronic and Ionitronic Computing Technologies, was delivered by Prof Stuart Parkins from IBM and Max Planck Institute. The year-long celebrations drew to a close on January 5th with an event featuring an in-house symposium participated by faculty, students and alumni. The highlight of the evening was a musical performance by master flautist, Pandit Hariprasad Chaurasia. Hon'ble Vice President of India, Shri M Hamid Ansari released a Memoir of JNCASR's 25 years during the Concluding Ceremonies of this momentous year.

It is, perhaps, only fitting that 2014 be the year that the Founder-Director of JNCASR, Prof CNR Rao, received the Bharat Ratna, the country's highest civilian honour. Equally appropriate is the Centre's being named the institution with the 'highest impact,' according to the Science Citation Index.

Over the years, JNCASR has filed 178 patent applications, and has been granted 31 patents from foreign countries and 7

patents from India. The Centre has also made substantial contributions to fields like nanotechnology and is involved in specialised research in areas of relevance, such as energy, cancer, HIV, Ebola etc.

Home to independent research, and several on-campus, multidisciplinary collaborations, JNCASR contributes about 200 papers each year to the world's finest scientific journals.

Members of the Centre's faculty have been recipients of international recognition and acclaim: Prof CNR Rao, Bharat Ratna, holds the singular distinction of being elected Fellow of many of the leading science academies in the world, while having received the Dan David Prize; the Queen's Medal of the Royal Society, London; the German Chemical Society's August-Wilhelm-von-Hoffmann-Denkünze Medal; the Order of Friendship, Russia; the India Science Prize; and a host of other awards. The highly-recognised Prof Roddam Narasimha is a Fellow of the Royal Society of London; the National Science Academy, USA; and the recipient of prestigious awards like the Trieste Science Prize, Italy. Prof Roddam Narasimha, Prof MRS Rao and Prof KS Valdiya are recipients of the prestigious Padma Awards of the Government of India. Other faculty members have also been honoured with highly esteemed prizes like the Shanti

tion

Swaroop Bhatnagar Award; the prestigious CRSI and MRSI Bronze Medals; the DAE Outstanding Research Career Award; the BM Birla Prize; the FICCI Award for Life Sciences. Adding to honours further, faculty members have also received fellowships from the Third World Academy of Sciences (TWAS), the Indian Academy of Sciences (IAS), the National Academy of Sciences (NASc), the Indian National Science Academy (INSA) and Department of Science and Technology, Govt. of India such as JC Bose, Swarnajayanthi and SERB Distinguished Fellowships.

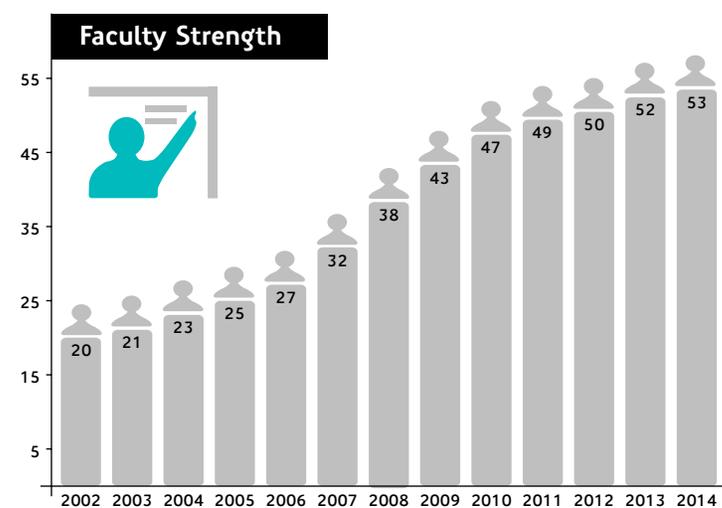
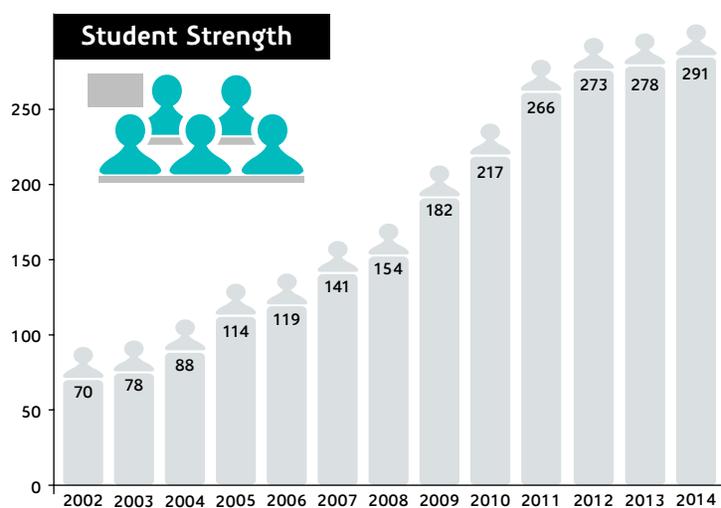
The JNCASR faculty-student ratio of about 1:5, as well as its state-of-the-art

facilities make it an ideal environment for research in the fields of Chemistry and Physics of Materials, Engineering Mechanics, Evolutionary and Organismal Biology, Molecular Biology and Genetics, Neuroscience, New Chemistry, Theoretical Sciences and Geodynamics.

JNCASR's International Centre for Materials Science (ICMS), the first of its kind in India, has been facilitating collaboration and networking on a global scale, and has attracted some of the finest international talent since 2008. The Centre itself enjoys rich and active collaborations with institutions like the NIMS, Japan; Purdue University, USA; and Northwestern

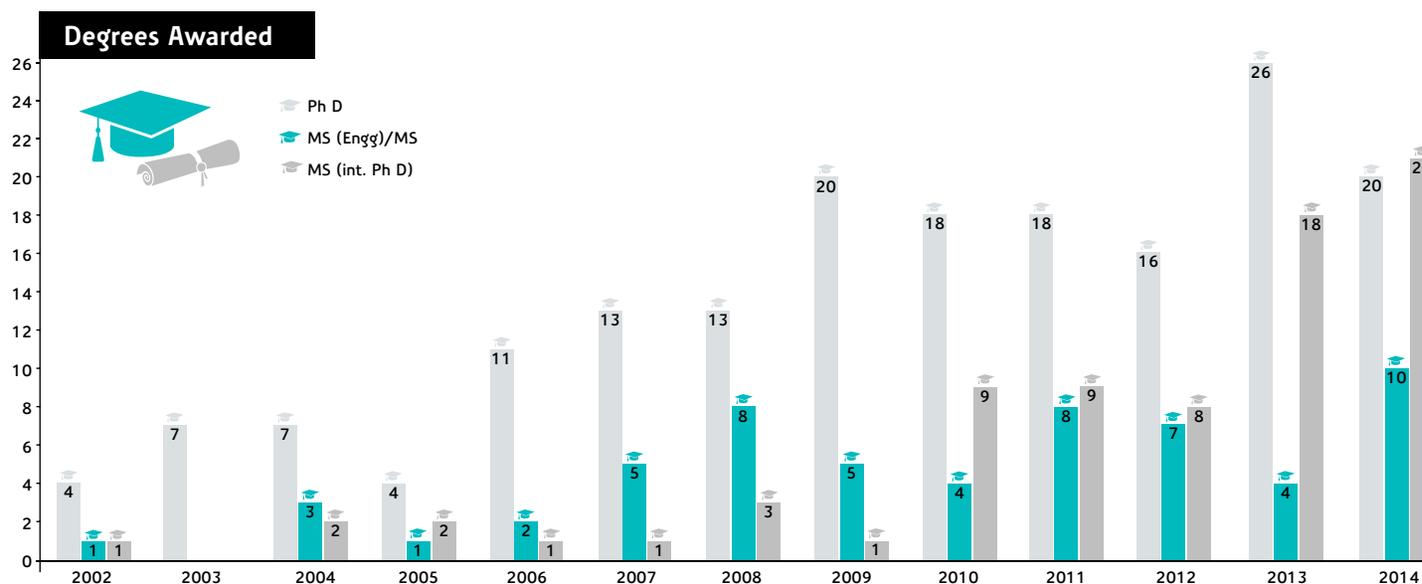
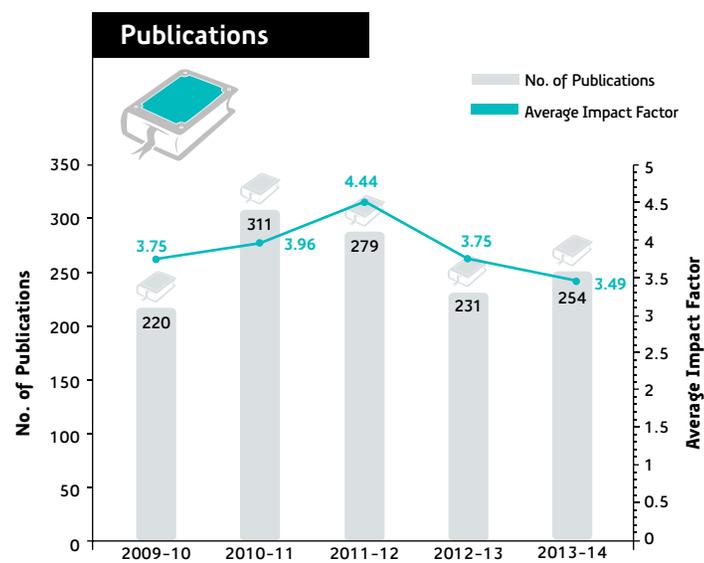
University, USA. The Centre offers short-term visiting fellowships, and has received 21 international visitors as part of this programme. In turn, several scientists from ICMS have visited other leading institutes.

In addition, the Centre's outreach activities reach audiences as diverse as science teachers, school students, undergraduates, and promising young chemists, and biologists, through programmes like the Summer Research Fellowships, Visiting Fellowships, Project-Oriented Biology Education (POBE) and Project Oriented Chemical Education (POCE). The JNCASR series of monthly lectures at the Madan Mohan Malviya Amphitheatre and the



CNR Rao Hall of Science on the campus are at the heart of the Centre's attempts at firing the scientific imagination of school students. They have resulted in conversations with almost two thousand school students each year.

The past 25 years have seen the Centre rise in reputation, as well as impact, and there is no reason to believe that the next 25 will be different. The spirit of fearlessness, and of scientific inquiry, will guide JNCASR, as it makes headway in devising solutions to some of the most challenging problems of the 21st century, whether in the areas of energy, materials science, healthcare, or engineering.



THE JEWEL OF THE NATION

The burnished bronze and platinum peepal-shaped medal, the Bharat Ratna, is the nation's highest civilian honour. It recognises exceptional service and performance of the highest order in any field of human endeavour.

In the year 2014, the honour was conferred upon Prof CNR Rao, Founder-President of the Jawaharlal Nehru Centre for Advanced Scientific Research.

Prof Rao is currently the National Research Professor, Linus Pauling Research Professor, and Honorary President of JNCASR, as well as the

Director of the International Centre for Materials Science (ICMS). He has been the Chairman of the Scientific Advisory Council to the Prime Minister of India.

Being one of the world's foremost experts in solid state and materials chemistry, his contributions to the field span five decades. The author of over 1,600 research papers, and 50 books, Prof Rao was one of the earliest to synthesize two-dimensional oxide materials such as La_2CuO_4 . His work has had a profound impact on fields like colossal magneto-resistance, high temperature superconductivity, and nanomaterials.





CHEMISTRY AND PHYSICS OF MATERIALS UNIT

**LINUS PAULING
RESEARCH PROFESSOR
AND FOUNDER CHAIR**

CNR Rao, FRS, FASc, FNA, FTWAS,
Hon FRSC, Hon F Inst P

PROFESSOR AND CHAIR

Balasubramanian S, FASc

PROFESSORS

Chandrabhas N, FNAsC
GU Kulkarni, FNAsC, FASc
Narayan KS, FNAsC, FASc, FNA
Shivaprasad SM*
Sundaresan A

ASSOCIATE PROFESSORS

Eswaramoorthy M
Tapas Kumar Maji

FACULTY FELLOW

Sarit S Agasti**

*Jointly with ICMS

**Jointly with NCU

**ASSOCIATE FACULTY
FROM ICMS**

Ranjan Datta
Rajesh Ganapathy
Sridhar Rajaram

**ASSOCIATE FACULTY
FROM TSU**

Shobhana Narasimhan, FNAsC
Swapn K Pati, FNAsC, FASc
Srikanth Sastry, FNAsC, FASc
NS Vidhyadhiraja
Umesh V Waghmare, FNAsC, FASc, FNA

Research in the Unit spans a wide variety and includes work on nanomaterials, multifunctional materials, organic solar cells, hybrid materials, catalysts, optoelectronic materials, and many aspects of biomaterials.

The Chemistry and Physics of Materials Unit (CPMU) is one of the earliest Units in the Jakkur Campus. Established under the stewardship of Professor CNR Rao, with a broad and singular objective to pursue research on materials with special emphasis on the nanoscale, soft matter, self-assembly, and advanced materials for energy and environmental applications. The goal in many of these studies is the design and synthesis of novel architectures and its relationship to properties emanating thereof. Members of the Unit's faculty are leaders in their areas and have contributed substantially to, both, broadening and enriching the discipline. The activities of the Unit are strengthened through close collaborations with associate members drawn from the International Centre for Materials Science and the Theoretical Sciences Unit.

RECENT HIGHLIGHTS OF OUR RESEARCH ARE:

Novel photocatalytic materials for splitting water and thus to generate hydrogen, synthetic routes to nanosheets of many inorganic layered materials, novel devices to improve light harvesting efficiency, simple chemical routes to develop transparent conducting electrodes, supercapacitors, a polymer optoelectronic interface which provides visual cues to a blind retina, development of SERS tools to study the nature of binding of medicinally relevant small molecules to enzymes, unravelling the microscopic interactions responsible for carbon dioxide adsorption in several porous materials using computer simulations, growth of stress and defect-free GaN nanowall networks using MBE which exhibit enhanced luminescence, the

synthesis of a flexible, fluorescent metal organic framework solid that is highly responsive to aromatic amines, reversible pore engineering (size and philicity) of microporous silica using charge-transfer modules, reentrant spin glass phenomenon and magnetodielectric effects in spiral magnetic oxides, a two-step glass transition exhibited by ellipsoidal colloidal particles, optical emission of lithium doped ZnO epitaxial thin films, enhancing the enantioselectivity in a Freidel-Crafts reaction by changing the conformation of the catalyst.

Researchers of the Unit actively engage themselves in collaborative efforts with groups in India and abroad. Protection of rights to intellectual property is diligently pursued which has resulted in a significant number of Indian and international patents awarded to the faculty.

The doctoral students of the Unit, currently numbering around 35, are exposed to both the fundamentals of the subjects as well as to recent advances through a rigorous course programme and technical seminars. Nearly 70% of them hold a fellowship granted by CSIR/UGC, based on their performance in the national level NET exam. The average time taken by a student of CPMU to submit her/his Ph D thesis is 5 years. Several of our alumni are now members of faculty in leading academic institutions and also serve as active researchers in industry.

Since 2007, the Unit has been offering an Integrated Ph D programme in Materials Science. Currently, 39 such students are in various stages of this programme. The Unit is fully committed to teaching and to the development of human resources. Seven technical staff members of the Unit ably support the research activity, not only in maintaining all the major experimental facilities, but also in finding innovative solutions to issues. The Unit also maintains a central workshop and a liquid nitrogen facility.

The following pages will provide a glimpse of our activities. For further details, please visit: www.jncasr.ac.in/cpmu

Computational Molecular Science



BALASUBRAMANIAN S

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Post-Doc: University of Pennsylvania, Philadelphia, USA

Computational Science has emerged as an independent approach to understand natural phenomena. Our Group studies molecular and macromolecular solids, liquids, and gases using advanced computational techniques. We develop and employ modern computing platforms, algorithms, and software towards this purpose. Techniques include: Molecular Dynamics, Monte Carlo and *ab initio* MD simulations, Density Functional Theory Calculations, QM/MM simulations and Quantum Chemical Calculations.

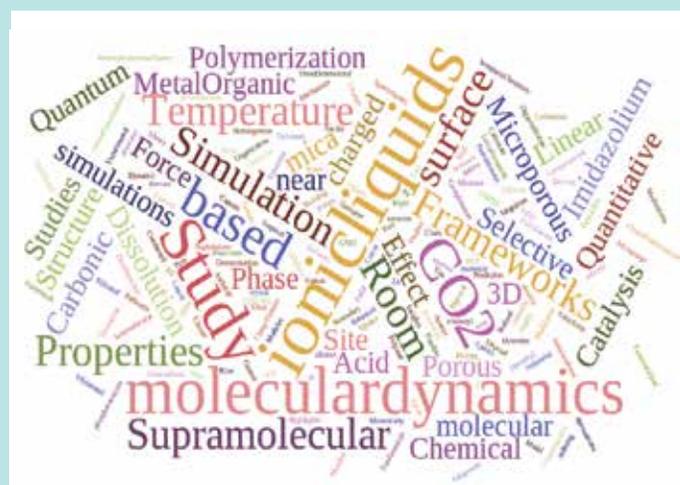


Fig.: Word-cloud of titles of research publications of our group during 2012–July 2014

CURRENT INTERESTS:

Environmentally Benign Solvents: Modelling supercritical carbon dioxide, room temperature ionic liquids and aqueous carbonic acid solutions.

Supramolecular Polymerisation: Modelling the thermodynamics, kinetics and mechanism of self-assembly of chromophores in organic solvents (along with Prof Subi George's group).

Gas Storage: Adsorption of gases in crystalline solids (metal-organic frameworks, covalent organic frameworks) and amorphous microporous polymers. We develop structural models as well (along with Prof Tapas Maji's group).

Biomolecules: Small molecule transport in proteins, enzymatic catalysis (along with Prof H. Balaram) and protein structure, function and dynamics. We strive to closely relate our work to experiments.

Programmable Molecular Materials in Imaging and Diagnostics



SARIT S AGASTI

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Ph D: University of Massachusetts, Amherst, USA

Post-Doc: Harvard University, Cambridge, USA

Our lab is interested in engineering programmable molecular materials to address challenges in bioimaging and clinical diagnostics. In the area of programmable molecular materials, we are specifically interested in synthetic DNA nanostructures (see Fig.). Our idea is to utilize their prescribed 3D geometry and large number of uniquely addressable features to organize sensor arrays for creating highly sensitive diagnostic systems.

The other exciting direction we are moving is to utilize the programmable nature of DNA hybridisation to generate probes for super-resolution microscopy (see Fig.). This imaging technique, called DNA-PAINT, accomplishes the necessary fluorescence ON/OFF switching for localisation-based super-resolution microscopy by using transient DNA hybridisation. Besides achieving ultra-high imaging resolution (~10 nm), this imaging technique, has an intrinsically scalable multiplexing ability (>100x). By integrating with a molecularly targeted affinity ligand (e.g. antibody), we envision that it would enable *in situ* proteomics imaging from single cells in the context of the tissue microenvironment.

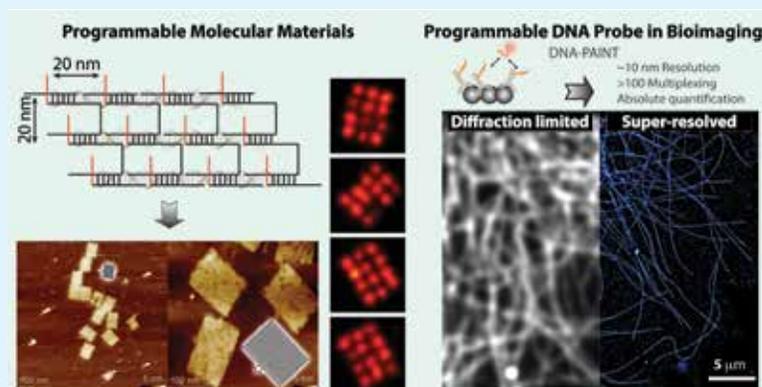


Fig.: Schematic showing the research activities in the lab.

KEY PUBLICATIONS

Ullal AV, et al., *Science Translational Medicine*, 6, 219ra9 (2014).

Agasti SS, et al., *Journal of the American Chemical Society*, 134, 18499–18502 (2012).

Raman, Brillouin Spectroscopy and High Pressure Research



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Ph D: Indian Institute of Science,
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Post-Doc: Cornell University,
New York, USA

Our Group is interested in the study of materials using optical spectroscopy under ambient and extreme conditions. Our Group activities can be divided into five categories: (a) Raman spectroscopy, (b) Surface enhanced Raman spectroscopy in nano-biotechnology, (c) Synthesis of novel metal nanostructures for SERS, (d) Brillouin scattering and (e) High pressure research using light and X-ray as probes.

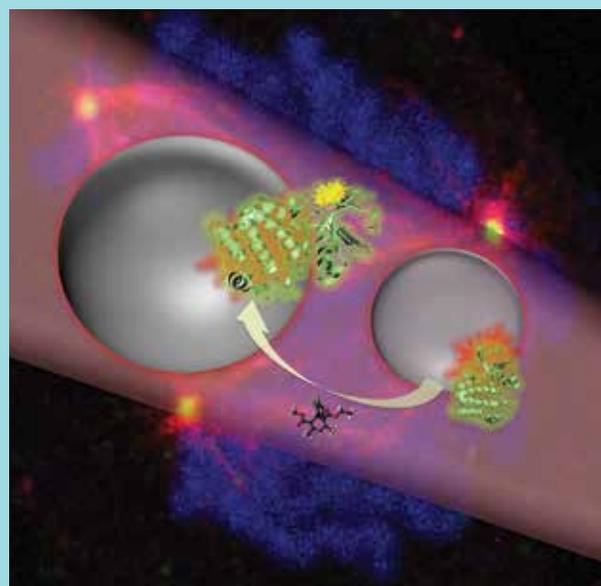


Fig.: The inhibition of oncogenic Aurora A Kinase by anti-hypertensive drug Felodipine captured by SERS

Vibrational spectroscopy has been an important component in the study of materials and of late with the recent advancements in lasers, Raman spectroscopy has evolved as an effective probe to study phase transitions, molecular structure, etc. Further, an advanced technique - SERS is used to investigate drug-protein interaction using metal nanoparticles. On the other hand Brillouin spectroscopy is a non-contact probe in understanding the mechanical properties of materials. High pressure Raman, Brillouin and XRD is used extensively by us to study materials under extreme conditions.

KEY PUBLICATIONS

Karthigeyan, et al., *Proceedings of the National Academy of Sciences*, (2014).

Gayatri Kumari, et al., *The Journal of Physical Chemistry Letters*, 3, 1130 (2012).

Nanomaterials and Catalysis



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Ph D: Anna University, Tamil Nadu

Post-Doc: AIST, Japan,
& Bristol University, UK

Our Group's efforts are directed towards four primary areas of research listed below:

Drug Delivery: Glucose-derived carbon-based materials have been extensively used in our Group as nanocarriers for nuclear targeting. Current interests are directed towards using these materials as brain theranostics, therapeutic-cum-diagnostic, for brain-related diseases.

Layered Materials: One of the main focus in this area lies in the synthesis and modification of clay and carbon based layered materials for light harvesting, drug delivery, gas separation and catalytic applications.



Fig.: Carbon-based materials as brain theranostics

Porous Materials: Our interests are focused towards combining conventional mesoporous silica with the functionally rich supramolecular chemistry to create new generation of hybrids capable to reversible switching of pore size and philicity. The modular nature of these materials allows for easy customisation of the pore properties. We also apply these materials for electrostatic gating of ion transport.

Catalysis: A variety of supports and catalysts are being explored for achieving high selectivity and conversion for oxidative dehydrogenation of higher alkanes and hydrogen peroxide synthesis.

KEY PUBLICATIONS

BVVS Pavan Kumar, et al., *Journal of the American Chemical Society*, 135, 10902-10905 (2013).

C Piyush, et al., *Journal of Materials Chemistry B*, 1, 939-945 (2013).

Nanomaterials, Nanofabrication and Devices



GU KULKARNI

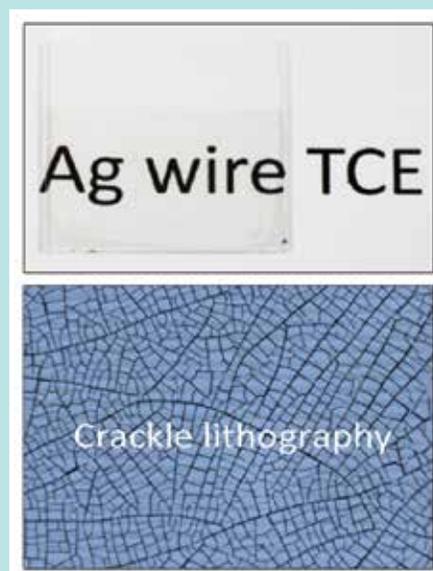
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Ph D: Indian Institute of Science,
Bangalore

Post-Doc: Cardiff University, Cardiff, UK

Our main theme of research is studying matter at the nanoscale and exploiting the properties realized in the study, for applications. Our research interests are focused on new strategies in synthesis of nanomaterials, nanopatterning and nano-device fabrication, including of molecular systems. Our recipes emphasize the importance of simple design, near ambient working conditions, solution-based processing as well as low-cost instrumentation. We strive to translate nano-research findings into affordable technology. The adjoining figure shows a photograph of a glass substrate hosting a highly interconnected silver nanowire network which is invisible to the naked eye; the wire network imparts its electrical conduction behavior to the insulating glass such that the composite system serves as a transparent conducting electrode. The electrodes thus formed exhibit optoelectronic properties that are superior in many ways, to those of conventional material (ITO) and are therefore considered important in futuristic technology.

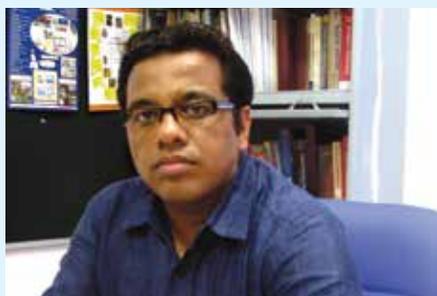


KEY PUBLICATION

KDM Rao, et al., *Advanced Materials Interfaces* (2014).

Fig.: Crackle lithography

Functional Organic/Organic-Inorganic Hybrid Materials



TAPAS KUMAR MAJI

ASSOCIATE PROFESSOR AND WARDEN

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Ph D: IACS, Jadavpur University, Kolkata
Post-Doc: Kyoto University, Japan

Our research work is focused on the design and synthesis of new solid state organic/organic-inorganic materials that addresses contemporary problem related to energy and environment. The hybrid crystalline porous solids are known as metal-organic frameworks (MOFs) or porous coordination polymers (PCPs) and organic porous solids are conjugated microporous polymers (CMPs) or covalent organic frameworks (COFs). We are also interested in soft materials like metallo-gels and stimuli responsive behaviour of such materials.

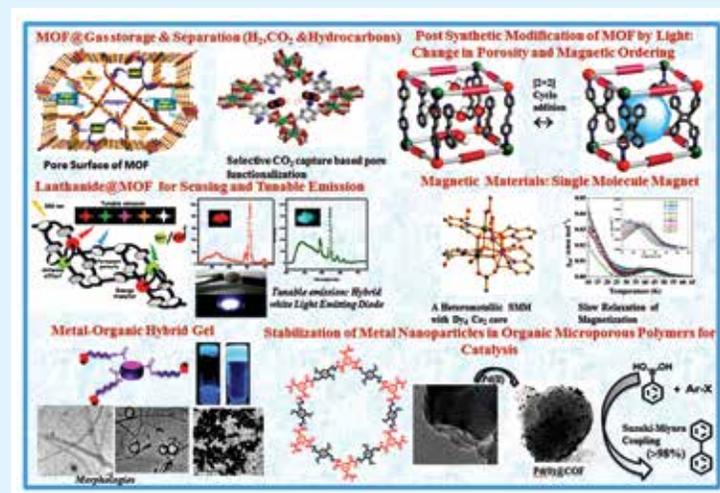


Fig.: Metal-organic/organic functional materials

Key areas of interests based on these solid materials:

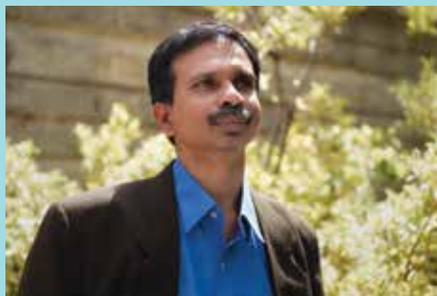
1. Hydrogen, Hydrocarbon storage and CO₂ capture in Porous Solid
2. Stabilisation of Nanoparticles in MOFs/COFs/CMPs for Catalysis and Gas Storage
3. MOFs/COFs at Nanoscale for Multimodal Imaging and Gas Storage and Separation
4. Porous Luminescent Materials for Sensing, Tuneable Emission and Light Harvesting
5. Molecule Based Magnetic Materials (SMM and Guest responsive Magnetic Materials)

KEY PUBLICATIONS

VM Suresh, et al., *Advanced Functional Materials*, Vol. 23, 5585-5590 (2013).

S Mohapatra, et al., *Chemistry of Materials*, Vol. 25, 1673-1679 (2013).

Organic Electronics, Photovoltaics, Device Physics and Bio-Electronics



NARAYAN KS

**PROFESSOR,
IN-CHARGE PRESIDENT AND
DEAN (RESEARCH & DEVELOPMENT)**

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Ph D: Ohio State University,
Columbus, USA
Post-Doc: Wright Patterson Air Force
Base, USA

(ORGANIC-POLYMER) ELECTRONIC DEVICES - PHYSICS AND APPLICATIONS

This research area spans a range of interdisciplinary fields, which brings in the scope of innovation and novelty in many of the approaches in the laboratory. Some of the current research activities, we are pursuing, are in the field of organic-polymeric electronics – with emphasis on photovoltaics and field effect transistors, bio-molecular electronics, soft lithography, nanodevices and development of near field microscopic techniques.

The approach to our research problems utilizes spectroscopic and microscopic techniques, transport measurements, device fabrication and characterization studies. Our research pursuit ranges from fundamental understanding of various optoelectronic phenomena in solution processible materials to applications in the field level. We actively collaborate with synthetic chemists, biomedical researchers, engineers and technology developers.

The two recent applications of our research outcome which are of impact to the community at large are in the area of low-cost polymer solar cells and polymer semiconductors as prosthesis elements for retina with non-functional photoreceptor.

KEY PUBLICATIONS

Anshuman Das and Narayan KS. *Advanced Materials*, 25, 2193 (2013).
Vini Gautam et al., *Advanced Materials*, 26,1751 (2014).

Chemistry of Materials



CNR RAO

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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. 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 characterisation, phase transformations, transition metal oxide systems, open-framework materials, nanomaterials and artificial photosynthesis.

Besides finding new methods of preparing different types of CNTs, NTs of various inorganic materials, graphene and related materials, inorganic analogues of graphene have also been synthesized by employing novel strategies. New hybrids of MOFs with graphene and BN have also been prepared and have shown improved gas adsorption and mechanical properties.

Artificial photosynthesis is considered to be a promising direction to solve the challenge of energy crisis. Inexpensive oxides of Co and Mn for O_2 evolution and MoS_2 , $MoSe_2$ and heterostructures of CdS for H_2 evolution have been identified as efficient catalysts.

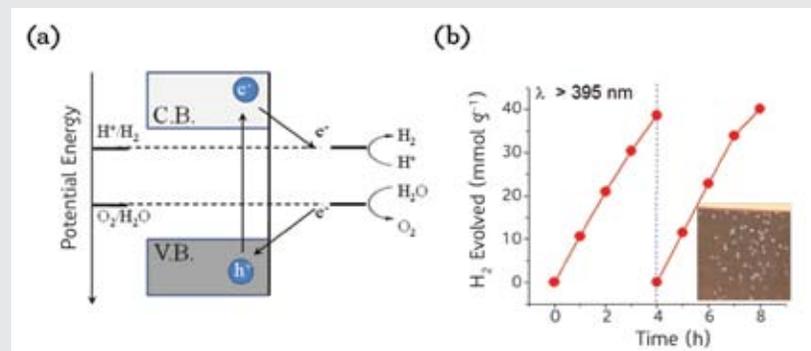


Fig.: (a) Schematic representation and (b) Hydrogen evolution with time

KEY PUBLICATIONS

Urmimala Maitra, et al., *Angewandte Chemie International Edition*, 52:49, 13057–13061 (2013).

SR Lingampalli, et al., *Energy Environmental Science*, 6, 3589–3594 (2013).

Novel Low-Dimensional Properties of GaN Thin Films



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In our Group, we address the issues related to the group III-nitride semiconductor systems. We attempt to form novel nanostructured materials that can lead to enhanced performance of devices that employ them. We have formed self-assembled nanostructures of GaN and InN thin films by Molecular Beam Epitaxy and measured their various optical, structural and electronic properties.

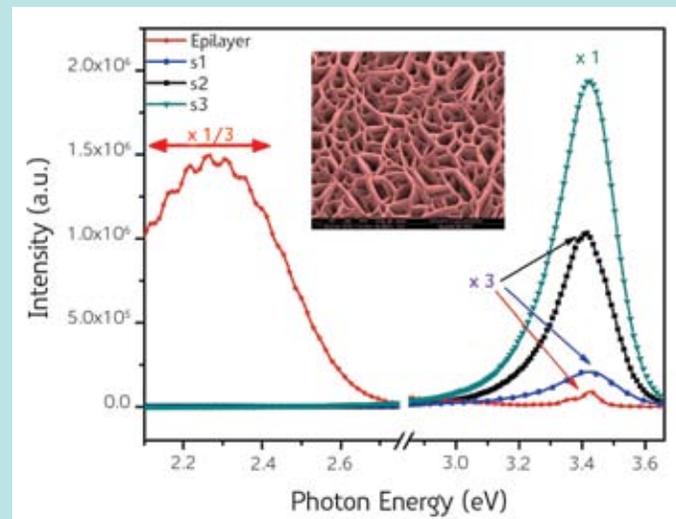


Fig.: Photoluminescence spectra of GaN thin films with different nano-morphologies, showing defect free and enhanced emission in the nanowall-network form.

In the process, we have discovered a novel self-assembled GaN nanowall network, which shows novel exciting properties that shows promise for several applications. In this configuration, GaN is defect-free and shows orders of magnitude enhanced photoluminescence, which can lead to high brightness LEDs and lasers. We have also observed directed band edge emission via aligned UV-pencils of about 100 nm diameter. The material yields unprecedentedly high mobility of electrons which we speculate is due to 2D electron confinement in these walls. We also observe ferromagnetism at the tip of these walls, making it a potential material for spintronics. We also see this morphology of GaN to be useful for enhanced bio-sensing by Surface Enhanced Raman Spectroscopy. Our endeavour now is to utilize these observations and demonstrate their utility for high performance devices and for novel applications.

Magnetism, Superconductivity and Multiferroicity



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The main focus of our research is to understand the relationship between structure and properties of materials. This involves both fundamental and applied aspects of chemistry and physics of solid state, and a spectrum of materials including superconductors, multiferroics and magnetic materials. The important finding of our Group and our collaborators, is the discovery of universal ferromagnetism in nano particles of otherwise nonmagnetic inorganic materials.

SURFACE FERROMAGNETISM

The nonmagnetic oxides such as CeO_2 , Al_2O_3 , ZnO , and MgO become ferromagnets at room temperature when they are made at the nanoscale. The unexpected ferromagnetism has been shown to be confined only to the surface of the nano particles and its origin was attributed to anion and/or cation vacancies at the surface. Based on this work, the ferromagnetism of nanoparticles was suggested to be an universal feature not only of oxides but also of nitrides and chalcogenides. With its origin at the surface of nanoparticles, it has been demonstrated that such ferromagnetism could coexist with other functional properties such as ferroelectricity and superconductivity at the core of the particles.

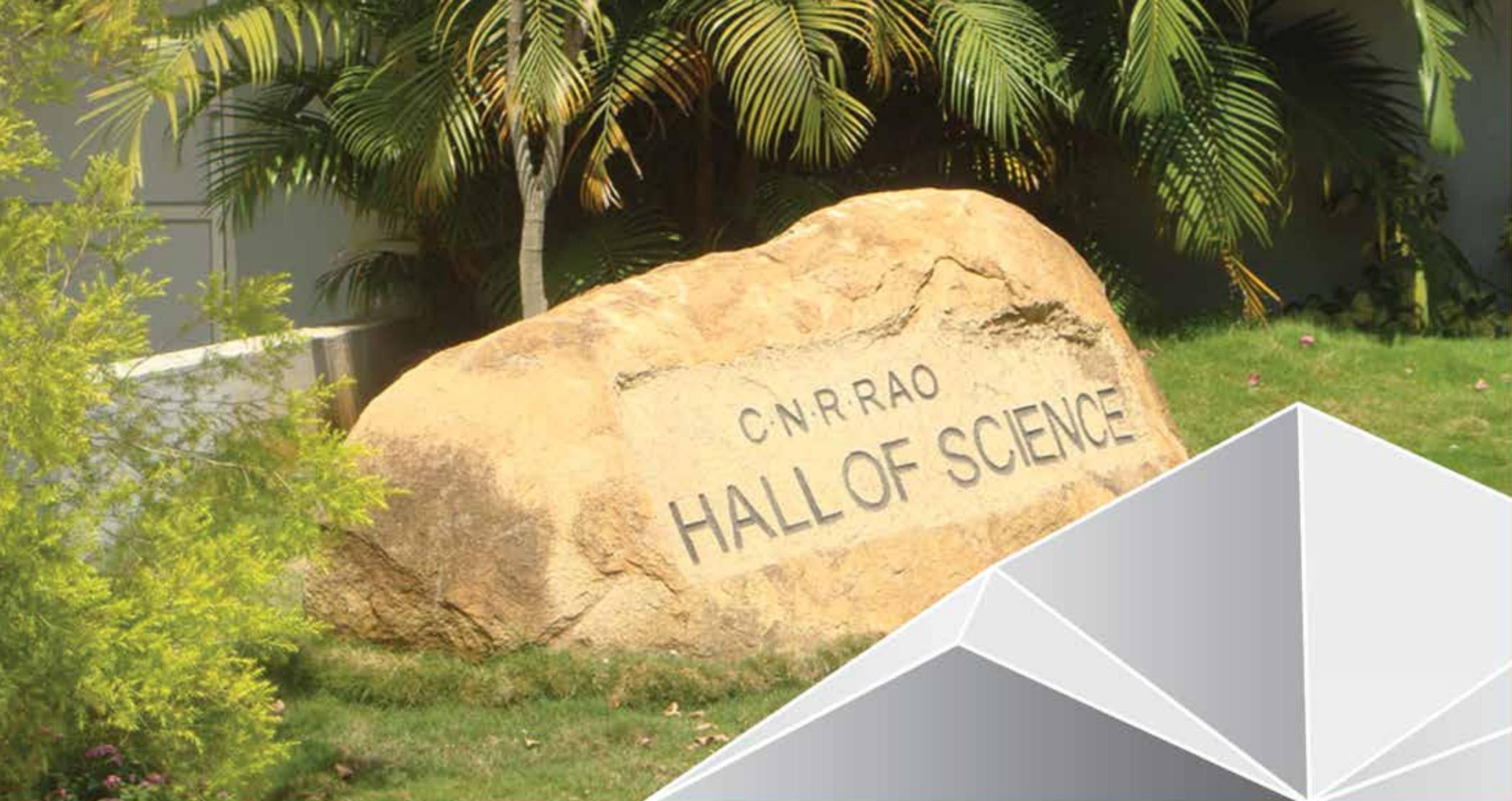
MULTIFERROICITY

Multiferroics are materials that exhibit magnetism and ferroelectricity simultaneously in the same phase. Magnetoelectric multiferroics are an interesting class of materials because of the coupling of the two order parameters that leads to new device application through the control of magnetism by an applied electric field, and control of electric polarisation by an applied magnetic field. Our focus is to explore new multiferroic materials where the ferroelectricity is induced by magnetism.

KEY PUBLICATION

Sundaresan A, et al., *Physical Review B*, 74, 161306 R (2006).





C.N.R. RAO
HALL OF SCIENCE

EDUCATION TECHNOLOGY UNIT

MEMBERS

V Krishnan, Honorary Professor & Chair

Indumati Rao, Coordinator (Honorary)

Jatinder Kaur, Sr Technical Officer

Sanjay SR Rao, Assistant (Multimedia)

The CNR Rao Hall of Science was established to have a dedicated venue for direct contact programs to popularise Science among students and to enhance the skills of science teachers.

Education Technology Unit was established in 1996. The focus of the Unit is to develop learning and teaching materials. It has developed and produced multimedia CD-ROMs in various science subjects in different languages. The Unit has undertaken translation, designing and formatting print-ready copies of books which it has published in collaboration with different publishing houses for use by teachers and students to improve science education in schools/colleges. In addition the Unit is actively involved in science popularisation 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-ROMs and books developed and produced at ETU are:

- **UNDERSTANDING CHEMISTRY** by Prof CNR Rao (Also available in Kannada and Hindi) (Book & CD-ROM).
- **LEARNING SCIENCE** by Prof CNR Rao and Mrs. Indumati Rao (2 CD-ROMs and 4 Books)
- **VIGNYANA KALIYONA** (4 CD-ROMs and books in Kannada)
- **VIGYAN SEEKHE** (4 books in Hindi)
- **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) (Book and CD-ROM)
- **CHEMISTRY TODAY** (Books in English, Hindi and Kannada)
- **RASAYAN VIGYAN KI DUNIYA** (Book in Hindi)
- **NANOPRAPANCHA** (Book in Kannada)

The CNR Rao Hall of Science was inaugurated by the Hon. Prime Minister Dr Manmohan Singh on December 3, 2008. It was established to have



a dedicated venue for direct contact programs to popularise Science among students and to enhance the skills of science teachers. ETU is located at the CNR Rao Hall of Science and is engaged in organizing/participating in the various activities of the CNR Rao Hall of Science. CNR Rao Hall of Science and Education Technology Unit have organized and conducted Teacher-student programs/workshops as part of the Science Outreach program. These programs have been conducted in Physics, Chemistry, Biology at the Madan Mohan Malaviya Amphitheatre, CNR Rao Hall of Science regularly from

the time of its inception. In all the above programs faculty from different institutes are invited to give lectures on a particular theme in the concerned subject and participate in an interactive question and answer session at the end of the program. Students and teachers from various schools and colleges in and around Bangalore, Bangalore Rural, Jawahar Navodaya Vidyalayas (Southern Region) and from different parts of Karnataka have attended these programs. In each of the above programs at least 200 - 225 students and teachers have participated.

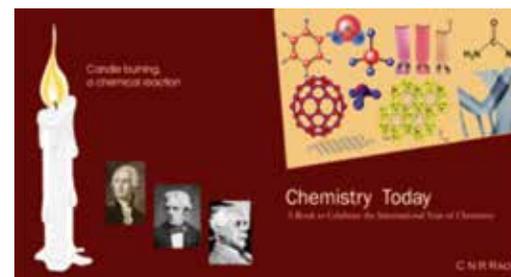
A few highlights of the Unit's activities are as given below:

ETU completed a project for Vision Group on Science and Technology, DST, Govt. of Karnataka in June 2010 of supplying 7500 multimedia CD-ROM titles (each containing six Kannada CD-ROM titles developed and produced by ETU) and 1500 Nanoworld books and CD-ROMs for distribution to schools/colleges in the state.

ETU designed the cover for the book titled 'Climbing the limitless ladder - A life in Chemistry' authored by Prof CNR Rao and was published by World Scientific. The book was launched by Shri Kapil Sibal, Hon. minister for Human Resource Development at New Delhi on July 16, 2010.

ETU designed and produced a print-ready copy of a book titled 'India as a global leader in science' for the Science Advisory Council to the Prime Minister. 5000 copies were printed. The book was released by the Hon. Prime Minister.

To commemorate the International Year of Chemistry (IYC-2011), ETU designed, formatted and produced the book titled 'Chemistry Today' authored by Prof CNR Rao. This was released at a function on January 1, 2011 by Prof CNR Rao at the JN Tata Auditorium. The book was distributed to all the participants. ETU organized and conducted several IYC-2011 programs in Chemistry for students and teachers. The book 'Chemistry Today' was translated into Hindi and Kannada and Print-ready copies were made available by ETU. These books were distributed in Schools/colleges.



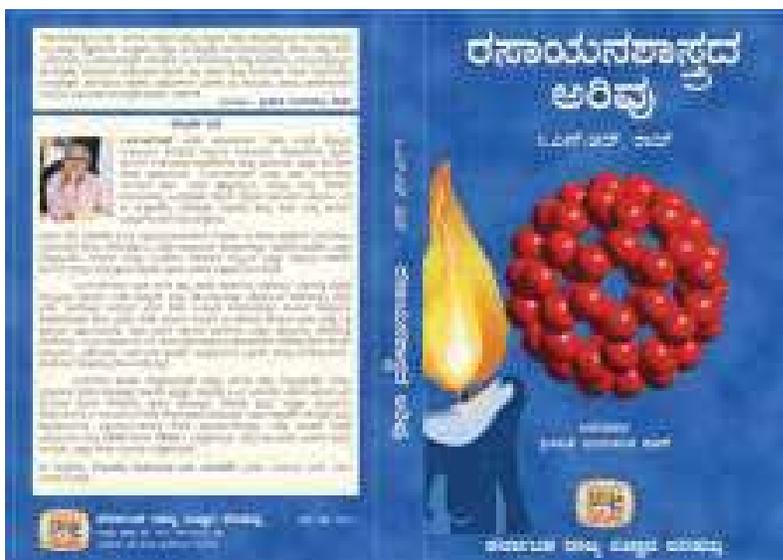
ETU completed the translation and produced the print-ready copies of the book 'Nanoprancha' in Kannada for NavaKarnataka Publications Ltd.



The book 'Mithiyillada Eani, Rasayanashastradalli Jeevana' (Kannada version of the autobiography 'Climbing the Limitless Ladder' written by Prof CNR Rao) was edited by Mrs. Indumati Rao for Karnataka Rajya Vijnana Parishath which published the book.



The CNR Rao Hall of Science & Education Technology Unit along with SOP-ETU took up a project sponsored by the Vision Group on Science & Technology, DST, Govt. of Karnataka of conducting four Workshops for 100 Pre-University Teachers from different places in Karnataka in using the College Chemistry Kit. The entire kit consists of 32 plastic/glass laboratory items, 85 solid and liquid chemicals for carrying out chemistry experiments. ETU undertook assembling of the Kits. Four workshops were conducted in batches of 25 teachers by SOP-ETU in April 2011. At the end of each workshop each teacher was presented with two Kits to take back to their colleges.

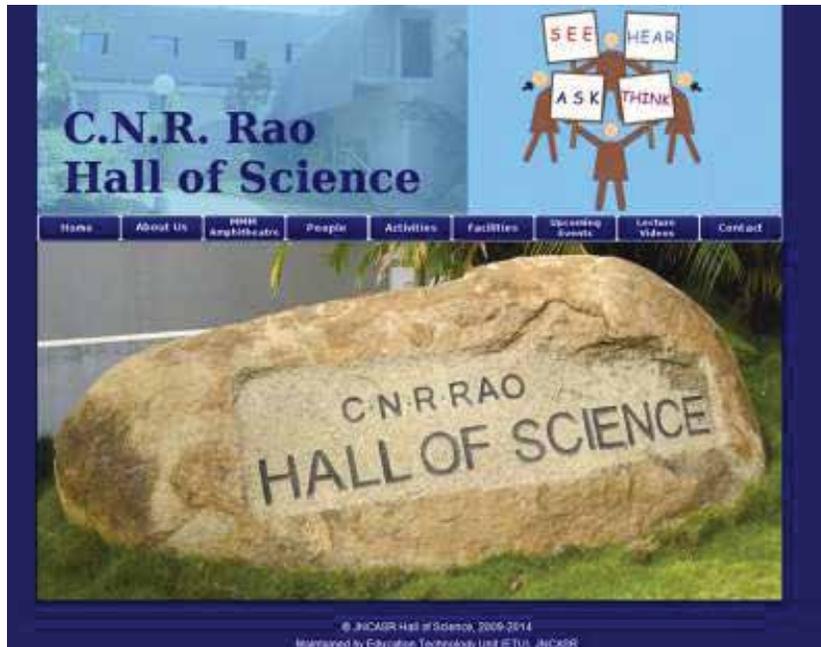


The Book 'Rasaayanshastrada Arivu' authored by Prof CNR Rao was translated by Mrs. Indumati Rao, made print-ready at ETU for Karnataka Rajya Vijnana Parishath (KRVP). To commemorate International Year of Chemistry-2011, the book was released at a function organised to commemorate the International Year of Chemistry on March 12, 2012.

ETU has collated and produced a document titled 'Science Outreach' listing all the Science Popularisation Programs organized by ETU under the joint auspices of JNCASR and various institutions across different parts of the country. These Programs for students and teachers were conducted by Prof CNR Rao and Mrs. Indumati Rao.

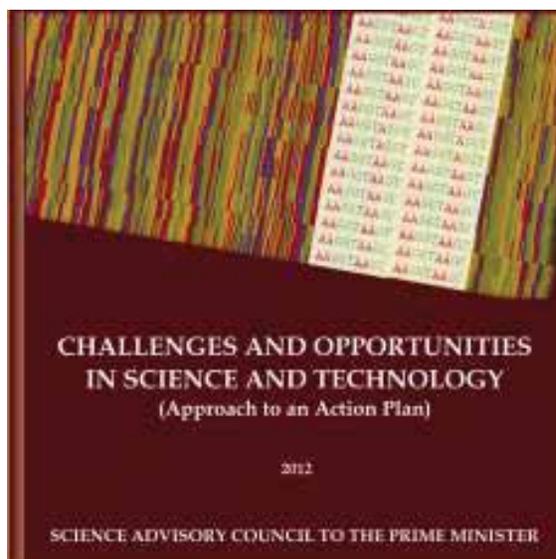
ETU has brought out a document 'Programs of the CNR Rao Hall of Science' on all the teacher-student programs/workshops organized by the CNR Rao Hall of Science and ETU as part of the Science Outreach Program. The compilation lists the Lecture Programs that have been conducted at the Madan Mohan Malaviya Amphitheatre, CNR Rao Hall of Science since its inception in 2009. The report also lists the Science Outreach Programs for students and teachers conducted annually in Uttarakhand.

ETU created a logo for the Hall of Science and a special poster for use in the Hall of Science Programs. These were made print-ready for poster printing.

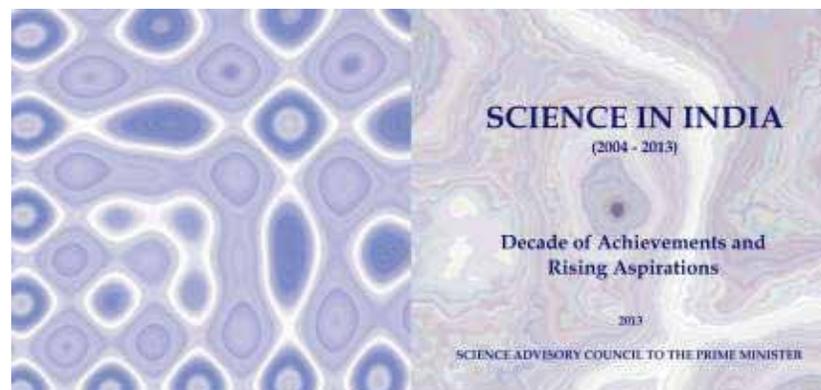


A Webpage for the Hall of Science was a project taken up jointly by ETU & CompLab. ETU designed the layout and the features of the Webpage. The preparation of the content material (both text and graphics) in the formats as required was completed for the CompLab by ETU.

The features of the Webpage are designed to be user-friendly and give information about the CNR Rao Hall of Science, people associated with it, its activities, facilities and information about upcoming programs. It has a special feature called 'Lecture Videos' where videos of the various lecture programs conducted at the Hall of Science are posted. These lecture videos are available in both High and Low Resolution formats to enable viewers to view these lectures at their convenience. The webpage also provides information about the activities of ETU-SOP-POCE.

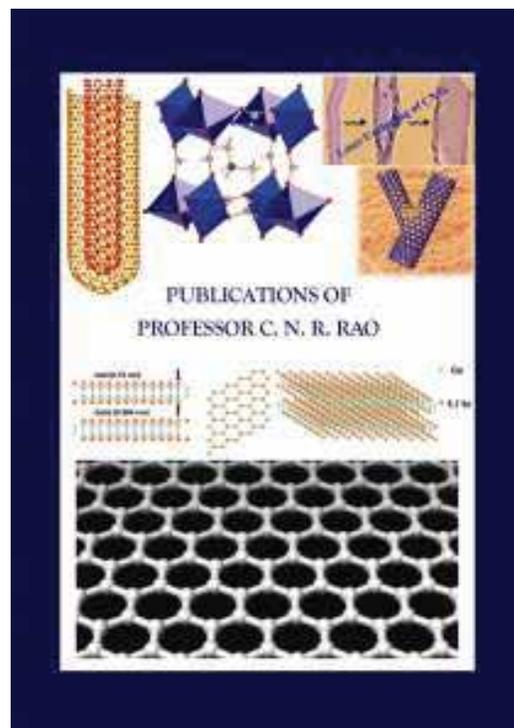
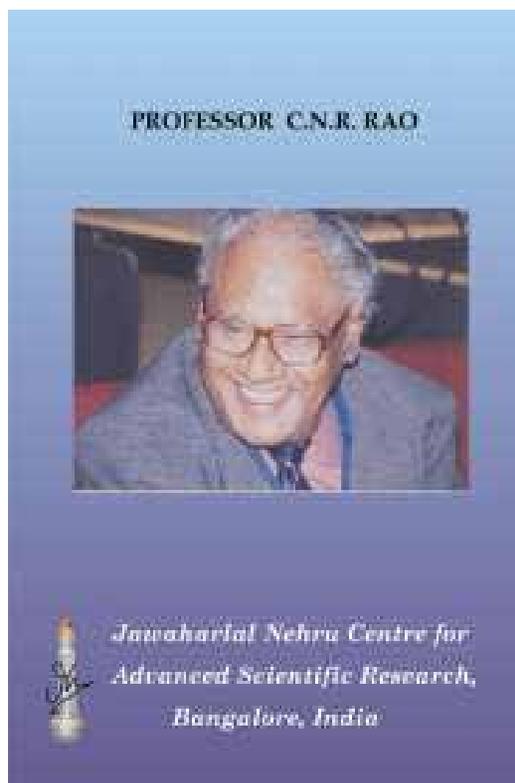


ETU designed and produced a print-ready copy of a book titled "Challenges and Opportunities in Science and Technology (Approach to an Action Plan)" for the Science Advisory Council to the Prime Minister. 10,000 copies were printed.



ETU was assigned the task of producing the print-ready copy of the book titled 'Science in India'. It consists of three parts starting with a Vision document followed by a brief presentation of the accomplishments and recommendations of the Science Advisory Council to the Prime Minister during 2004-2013. Part 3 deals with the challenges and opportunities in science and technology along with an approach to an action plan. A print-ready copy of the book was designed and produced by ETU. The book was released in New Delhi by the Hon. Prime Minister on July 8, 2013. 2150 copies were printed. A soft copy of the same was sent to SAC-PM office for uploading it on the DST Webpage and the PMO Webpage.

The cover designs for the books titled "Readings in Solid-state and Materials Chemistry (A selection of research papers of CNR Rao)" and Chemistry of Nanomaterials' Selected papers of CNR Rao were designed and print-ready copies were sent to M/s World Scientific who published the books.



The book 'Professor CNR Rao' (a short biography) was redesigned and a print-ready copy was made ready by ETU. 1000 copies of the book were provided to the 'Directions in Materials Science (DMS)' Conference for distribution to the participants. The book 'Publications of Prof CNR Rao' was designed, formatted and print-ready copy was completed at ETU. 200 copies were provided to the DMS conference.



In the area of science popularisation, 'Nanoworld', 'Learning Science' 'Celebration of Chemistry' and 'Vignyana Kaliyona' (a science popularisation program in Kannada for the benefit of Kannada medium school children) programs were conducted at different places in the country.



The Summer Science Outreach Program sponsored by the CNR Rao Hall of Science, JNCASR is conducted in association with Himalyan Gram Vikas Samiti, Gangolihat by Prof KS Valdiya, Prof CNR Rao and Mrs. Indumati Rao and several Faculty members of JNCASR actively participate in these programs.



The CNR Rao Hall of Science and Education Technology Unit conducted 10 lecture programs for students and teachers during 2013. In addition to the planned programs, a program for INSPIRE students and a four-day Science Orientation Workshop for Jawahar Navodaya Vidyalaya students were conducted at the MMM Amphitheatre, CNR Rao Hall of Science. These students and teachers were from different JNV's of Karnataka. 72 students and 8 teachers participated in the four-day workshop conducted on October 22-25, 2013.

The Karnataka State Council for Science and Technology, IISc, Bangalore, Royal Society of Chemistry, London and the CNR Rao Hall of Science & ETU, JNCASR jointly organized and hosted the Knowledge Exchange Workshop – Chemistry on October 3-5, 2013. Prof MRS Rao inaugurated the workshop. Chemistry teachers from various high schools from Bangalore and North Karnataka participated in the three-day workshop.

All the above programs were conducted at the Madan Mohan Malaviya Amphitheater, CNR Rao Hall of Science, JNCASR.

A program for students of Classes XI and XII was organized by IIT/Indore on 31st January 2014 at the Daly College Auditorium, Indore as part of the 'Frontier Lecture Series in Chemistry'. Prof CNR Rao gave the lecture titled 'Chemistry: Glorious Past and Exciting Future' and Mrs. Indumati Rao presented excerpts from the CD-ROM 'Nanoworld'. Around 1200 students and teachers attended the program. On February 15, 2014 Prof Rao gave the lecture 'Intuition & Inspiration – Story of Science' to students and teachers at the Basaveshwar Science College, Bagalkot and Mrs. Indumati Rao presented excerpts from the CD-ROM 'Nanoworld' for 30 minutes.

The Summer 2014 Science Outreach Program sponsored by the CNR Rao Hall of Science, JNCASR was conducted in association with Himalayan Gram Vikas Samiti, Gangolihat by Prof KS Valdiya during April 19-25, 2014. The CNR Rao Hall of Science and ETU presented a 30 minute multimedia presentation in Hindi. Mrs. Indumati Rao presented excerpts from the CD-ROM title "Understanding Chemistry" in Hindi. ETU also prepared a PowerPoint presentation 'Rasayan Vigyan Manana' with both Hindi and English subtitles for Prof CNR Rao's lecture to students and teachers. Prof Rao gave the lecture titled 'Nanoworld'.

The CNR Rao Hall of Science and ETU commenced the teachers-students programs/workshops conducted under the auspices of the Science Outreach program for this year on June 30, 2014. The Science Teachers Award Function cum lecture program was organized and conducted at the Madan Mohan Malaviya Amphitheatre. The recipients of the CNR Rao Education Foundation sponsored prizes for Outstanding Science Teachers for 2013 were Shri Narayan Vitthalrao Babanagar and Dr Shripal Rathi. The Lecture Program had one lecture in Chemistry and one in Biology. Around 230 students and teachers attended the program. ETU and the CNR Rao Hall of Science organized and conducted the 'Program in Physics for students' on July 17, 2014, a 'Program in Biology for students' on August 22, 2014.

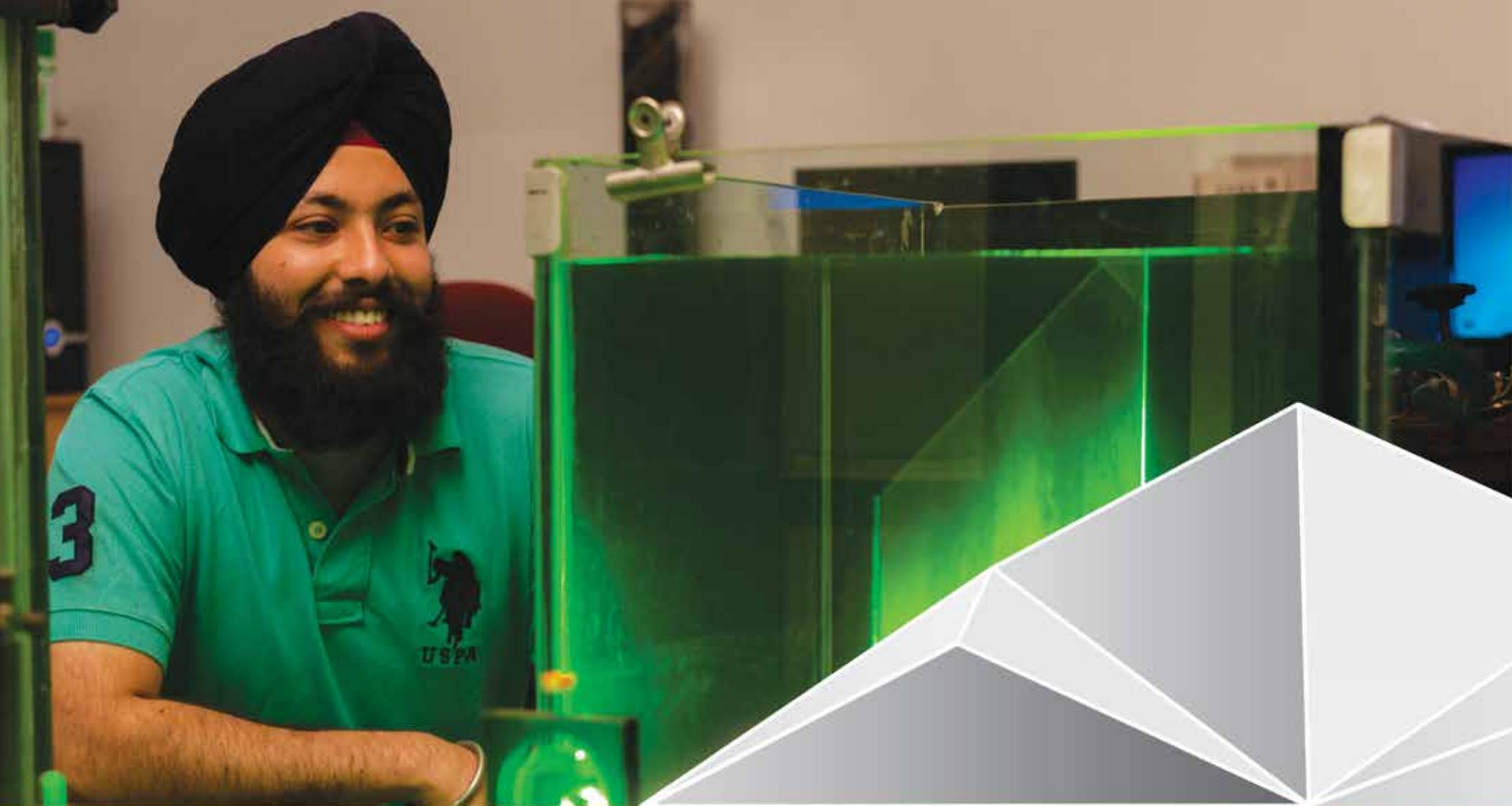
Students doing the PGDSE course took up the multimedia course. The students had to complete and submit a multimedia presentation in their chosen subject (Physics, Chemistry and Biology). They were introduced to the basics in Multimedia and were then assigned the task of selecting a theme/topic of their choice for developing into a multimedia presentation. Accordingly, the students were guided into preparing the script, creating or sourcing graphics/visuals, making videos and doing the voice-over for a 30-40 minute lecture presentation. This year the students submitted their presentations in Physics.

SOP-POCE has conducted Eleven Workshops on 'Experiments using College Chemistry Kit' between July 2013 – January 2014 for the Science Pre-university students and teachers from different colleges of Karnataka. 256 students and 16 teachers participated in these workshops.

The CNR Rao Hall of Science and Education Technology Unit will be organizing teachers/students workshops/programs in different subjects like Physics, Chemistry, Biology and Nanoscience as part of the Science Outreach program. It is proposed to have lectures and demonstrations with different themes in a particular subject.







ENGINEERING MECHANICS UNIT

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**HONORARY PROFESSOR/
DST YEAR-OF-SCIENCE PROFESSOR**

Roddam Narasimha, FRS, FNASc, FNA, FASc, FNAE, FTWAS

The Engineering Mechanics Unit pursues research on a variety of topics where fluid flow and heat transfer play a critical role in providing insight into various physical phenomena.

Research done in the Unit has both fundamental relevance, in terms of attempting to explain the underlying basis of natural phenomena, and in addition, is relevant to several technological applications.

Research endeavors currently underway concern the study of both complex microstructured fluids (suspensions and emulsions, granular gases, polymer solutions/melts, active matter) and complex flows (turbulence, non-linear development of hydrodynamic instabilities, pattern formation), spanning an enormous range of length scales from the microscopic to the geological/astrophysical, via a combination of experiments, large-scale computation and theoretical analyses.

Research on rapid granular flows has helped in understanding the origin of shear-banding instabilities, and shown that vorticity banding can appear both as first and second-order transitions. Recent research on emulsions and suspension of anisotropic particles has highlighted the crucial role of micro-scale inertia on the dynamics and rheology of these materials. Analytical theory and large-scale simulations of a suspension of microscopic swimmers, an experimental realisation of active matter, have aided in understanding the nature of fluctuations in these non-equilibrium systems. While the role of polymers in essentially modifying turbulence is well known (turbulent drag reduction), recent experiments with dilute polymer solutions have identified the ability of polymer molecules, at small concentrations, to even stabilize inflectional laminar flows.

Research activities relevant to geophysical processes include modelling mantle convection, cloud dynamics, the dynamics and stability of large-scale vortical structures, and the thermal structure of the nocturnal boundary layer. The unusual entrainment characteristics of cumulus clouds have been explored via a combination of experiments and direct numerical simulations. The study of the nocturnal boundary layer has helped in both identifying a crucial error in radiation-codes used routinely for atmospheric calculations, and in solving an 80 year old micro-meteorological mystery – the origin of the Ramdas layer. Experiments have conclusively demonstrated the importance of aerosol-induced radiative forcing in shaping the near-surface nocturnal temperature profiles, and their importance in the energy budget of the nocturnal boundary layer. Ongoing efforts are attempting to develop a mathematical model as well as the instrumentation towards predicting radiation fog. Recent analytical research has shed light on the 'missing modes' that govern the interaction of large-scale vortices with ambient turbulence, thereby completing the solution to a classical problem first studied, more than a century ago, by Lord Kelvin. The research has been extended to analyze the general role of so-called continuous spectrum in hydrodynamic stability.

The aerodynamics of insect flight is currently being investigated via a combination of experiments and computations. This has led to the identification of a new mechanism of lift generation and its enhancement by controlled wing flexibility, a finding of relevance to the design of micro air vehicles.

The expected arrival of Exascale computing will enable the execution of advanced simulation algorithms for Computational Fluid Dynamics (CFD), thereby providing new insight into complex phenomena such as turbulence. The primary challenge in utilizing this potential of emerging computing systems is the successful handling of intensive floating point computations coupled with increased data movement operations on systems consisting of millions of lightweight processing cores. Thus, direct numerical simulation of fluid dynamics for engineering applications requires highly efficient and accurate methods for CFD. In this regards, a new class of CFD algorithms, rooted in kinetic theory (the Boltzmann equation) has been developed which enable simulations of complex flow problems with reasonable computing requirements.

Fluid Mechanics and Heat Transfer



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Our Group is working on research problems in the areas of unsteady aerodynamics of insect flight, modelling radiation-fog, polymer drag reduction, entrainment and mixing in cloud-like flows, development of a high-efficiency heat exchanger, and heat transfer and sustainable use of water in greenhouses.

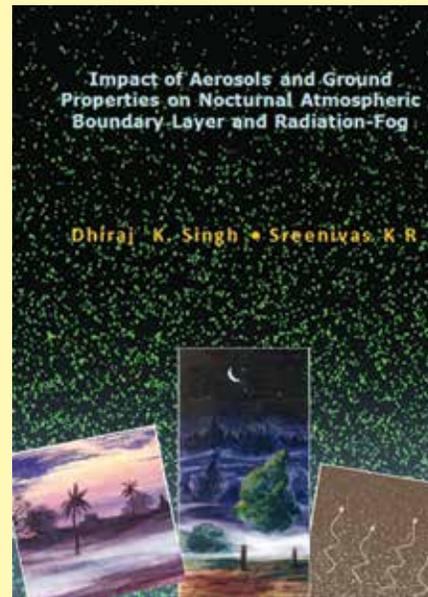


Fig.: Monograph on the study of Nocturnal Boundary Layer and Radiation-Fog

Results from the study on nocturnal boundary layer are being published as a monograph – Impact of Aerosols and Ground Properties on Nocturnal Boundary Layer and Radiation-Fog.

KEY PUBLICATIONS

V Mukund, et al., Quarterly Journal of the Royal Meteorological Society, 140(678), 151-169 (2014).

SS Diwan, et al., Bulletin of the American Meteorological Society (2014).

Mechanics of Granular Matter and Nonlinear Dynamics



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Post-Doc: University of Stuttgart,
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California, San Diego, USA

Granular/particulate matter can exist in gaseous or liquid or jammed states depending on external forcing. I am interested in the application of the basic principles of mechanics and physics to understand the dynamics of granular matter, suspensions and related non-Newtonian fluids. Bulk of my work is theoretical and computational in nature, with a focus to come out with better mathematical models using ideas from statistical mechanics, kinetic theory, nonlinear dynamics and asymptotic methods. Recently I have set up a laboratory where my students carry out table-top experiments on granular matter and multiphase flows.

CURRENT RESEARCH TOPICS

1. Kinetic theory and non-Newtonian rheology of granular matter. Jamming and isostaticity.
2. Nonlinear stability, bifurcation theory and patterns: Ginzburg-Landau formalism.
3. Buoyancy-induced flows and mixing: experiments with PIV and PLIF.

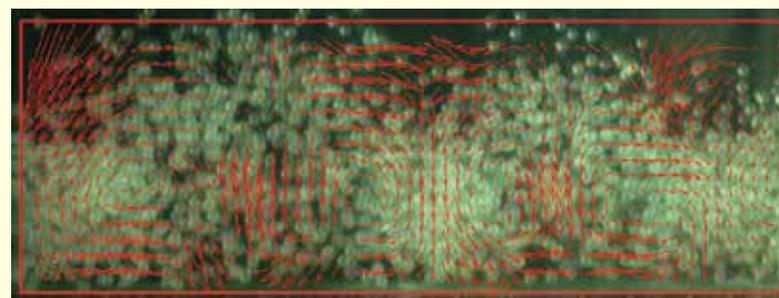


Fig.: Convection rolls in a vibrated granular matter – analogue of classical Rayleigh-Benard convection

KEY PUBLICATIONS

R Rongali and M Alam. Physical Review E, Vol. 89, 062201 (2014).

M Alam and P Shukla. Journal of Fluid Mechanics, Vol. 716, 349-413 (2013).

Computational Physics



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Post-Doc: ETH Zürich, Switzerland

My Group works on development and application of new algorithms which are based on blending of three key ideas: 1) Conservation laws and entropy inequalities should be preserved at discrete level too, 2) Physical symmetries and isotropy should be respected as much as possible by discrete models, and 3) Discrete models should preserve memory locality as much as possible. The hope is that numerical schemes, which respect structures and symmetries of original equations, tend to be more efficient than usual schemes. In order to develop such models, we often use the notion of quasi-equilibrium and separation of time scales – ideas developed in context of kinetic theory of gases.

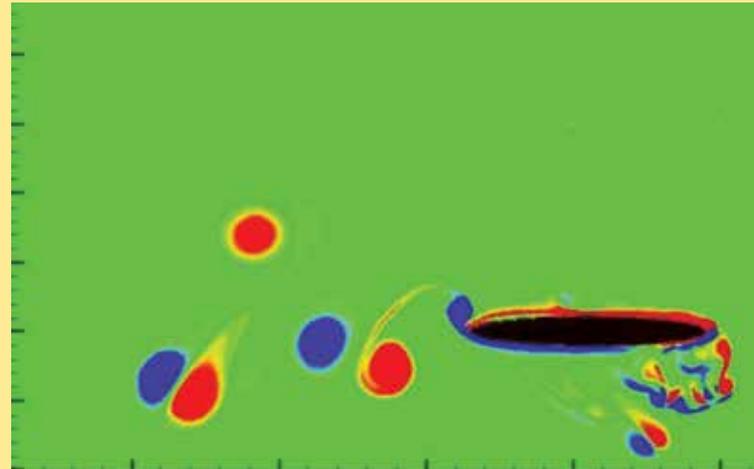


Fig.: Vorticity contours computed close to an elliptical cylinder flapping at $Re = 1000$

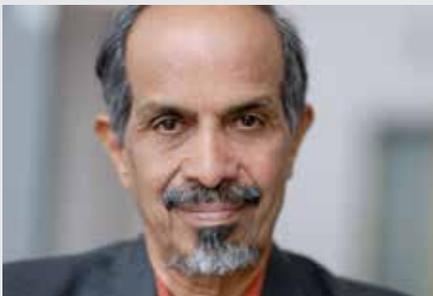
The other important part of my research theme is to apply these algorithms to practical problems. In this context, we have recently performed large-scale direct numerical simulation to get better understanding of the time dynamics in context of turbulence and extract new scaling laws.

KEY PUBLICATIONS

AG Shet, et al., *Physical Review E*, 88, 013314 (2013).

T Chakradhar, et al., *Journal of Fluid Mechanics (Fast Track, Rapid)*, 728, R4 (2013).

Aerospace and Atmospheric Fluid Mechanics



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Post-Doc: California Institute of Technology, California, USA

The dynamics of turbulent flows has an interesting link with the statistical mechanics of a vortex gas, which is a Hamiltonian system of parallel line vortices in an inviscid fluid. From the most extensive numerical simulations to date of a temporal free-shear layer, it is found that (i) the bulk parameters of the vortex-gas solutions (mixing excluded) are close to experimental observations in plane mixing layers, and (ii) classical fluid dynamics represents an 'explosive' phase of an otherwise slow relaxation to equilibrium in the vortex gas, exhibiting in this phase a universality in the growth rate of the shear layer independently of widely-varying initial conditions.

1. An alternative approach to a free-shear layer is via the evolution of a plane continuous vortex sheet, which is known to encounter a finite-time singularity during evolution. Taking the solution past the singularity invoking a viscosity 'switch' shows that such singularities keep appearing and disappearing over time in different parts of the flow region.
2. Considerable progress has also been recently made in DNS studies of the complex flow past a gas turbine blade, involving transition, relaminarisation, separation bubbles and retransition, and of cumulus cloud flows.

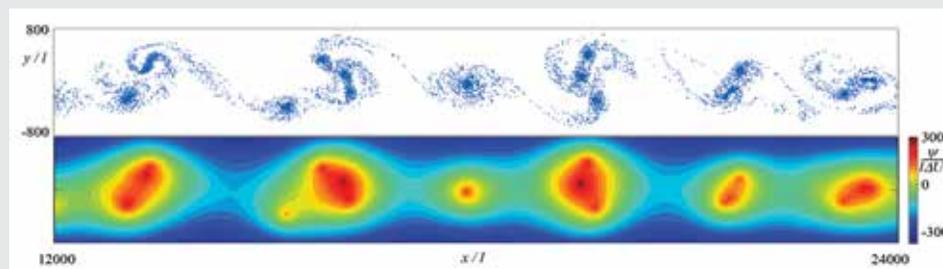


Fig.: Vortex-gas solution, temporal turbulent free shear layer; vortex positions and stream function

KEY PUBLICATIONS

S Suryanarayanan, et al., *Physical Review E*, 89 (2014).

U Paul and R Narasimha, *Physica Scripta*, T155 (2013).

Complex Fluids and Flows



GANESH SUBRAMANIAN

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Our research endeavours span a range of phenomena in complex fluids, hydrodynamic stability and the atmospheric (nocturnal) boundary layer. Topics of interest include active and passive suspension rheology, the role of inertia and viscoelasticity in micro-scale transport phenomena, and the significance of the continuous spectrum in vortical flows. We use a combination of analytical theory and numerical simulations to attack the problem of interest.

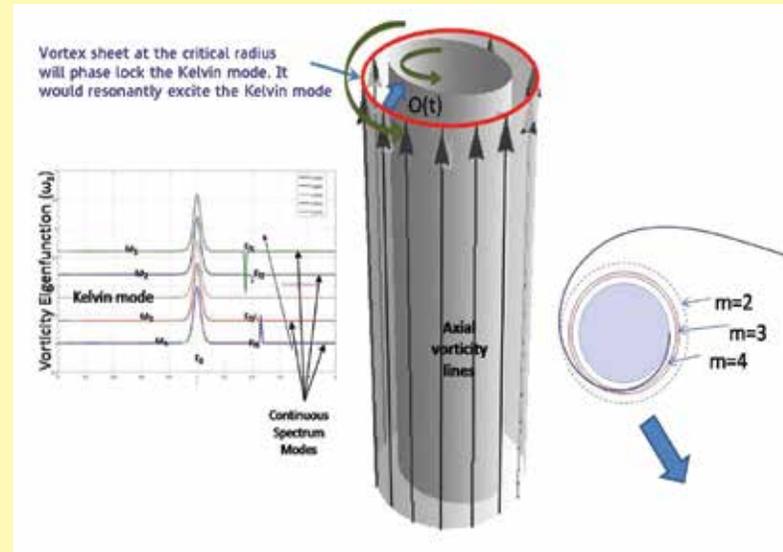


Fig.: Vortex Column Resonance

To quote two instances:

1. We have found a novel instability in a bacterial suspension that may play a key role in determining the level of velocity fluctuations in such non-equilibrium systems;
2. Our research has shown a profound asymmetry between the orientation dynamics of rod-shaped and disk-shaped particles in shearing flows.

KEY PUBLICATIONS

G Subramanian, et al., *Current Science*, 98(8), 1103-1108 (2010).

Roy A and Subramanian G, *Journal of Fluid Mechanics*, 741, 404-460 (2014).







EVOLUTIONARY AND ORGANISMAL BIOLOGY UNIT

PROFESSOR AND CHAIR

Vijay Kumar Sharma, FASc, FNA

PROFESSOR

Amitabh Joshi, FASc, FNAsc, FNA

FACULTY FELLOW

TNC Vidya

ASSOCIATE FACULTY

Sheeba Vasu

Our Unit is one of the principal centres in the country for research and training in chronobiology, evolutionary genetics, population ecology, behavioural neurobiology, behavioural ecology and phylogeography.

Biological systems are organised in a 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 at 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 are, consequently, best posed in the context of an organism embedded in its ecology.

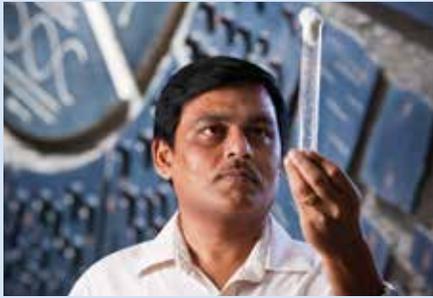
In Organismal Biology, the organism is the entity around which (a) questions regarding functionality in biological systems are framed, and (b) information gleaned from studies at various

structural levels of biological complexity is welded together in an attempt to answer such questions. Actually, 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 one of the principal centres in the country for research and training in chronobiology, evolutionary genetics, population ecology, behavioural neurobiology, behavioural ecology and phylogeography. We do mostly empirical research, both in the lab and in the field, 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 labs for routine handling of large numbers of *Drosophila* populations, labs for experiments in physiology, biochemistry, molecular biology, genomics 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 3,500 channels, our activity recording system for insects and small mammals is the largest such facility in the world. The Unit also maintains a field station in HD Kote Taluk, Karnataka, for facilitating research in wildlife biology.

Circadian Rhythms in Fruit Flies and Ants



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Post-Doc: IISc, Bangalore;
NTNU, Trondheim, Norway;
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We are interested in both experimental and theoretical aspects of circadian (daily) rhythms. We ask questions regarding: (i) association between clock precision, phase, and period, (ii) adaptive significance of circadian clocks in fruit flies (*Drosophila melanogaster*), (iii) evolution of morning and evening chronotypes, and evolution of clock precision in *D. melanogaster*, (iv) role of circadian clocks in regulating life history traits in fruit flies and ants, (v) circadian consequences of social interactions in fruit flies and ants, (vi) role of the olfactory receptor neurons *Or47b* in socio-sexual interactions in *D. melanogaster*, (vii) cradle effect in sleep: role of mechanosensory receptors in promoting sleep in *D. melanogaster*, (viii) neurogenetics of egg-laying rhythm in *D. melanogaster*, (ix) study of circadian rhythms in nature, and (x) role of temperature in mediating circadian phenotypes in *D. melanogaster*.

Our work has led to major new results and ideas in several areas of adaptive evolution, chronobiology, sociobiology and neurogenetics. Our studies have demonstrated that: (i) clock properties such as precision, phase, and period are correlated, (ii) circadian clocks provide adaptive value to organisms, (iii) circadian clocks can evolve in the lab, (iv) circadian clocks time pre-adult developmental stages, (v) social interactions result in short and long term changes in circadian clocks, (vi) *Or47b* mediate male-dependent nocturnal sex drive and mating efficiency, (vii) cooler temperatures promote strong-type phase response behaviour, (viii) genetic architecture mediating morning and evening emergence in the *early* and *late* populations of *D. melanogaster* is primarily autosomal, and both additive and non-additive genetic interactions contribute to chronotype divergence, and (ix) temperature plays a major role in enhancing chronotype divergence in the *early* and *late* populations of *D. melanogaster*.

KEY PUBLICATIONS

KM Vaze, et al., *Heredity*, 111, 265-274 (2013).
J De, et al., *Proceedings of National Academy of Sciences, USA*, 110, 8984-8999 (2013).

Evolutionary Genetics, Life-History Evolution and Population Dynamics



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My principal interest is in trying to better appreciate and understand adaptive evolution as a dynamic process in which the interaction of the ecology and genetics of a population shapes its evolution. I am also interested in understanding the dynamics of population size, especially in spatially structured populations. Most of my research is empirical and laboratory based, using fruitflies (*Drosophila* spp) as a model system. I occasionally do theory too, but my theoretical work is very strongly motivated by and grounded in empirical studies. More recently, I have been intrigued by the possibility that the existing conceptual framework we have for describing and understanding evolution might have some serious shortcomings, and that new conceptual approaches may need to be developed to overcome them. This leads to a nascent but growing interest in many philosophical issues in evolution. I also have serious interests in poetry (urdu, english, and to a more limited extent farsi, braj and punjabi), history, military science, philosophy, and many kinds of music, especially traditional qawwali.

My work on evolutionary genetics over the last decade has largely been built around selection experiments with *Drosophila*. Through selection, we have created populations with markedly reduced egg to adult development time. Comparison of the pre-adult traits evolved in these populations with those earlier seen to evolve in populations subjected to high larval crowding showed clearly that faster development and competitive ability are actually negatively correlated within populations and comprehensively changed our understanding of the relationship between rapid development and competition in *Drosophila*. We are now using these populations to try and understand the genetic control of timing of key developmental events, as well as the developmental underpinnings of evolutionarily important variation in life-history related traits, an approach we have labelled developmental evolutionary biology or devo-evo. Other selection experiments are aimed at understanding the ways in which *Drosophila* adapt to extreme larval crowding, and the effects that such adaptations may have on population stability.

KEY PUBLICATION

LD Mueller, et al., *Stability in Model Populations*, Monographs in Population Biology, 31 (2000).

Animal Behaviour and Sociogenetics



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I am primarily interested in animal behaviour and sociogenetics, but also in phylogeography. We, in my lab, work on the social organisation and behaviour of Asian elephants. We try to: a) understand the complexity of social organisation in this species, which shows a fluid, fission-fusion society, and b) find out how ecological factors and genetic relatedness between individuals influence associations, patterns of movement, and dominance relationships. Field data for this study comes from individually identified elephants that we are monitoring in Nagarahole and Bandipur National Park.

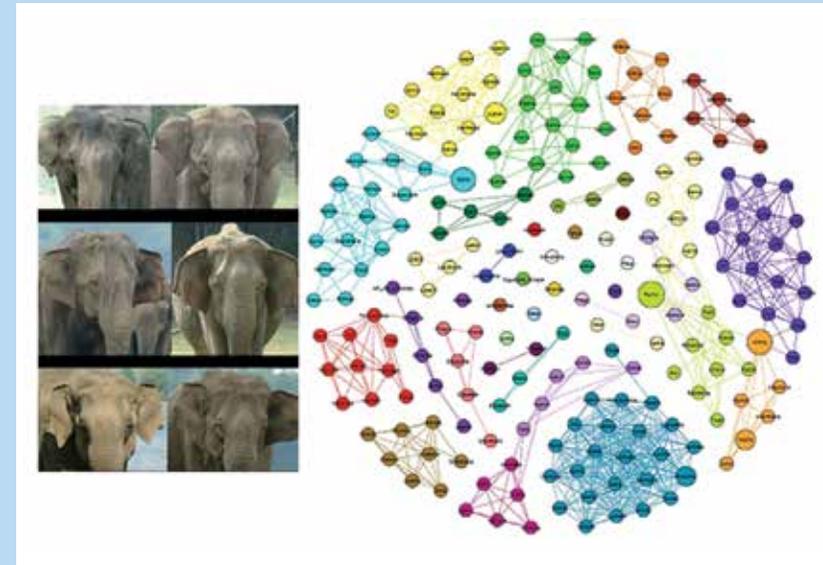


Fig.: Association network of adult female elephants (right) and some identified females (left)

We also work on communal roosting in mynas and on the comparative phylogeography of large mammals in the Western Ghats.

KEY PUBLICATIONS

S Chakraborty, et al., *Conservation Genetics*, 15, 897-907 (2014).

M Sarangi, et al., *PLOS ONE*, (2014).





GEODYNAMICS UNIT

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AND CHAIR**

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SENIOR ASSOCIATE

CP Rajendran

PRINCIPAL INVESTIGATOR

Jaishri Sanwal Bhatt

The Unit integrates data from diverse fields as seismology, geology, geochronology, geodesy and geomorphology, to gain insight into the tectonic processes of the Indian subcontinent by assessing their role in molding landscape and environment, and their earthquake hazard potential.

The paradigms that developed solid Earth sciences are essentially rooted in geodynamic concepts. The first of these is plate tectonics, the well-known suite of processes that underline the crustal evolution. The second is centered on the mantle convection – the fundamental process that governs the planet's internal workings. The third is the dynamical relationship between these deeper processes and faulting and earthquakes. The geodynamo that controls and sustains the magnetic field represents the fourth paradigm. All modern researches in solid Earth sciences are grounded essentially on these four fields. Although these paradigms explain varied Earth observations, there are many unresolved questions like the complex linkages between geodynamics, tectonics and various other processes such as the evolution of climate and life sustaining environment. India, with its tumultuous geodynamic past and varied tectonic environments, offers an excellent natural laboratory to study and understand these processes.

The Indian landmass is an amalgamation of diverse tectonic components that range in age from the Archaean (4.0–2.5 billion years) to the Recent. Its northern boundary defined by the Himalaya that resulted from continent-to-continent collision, whereas the eastern margin consisting of the Andaman arc was formed by the ongoing subduction of the Indian plate. The peninsular region, itself a mosaic of Archaean cratons was rejuvenated during the fragmentation of the Gondwana supercontinent in the Mesozoic (252–66 million years). Such an eventful past generated hotspots of relatively higher

stress concentrations and tectonically active domains. The hazards emanating from such processes have direct impact on human populations. We focus on tectonic processes of the Indian subcontinent by assessing their role in molding landscape and environment, and their earthquake hazard potential.

The advent of Global Positioning System (GPS) has revolutionized the study of plate boundary processes, but real time strain measurement covers only a fraction of one strain cycle. To address some key questions in seismology in plate boundaries like the Himalaya and the Andaman and Nicobar, we need longer earthquake record that overlaps multiple strain cycles that runs into thousands of years. We use both GPS-based techniques and geological methods to understand the tectonic processes in the Himalaya, Andaman and peninsular India. We employ techniques and methodologies of Quaternary sciences to develop constraints on major earthquakes and also on other extreme natural events including tsunamis that have left their imprints in the geological archives. Tectonic deformations during the Quaternary times (2.588 million years ago to present) preserved in the geological and geomorphological records have the potential to bridge gaps in information, necessary for construction of not only the earthquake time series but also on past climatic variability. Understanding the relation between climate and tectonics are of considerable

research interest, for which the Himalaya provides the perfect tectonic setting. We apply methods in tectonic geomorphology to analyze river profiles and course anomalies to understand the tectonic rejuvenation of landforms, as a window to underlying fault activities. We integrate data from diverse fields as seismology, geology, geochronology, geodesy and geomorphology, to gain insight into the tectonic processes.

Current activities also include outreach programs, which include writing of books for students, teachers and researchers in geology, on the geodynamic history of the Indian continent, natural hazard mitigation, state of the natural environment of India. We are involved in the Science Outreach Program in remote regions of Uttarakhand, sponsored and funded by the CNR Rao Hall of Science.

Neotectonics and Environmental Geology



KS VALDIYA

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Post-Doc: Johns Hopkins University,
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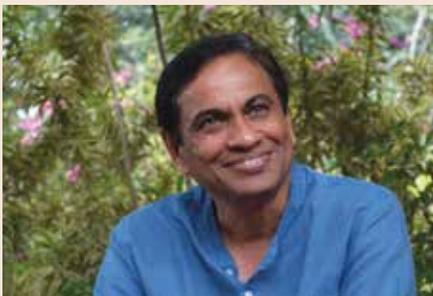
The identification of belts where sudden and swiftly occurring geological phenomena often destabilize the natural configuration of life, and threaten the balance of ecosystems, is the principal objective and the main thrust of activities of this one-man Unit. Regions vulnerable to landslides and occurrence of earthquakes repeatedly in the central sector of the Himalayan arc, including the Indo-Tibetan border region, Kumaun (Uttarakhand, Himalaya), the Biligirirangan Range in south-eastern Karnataka, the Sahyadri Range, and the coastal belt in western Karnataka and central Kerala were taken up for studies. Various signs of physical changes taking place in the natural systems in the study areas were interpreted through the 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 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; and the development of mountain or hill barriers along active faults in south-eastern Karnataka and adjoining Tamil Nadu, the southern Sahyadri and its foothill belt in central Kerala, and in the Sor Valley in eastern Kumaun in Uttarakhand, 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 a 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.

KEY PUBLICATIONS

KS Valdiya, *Geology, Environment and Society*, Universities Press, Hyderabad (2004, 2011).
KS Valdiya, *Journal of Geological Society of India*, 65, 537-552 (2006).

Fault Zone Studies, Active Tectonics and Seismic Hazard



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Post-Doc: University of South Carolina,
Columbia, USA

The focus of his studies is to understand the earthquake source zones and fault zones of India and contiguous areas thereby assisting the seismic hazard evaluation of the region. He and his Group contribute in the areas of earthquake seismology, active tectonics, earthquake geology, paleoseismology, tsunami geology and tectonic geomorphology. To address the key questions in seismology like the seismic gap hypothesis, and characteristic earthquakes (slip-predictable or time-predictable models) or spatial and temporal clustering of earthquakes (explained as due to stress triggering and fault interaction), it is important to understand how seismic sources behave in the longer term. His work is mainly focused on developing an extensive database on spatial and temporal earthquake recurrence patterns for various fault systems, which will help to draw realistic statistical conclusions and develop tectonic models of earthquake kinematics. His research also targets to further the knowledge on the earthquake generation along the plate boundary systems like the Himalaya and Andaman-Nicobar tectonic zones, major potential sources of damaging earthquakes in India.

KEY PUBLICATIONS

J Paul, et al., *Bulletin of the Seismological Society of America*, 104, 10.1785/0120130220 (2014).
CP Rajendran, et al., *Journal of Geophysical Research*, 118, 10.1002/jgrb.50122 (2013).





INTERNATIONAL CENTRE FOR MATERIALS SCIENCE

DIRECTOR

CNR Rao, FRS, FASc, FNA,
FTWAS, Hon FRSC, Hon F Inst P

PROFESSOR

SM Shivaprasad*

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Rajesh Ganapathy
Sridhar Rajaram
Ranjani Viswanatha**

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GU Kulkarni, FNAsc, FASc
Narayan KS, FNA, FASc, FNAsc
Sundaresan A
Tapas Kumar Maji

HONORARY FACULTY FROM IISc

AK Sood, FASc, FNA, FTWAS
U Ramamurthy, FASc

* Jointly with CPMU
** Jointly with NCU

The International Centre for Materials Science (ICMS), at the Jawaharlal Nehru Centre for Advance Scientific Research, is devoted to carrying out high impact interdisciplinary research, promote collaborations and personnel exchange, organize discussions and meetings and promote Advanced Materials Science education.

ICMS was dedicated to the nation by then Prime Minister of India, Dr Manmohan Singh, on December 03, 2008. The Centre is financially supported by the Department of Science and Technology (DST), Government of India and directed by Professor CNR Rao, FRS.

The ongoing research programs are Chemistry of Materials, Surface Physics, Soft Condensed Matter and Low-dimension materials and other aspects of Materials Science. The Centre now houses several sophisticated research facilities such as Molecular Beam Epitaxy and other growth systems, ultra high resolution TEM and state-of-the-art optical, electrical and magnetic characterisation probes.

ICMS supports Ph D and MS degree programmes, Short-term visits and offers Post-Graduate Diploma in Materials Science.

The centre has established several collaborations and has signed Memoranda of Understanding with leading international research institutions such as Weizmann Institute, Germany, SISSA, Italy, RMIT-Australia, University of Waterloo Canada etc, under which there is a constant exchange of students and researchers in addition to frequent technical meetings and workshops. The centre is a member of several International fora like EICOON, WMRIF and IUSSTF.

International Centre for Materials Science also conducts several annual lecture series by eminent scientists from all over the world. This year the sixth 'International Materials Science Lectures' was delivered by Prof Mercuri G Kanatzidis,

Northwestern University, the 'Annual Materials Lecture' by Prof Ashutosh Sharma, Indian Institute of Technology, Kanpur and the 'Sheikh Saqr Materials Lecture' by Prof Sir Andre Geim, FRS Kt, University of Manchester.

Two semester (one year) Post-Graduate Diploma in Materials Science at ICMS has been specially designed to encourage research among students and teachers from rural areas with limited resources. Ph D stream, and under developed countries under this programme. ICMS also encourages students from developing and under developed countries under this programme. The students completing the program successfully are awarded with a Post-Graduate Diploma degree certificate. Nine students have graduated until now under this and at present, three students are enrolled.

SHEIK SAQR LABORATORY

The financial support provided by Ras al Khaimah Centre for Advanced Materials has been used to establish the Sheikh Saqr Laboratory (SSL) here, in the premises of the International Centre for Materials Science. This laboratory supports various fellowship programmes and conferences to encourage front-line research and international co-operation. The new CCMS building that houses the Sheikh Saqr Laboratory and the Sheikh Saud Lecture Hall, was inaugurated by His Highness Sheikh Saud Bin Saqr Al Qasimi

on August 26, 2013. The Sheikh Saqr Laboratory houses the state of the art research facility that complement the facilities at ICMS. These include a 3-D projection seminar hall, analytical facilities, facility for synthesis of organic materials for optoelectronic devices, a class room for practicals and more. In addition to conferences, schools, short term visits and exchange programmes, the SSL grant also supports various fellowship programmes. This year Prof Shobhana Narasimhan and Prof Balasubramanian Sundaram have been awarded the Sheikh Saqr Senior Fellowships. While Dr Subi George and Dr T Govindaraju have been awarded the Sheikh Saqr Career Award Fellowships. The Sheikh Saqr Junior Fellowships have been awarded to Mr Rana Saha and Mr BVVS Pavan Kumar.



TUE-CMS THEMATIC UNIT OF EXCELLENCE ON COMPUTATIONAL MATERIALS SCIENCE

MEMBERS

Balasubramanian S, FASc (Coordinator)
Shobhana Narasimhan, FNASc
Swapan K Pati, FNASc, FASc
Meher Prakash
Srikanth Sastry, FNASc, FASc
Umesh V Waghmare, FNASc, FASc, FNA

STAFF

Vijay Amirtharaj A
Ananda Raman A
T Basavaraj
K Venkatesh

RESEARCH STAFF

Anant D Kulkarni, Research Scientist D (Program Support)
Somesh Kr Bhattacharya, Research Associate
Premkumar Leishangthem, Research Associate
Devina Sharma, Research Associate

Members of TUE-CMS carry out research in the broad area of computational materials science, using a variety of analytical and computational tools.

The Thematic Unit of Excellence on Computational Materials Science (TUE-CMS) is a project funded by the Nano Mission of the Department of Science and Technology. It was established in January 2012. This TUE continues and expands the activities carried out under the Centre for Computational Materials Science (CCMS) which was established in 2006. CCMS too was supported by the Nanoscience and Technology Initiative of DST. TUE-CMS operates under the International Centre for Materials Science at JNCASR.

Members of TUE-CMS carry out research in the broad area of computational materials science, using a variety of analytical and computational tools. They have strong interactions with groups engaged in experimental research in materials and biology. 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, multifunctional materials, spintronic materials, disordered systems, complex and molecular liquids, biomimetic systems and biomaterials. The techniques employed include *ab initio* calculations, molecular dynamics simulations, multiscale modelling and many body theory. Research

is also carried out on developing various techniques and codes such as Monte Carlo simulations to predict gas adsorption isotherms in porous solids, enhancements in capabilities of first principles techniques and combined atomistic and continuum methods to study meso-scale problems in materials. Around 50 original research articles are published by members of TUE-CMS every year.

The High Performance Computing Facility of TUE-CMS has three Infiniband based clusters, two are of 6 TFLOPS & one of 10 TFLOPS computing capability. A stereoscopic projection facility to visualize results of complex molecular simulations has been established. A 1,800 sq. ft. advanced data centre is being established which will house a 100 TFLOPS computer in the first phase.

Along with supporting the research programmes of its members, TUE-CMS 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. TUE-CMS is also committed to establishing international collaborations with institutions of equivalent high quality in the area of computational science.

www.jncasr.ac.in/ccms



TUE-NANO THEMATIC UNIT OF EXCELLENCE IN NANOCHEMISTRY

FACULTY

GU Kulkarni

Narayan KS

CNR Rao, FRS, FASc, FNA,
FTWAS, Hon FRSC, Hon F Inst P

SM Shivaprasad

Ranjan Datta

Eswaramoorthy M

Rajesh Ganapathy

Subi Jacob George

T Govindaraju

Jayanta Haldar

Tapas Kumar Maji

Sebastian C Peter

Sridhar Rajaram

Ranjani Viswanatha

TECHNICAL ASSISTANCE

NR Selvi (FESEM)

Govindan Kutty

In order to boost research interest in nanoscience, many academic activities such as courses in nanoscience, discussion meetings and symposia are being conducted.

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.

The main activities of the Unit are as follows: 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.

Graphene, graphene derivatives and graphene analogues of inorganic layered material; synthesis, and properties, graphene based SETs and photo detectors.

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, mesoscale assemblies.

Patterned nanomaterials, Electron beam and AFM-based high-resolution nanolithography.

Thin films of novel functional oxides, transition metal oxides of interest in high Tc superconductivity, synthesis using RF magnetron sputtering, characterisation and processing.

Characterisation of nano objects using electron and scanning probe microscopy techniques, UV-Vis spectroscopy, X-ray photoelectron spectroscopy.

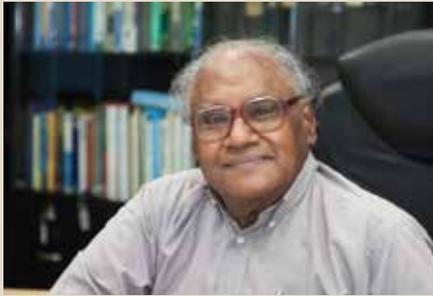
Characterisation of nanomaterials using high-resolution powder X-ray diffraction, RDF from Rietveld analysis, Reflectivity studies on films.

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, Surface-enhanced Raman spectroscopy (SERS) by tagging gold and silver nanoparticles to proteins, polypeptides, etc., Diagnostic tools for biology.

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, modelling advanced materials showing rectification and those of interest in spintronics.

Chemistry of Materials



CNR RAO

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RESEARCH INTERESTS

Oxide Materials: Multiferroics, Electronic Phase Separations, Colossal Magnetoresistance (CMR)

Carbon Materials: Nanotubes and Graphene

Nanomaterials: Of all dimensionalities

Organic-Inorganic Hybrid Materials: Including Kagome structures

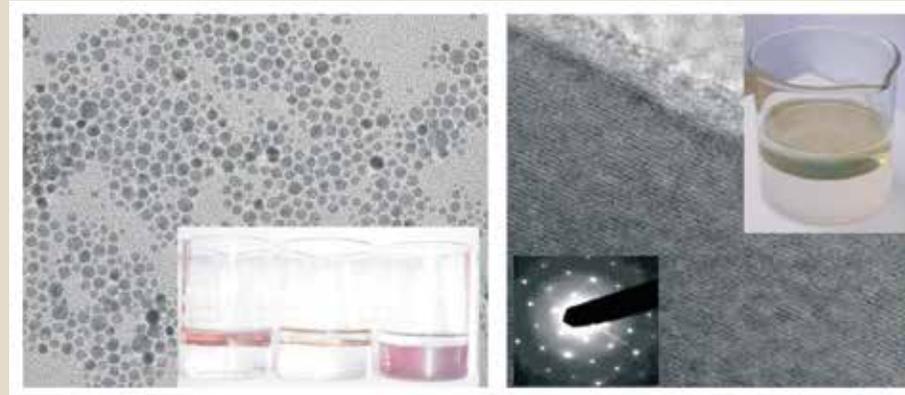


Fig.: Organic-water interface for large scale syntheses of nanocrystals and single crystalline films

KEY PUBLICATIONS

CNR Rao, et al., *Chemical Physics Letters* (Frontiers article) 609, 172 (2014).
U Gupta, et al., *Applied Physics Letters* (Mater) 2, 092802 (2014).

HRTEM, HREELS, Semiconductors, Thin Film Growth



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ABERRATION-CORRECTED HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPE

This particular microscope has both Cs corrector (HRTEM) and probe corrector (for HAADF-STEM) which yields spatial resolution $\sim 0.8 \text{ \AA}$ and in principle, can resolve the atomic arrangement of atoms in crystals with the smallest inter-atomic bonds.

Negative Cs helps in imaging light atoms like O, N with white contrast with the possibility of quantifying their occupancy in the lattice. Besides, this microscope is equipped with EELS and energy filter components, with energy resolution better than 0.2 eV.

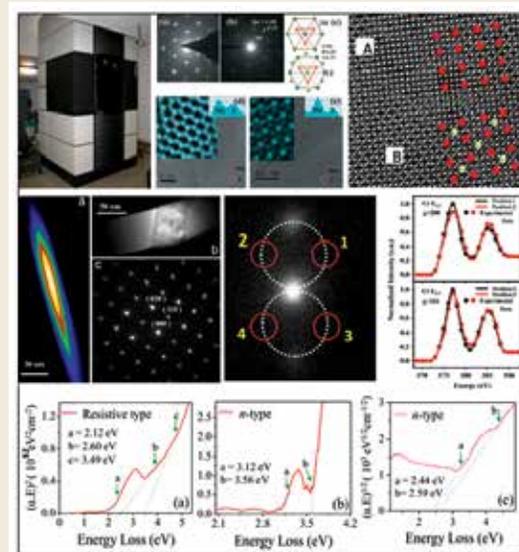


Fig.: Image of the electron microscope, high-resolution images, EMCD and optical band gap by EELS

MAGNETISM AND OPTICAL STUDY BY HR-EELS

Electron magnetic circular dichroism (EMCD) in a TEM is a new idea and useful to characterize magnetic system at the nano and atomic scale. EELS can also be used for optical band gap study as well as plasmon study in principle at the atomic resolution.

OPTOELECTRONIC MATERIALS

Pulsed laser deposition (PLD) thin film growth of ZnO semiconductor. Issues being pursued are p-doping problem, understanding formation and role of point defects. Other materials include various spinel oxides, Heusler alloys, MoS_2 , ReS_2 etc.

FIRST PRINCIPLE-BASED THEORETICAL CALCULATION

First principle-based electronic structure and EELS spectra simulation.

Experimental Soft Condensed Matter Research



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Experimental research in our Group strives to unravel the physics of soft condensed matter. From particle laden suspensions that make up toothpaste to biological cells and the slender organic molecules in a liquid crystal display, soft materials are ubiquitous in our daily lives. In spite of this remarkable diversity, a unifying attribute of these materials is that they comprise of mesoscopic structures held together by weak entropic forces. Consequently, weak external perturbations couple strongly to their microstructure which, in turn, determines their macroscopic response. Understanding this structure-response relationship is central to identifying properties exclusive to this class of condensed matter and will have a direct impact on the development of tailor-made materials.

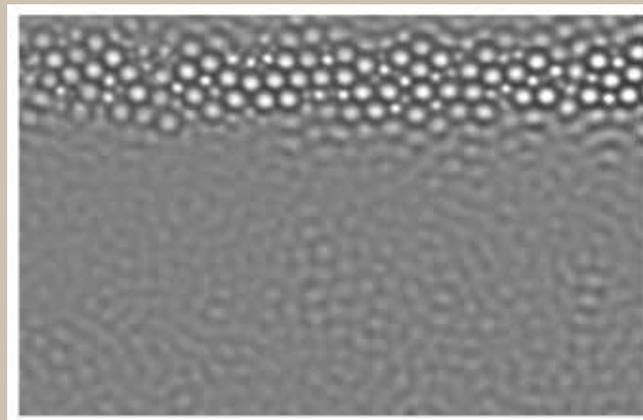


Fig.: Glassy dynamics near an optically pinned colloidal wall

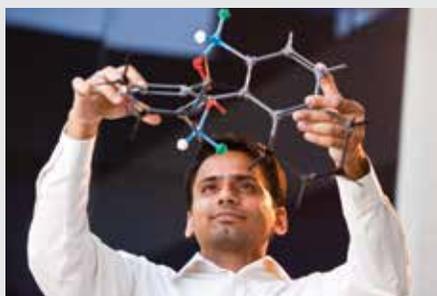
Our research efforts can be classified under two broad themes. First, exploring the role of shape/interaction anisotropy and the nature of the interaction between the fundamental building blocks on material properties. The second theme is to unravel the link between the microstructural dynamics of soft matter at sub-micrometer length scales to their macroscopic response when subjected to external fields.

KEY PUBLICATIONS

CK Mishra, et al., *Physical Review Letters*, 110, 188301 (2013).

Gokhale, et al., *Nature Communications*, (2014).

Organic Semiconductors and Asymmetric Catalysis



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The high cost associated with the production of inorganic semiconductors has been a barrier for the development of low cost electronic devices. Solution processable organic semiconductors provide a cost-effective alternative mainly due to the reduction in processing costs. However, in order to realize the promise of low-cost electronics, the performance of organic electronic devices has to be improved. In our Group, this will be addressed using the toolkit of synthetic chemistry. As part of this approach, we have utilized non-planar perylene diimides as alternatives to fullerenes in organic solar cells. Further studies using transient absorption spectroscopy have shown that the charge generation characteristics are similar to that of fullerenes. Mobility measurements also indicate the charge transport is as facile as fullerenes.

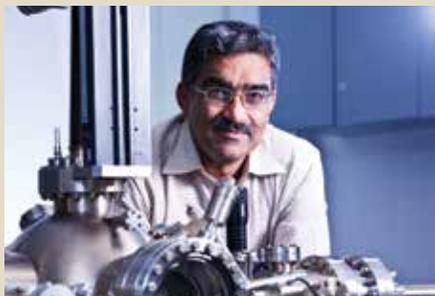
In the area of catalysis we are looking to develop environmentally benign approach for the synthesis of amino acids. In this context, we are developing an alternative to the Strecker reaction that avoids the use of cyanide. We have also developed a novel method to control the conformation of hydrogen bonding catalysts.

KEY PUBLICATIONS

S Rajaram, et al., *Journal of Physical Chemistry Letters*, 3, 2045-2048 (2012).

R Shivanna, et al., *Energy & Environmental Science*, 7, 435-441 (2014).

Obtaining High Mobility Indium Nitride and InGaN Thin Films



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In recent years along with research on nanostructured GaN, we have undertaken extensive work on InN and InGaN thin films, that have great potential for applications, such as full spectrum solar cells and LEDs. We have extensively addressed the issue of forming high quality epitaxial InN, which is hindered by its low dissociation temperature. By careful and systematic studies we have found the relation between the charge carrier concentration, the position of Fermi level and the morphology of the films. By kinetic control we have formed InN with fewer grain boundaries.

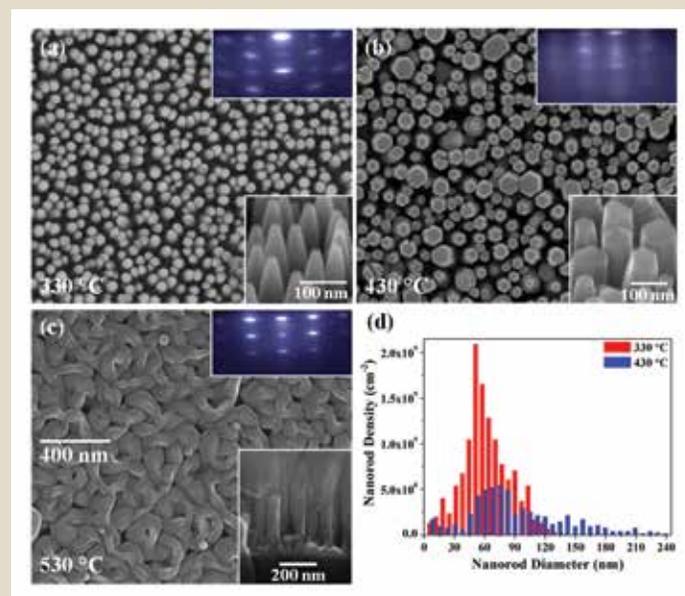


Fig.: Kinetically controlled morphology dependence of InGaN films with different In incorporation.

The highlight of our work is in forming a novel approach of Superlattice matched Epitaxy of InN on Si (111) surface, which reduces the interfacial defect and lattice mismatch, and yields high quality InN. We have also achieved almost defect free InN thin films and nanorods, by growing them on a GaN nanowall network template. In this system we have initial results that show highest reported mobility of electron, and also a room temperature terahertz emission. We are forming InGaN nanostructured films with variable In incorporation, for band-gap engineering coupled with low-dimensional properties. We are pursuing this approach to form templates for growth of III-Nitride films for high performance devices.

Semiconductor Nanocrystals: Electronic Structure Study



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The primary focus of our research is the synthesis and the study of electronic structure of transition metal doped and undoped semiconductor nanocrystals and metal-semiconductor hybrid structures. Current interests range from the synthesis of novel materials in the 3D confined regime using colloidal synthesis, the study of their properties and use of these materials for applications. Specifically, we are working on the study of magnetic, optical and magneto-optical properties of doped II-VI semiconductor nanocrystals and their effect on the host nanocrystals for sizes ranging from 3 nm to 50 nm. Interesting size and shape dependent observations that can be used to tailor make the nanocrystals for the application of interest have been made and the mechanism of these properties are being explored. The use of these properties to design better stable and low cost devices for LED and solar cell applications is an additional focus of the lab.



Fig.: Properties of down conversion Phosphor obtained from Cu doped CdS Nanocrystals.

KEY PUBLICATIONS

A Saha, et al., *Journal of Materials Chemistry C*, 2, 3868-3872 (2014).

GK Grandhi, et al., *ACS Nano*, 6, 9751-9763, (2012).





MOLECULAR BIOLOGY AND GENETICS UNIT

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Kaustuv Sanyal

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MRS RaO, FASc, FNA, FNAsc, FAMS, FTWAS

Molecular Biology and Genetics Unit (MBGU) conducts research and training in several key areas of biology with an emphasis on human health and disease.

Current focus of our research activities includes infectious diseases (AIDS and Malaria), genetic disorders (brain disorders, deafness and cancer), mammalian stem cells, cardiovascular development, transcription regulation, protein engineering, biochemistry, developmental biology, genome biology, autophagy and molecular mechanisms of centromere formation and chromosome segregation. A new research initiative of the centre in the area of neurosciences is being currently hosted in the Unit.

Our research is supported by grants from several funding agencies and from biotechnology industry. Many research themes in MBGU are build up on an active interface of biology and medical specialties and are being carried out in collaboration with clinician colleagues from a number of major medical organisations in the country. In the last 20 years or so, there has been active exchange of research ideas and facilities among scientists in MBGU and other colleagues in the centre, who are chemists, physicists and engineers. It is very heartening to see such collaborations within and outside JNCASR take roots and mature. Scientific outcome of these efforts is amply reflected in multidisciplinary nature of our publications.

Each laboratory in MBGU is well equipped for their individual requirements and certain major research facilities including a multi-photon confocal microscope, DNA sequencing, mass-spectrometer, microarray scanner and cell sorters operate as shared platform facilities. An animal facility provides suitably regulated access to small animals, rats, mice and rabbits. High-speed internet access and computation-related technical support to the Unit is provided by a central computer laboratory.

MBGU attracts some of the best students from all over the country. Students for the Ph D, Integrated Ph D, POBE, MS-Ph D and SRF are selected through national-level competitive selection process. At present, 45 Ph D and 29 Integrated Ph D students are enrolled in MBGU.

Our academic goal is to provide training in a range of genetic, biochemical, cell and developmental biology approaches for basic and translational research. The essence of these research programmes is to give students ample flexibility and opportunity for pursuing a contemporary research theme and a broad-based training in multidisciplinary research areas. MBGU has created a vibrant and interactive research atmosphere for its

students, who find themselves immersed in multiple academic activities including research work presentations, journal club discussions, training workshops, thematic conferences and lectures by visiting scientists, throughout the year. Students are encouraged and supported to present their results at the scientific meetings. A number of students who have graduated from the MBGU, have gone on to build their independent careers in the academic organisations in the country and abroad as well as biotechnology industries.

MBGU faculty can be directly contacted through our web site www.jncasr.ac.in/mbgu.

Molecular and Cellular Mechanisms of Human Genetic Disorders



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The main focus of research in my laboratory is to explore the molecular and cellular basis of common human disorders: genetic generalized epilepsies, sensory epilepsies, neuropsychiatric disorders and congenital hearing loss. We have discovered several novel genes and genetic loci for epilepsy (2q33-q36, 3q13-q21, 5q12-q14, 5q33-q35, 4q24-q28, 10q21-q22), deafness (9p31-21, 11p14-q12, 18q 12-21), bipolar affective disorder (1p32.1, 6p24.3-ter). These genes/loci are currently being studied to isolate disease-causing mutations. We have also identified a wide spectrum of pathogenic mutations in several deafness-causing genes and examined the molecular basis of non-syndromic hearing impairment in Indian populations. The identification of over four dozen pathogenic mutations in the Cx26, Cx30, Tmprss3, Tmc1, Har, Cdh23, Slc26a4, Otof and Tmie genes has substantially extended our understanding of allelic heterogeneity at these genes

and provided a number of new alleles for potential use in cell biological, biochemical and structure-function correlation studies. Knowledge of the relative contributions of these genes to the load of hereditary hearing loss has helped devise a 'genetic algorithm' that has important utility for early detection of the disorder and implementation of suitable intervention therapies.

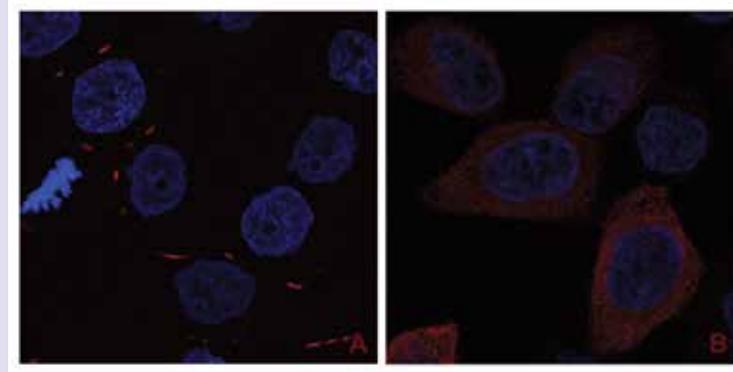


Fig.: Sub-cellular localisation of the wild type and mutant CONNEXIN 26 proteins. Wild type CONNEXIN exhibits characteristic gap-junction plaques at the junction of two contacting cells (A). Localisation of the defective CONNEXIN occurs in the cytoplasm and no gap-junction plaques are observed (B)

KEY PUBLICATIONS

R Ratnapriya, et al., *Human Genetics*, (2010).
R Ratnapriya, et al., *Human Genetics*, (2009).

Molecular Parasitology and Molecular Enzymology



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My laboratory focuses primarily on molecular enzymology and specific aspects of metabolism in *Plasmodium falciparum*. The malaria-causing *P. falciparum* is one of the most pathogenic microbes that continues to pose health hazards in many parts of the world. As a parasite that is largely intracellular, residing within host cells, it has evolved a unique set of biochemical pathways to adapt to the milieu of its growth. Metabolic pathways that are indispensable for parasite survival serve as ideal 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. We have characterized the purine salvage enzymes, HGPRT, ADSS, ASL, GMPS and 5' purine nucleotidase of *P. falciparum*, human and *M. jannaschii*. The laboratory has also been examining the crosstalk between purine nucleotide and tricarboxylic acid (TCA) cycles as the adenylate arm of purine nucleotide synthesis generates fumarate. *P. falciparum*, during its intraerythrocytic stages generates ATP primarily from glycolysis. In this context, the fate of metabolites produced by diverse pathways that feed into the TCA cycle merits study. Tools of genetics, cell biology, biochemistry and biophysics are used to address the various issues under study.

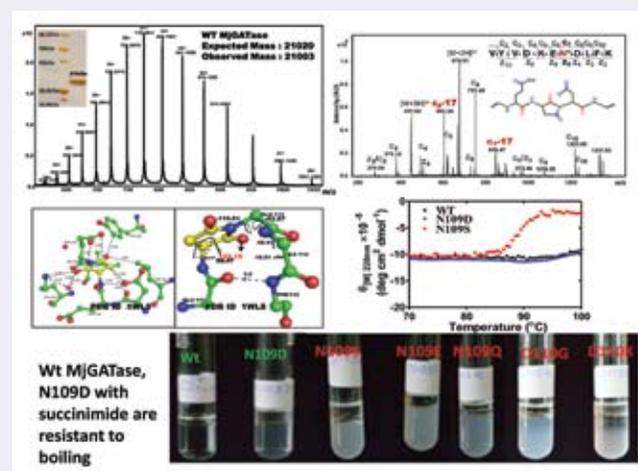


Fig.: Hperthermophilicity in *M. jannaschii* GATase conferred by an unusually stable succinimide

We have characterized the purine salvage enzymes, HGPRT, ADSS, ASL, GMPS and 5' purine nucleotidase of *P. falciparum*, human and *M. jannaschii*. The laboratory has also been examining the crosstalk between purine nucleotide and tricarboxylic acid (TCA) cycles as the adenylate arm of purine nucleotide synthesis generates fumarate. *P. falciparum*, during its intraerythrocytic stages generates ATP primarily from glycolysis. In this context, the fate of metabolites produced by diverse pathways that feed into the TCA cycle merits study. Tools of genetics, cell biology, biochemistry and biophysics are used to address the various issues under study.

KEY PUBLICATIONS

Srinivasan B, et al., *FEBS Journal*, 281, 1613-28 (2014).
Ali R, et al., *Biochemistry*, 52, 4308-23 (2013).

Stem Cell Potency and Cardiovascular Development



MANEESHA S INAMDAR

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Post-Doc: University of North Carolina, Chapel Hill, USA

Cardiovascular defects and diseases are the leading cause of prenatal, postnatal and adult mortality. The promise of stem cells and regenerative medicine is to repair and restore defective or diseased parts of the human body. A better understanding of development and disease progression could provide control over the outcomes of these engineered therapies.

By a comparative approach using human and mouse pluripotent stem cell models, knockout and transgenic mice, and *Drosophila* genetics, we have deciphered the roles of novel genes expressed early in the cardiovascular system. We showed that the conserved protein Rudhira/BCAS3 is essential for directional cell migration during developmental angiogenesis. We also showed that the endosomal protein Asrij interacts with ubiquitous proteins such as ARF1 promoting novel tissue-specific interactions. The Asrij-ARF1 axis regulates activation of JAK/STAT and Notch pathways to maintain the stem cell state. We established a new concept in stem cell biology, which has thus far focused on cytosolic proteins and transcription factors. This conserved nodal control on stem cells will help improve strategies for stem cell expansion, differentiation and cell reprogramming.



Fig.: Cardiovascular system in a mouse embryo. Heart and blood vessels are red due to presence of blood.

KEY PUBLICATIONS

RJ Khadilkar, et al., *Proceedings of the National Academy of Sciences*, 111: 4898-4903 (2014).
A Sinha, et al., *Cell Reports*, 4: 649-658 (2013).

Transcription Regulation and Chromatin Dynamics



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The Transcription and Disease laboratory of MBGU, JNCASR, focuses to understand how chromatin dynamics regulated by non-histone chromatin proteins (eg: PC4, HP1 etc) and histone chaperones are critical for gene regulation and its possible links to diseases (e.g.: oral/breast cancer and AIDS). The epigenetic language (especially histone modifications) responsible

for the underlying gene expression related to malignancy and differentiation (muscle and neuroglial) are being elucidated. Recently we have also initiated to investigate the role of Aurora Kinases in transcriptional regulation and differentiation processes. Several small molecule modulators of epigenetic enzymes (e.g.: KATs and arginine/lysine methyltransferases) have been discovered. At present, their potential in therapeutics and as a tool to understand gene networks in differentiation are also being studied.

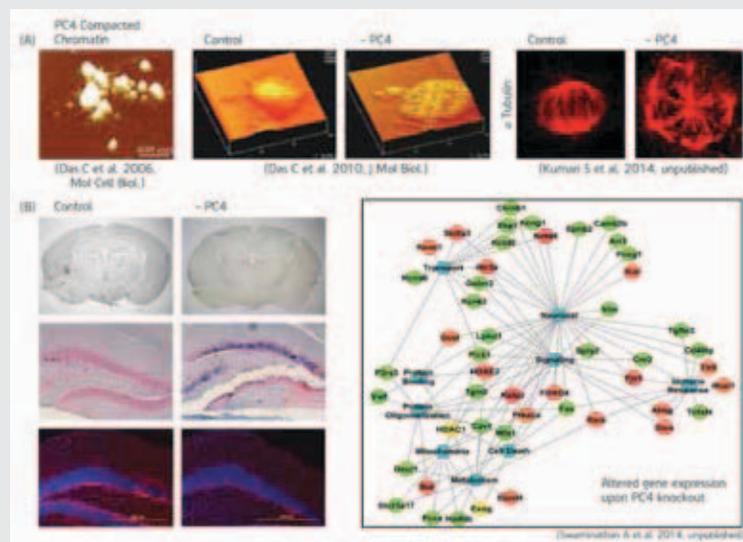


Fig.: Chromatin protein PC4 critical for neural development and memory

KEY PUBLICATIONS

Karthigeyan D, et al., *Proceedings of the National Academy of Sciences USA*, Vol.111(29), 10416-10421, (2014).
R Modak, et al., *ACS Chemical Biology*, 21:8 (6):1311-23. (2013).

Autophagy and Autophagy Related Pathways



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Every cell in our body is equipped with a form of housecleaning machinery called autophagy. Autophagy is universally present in all cells from yeast to humans. During nutrient starvation, autophagic processes promote cell survival by degrading superfluous cytoplasmic proteins and organelles.

IMPORTANCE OF AUTOPHAGY

As autophagy is not only involved in clearing superfluous and unwanted cellular components, it is also known to degrade several intracellular pathogens including bacteria and viruses (xenophagy). Autophagy also serves a neuroprotective role, as it clears large aggregates of mutant polyubiquitylated proteins resistant to proteasomal degradation – a process known as aggrephagy. Furthermore, autophagy is involved in several diseases including cancer.

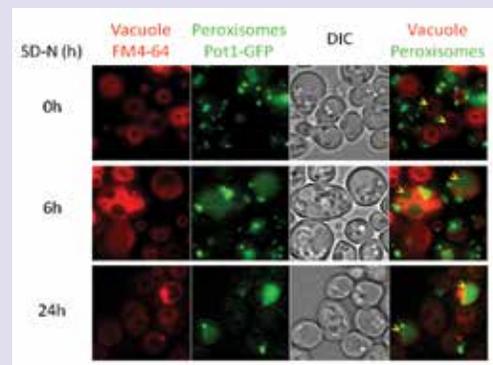


Fig.: Autophagy of peroxisomes in yeast

LAB APPROACHES TO STUDY AUTOPHAGY

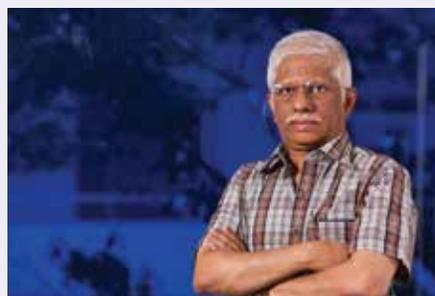
The laboratory currently focuses on using yeast (*Saccharomyces cerevisiae* and *Pichia pastoris*) and mammalian model systems to explore autophagy and autophagy related pathways. We employ high throughput assays to discover small molecule inhibitors and activators of autophagy. We have also performed screens to identify new molecular players that are required for autophagy. The information gained from such work is used to study the role of autophagy in, among others, xenophagy, aggrephagy and unconventional protein secretion.

KEY PUBLICATIONS

K Rajasekhar, et al., *ChemPlusChem*, 79, 25 (2014).

S Singh and Manjithaya R. In: Hayat, MA. *Autophagy*, Elsevier, 105, (2013).

Chromatin Biology and Genomics



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Post-Doc: Baylor College of Medicine,
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We have carried out a detailed analysis of PTMs of the testis specific histone variant TH2B by Mass spectrometry. We have also identified the repertoire of PTMs of the two transition proteins TP1 and TP2. We have shown that PRMT4 catalyzes the arginine methylation of TP2. The genome wide occupancy of the linker histone H1LS on spermatid chromatin has been mapped by ChIP-seq analysis.

We had previously discovered a novel non-coding RNA, mrhl RNA encoded in the mouse genome which negatively regulates wnt signaling by interacting with p68/Ddx5 helicase. We have now mapped the genome wide occupancy of mrhl RNA on spermatogonial genome by the ChOP technique and have shown that it regulates a sub set of genes that are involved in spermatogenesis. The putative homologue of mrhl RNA encoded in the human genome is now being investigated. Mrhl RNA is also expressed in mouse ES cells and during early development of mouse embryo.

Aebp1 is a transcriptional repressor that is involved in adipogenesis. Aebp1 is over expressed in primary glioma. We have shown earlier that Aebp1 is an anti-apoptotic protein. A detailed mechanistic analysis of Aebp1 has now shown that depletion of Aebp1 functions in glioma cells down regulates PI3K beta and in turn triggers AIF release from mitochondria that bring about nuclear chromatinolysis resulting in cell death. Thus Aebp1 offers as a potential candidate for therapeutic intervention in clinical management of glioma.

KEY PUBLICATIONS

G Gayatri, et al., *Molecular and Cellular Biology*, 32 (15), 3140-3152 (2012).

J Ladha, et al., *Molecular Cancer Research*, 10, 1039-1051 (2012).

Genetic and Epigenetic Definition of Centromeres



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Several proteins bind to centromere (CEN) DNA to form kinetochores, which help in the attachment of chromosomes to the spindle microtubules during mitosis and meiosis. The main focus of our laboratory is to understand the mechanism of chromosome segregation in pathogenic yeasts. Several lines of evidence suggest that CEN formation in most organisms is not entirely a sequence-dependent phenomenon. We discovered that a three-dimensional chromosomal scaffold is probably an epigenetic factor that determines CEN identity. We showed that the presence of an early replicating origin also determines centromere location. Functional cloning and comparative genomics studies in our laboratory revealed the CEN sequence and DNA elements are rapidly evolving although the relative location of the CEN region remains evolutionarily conserved in related species. Finally, we showed that an interdependent protein circuitry ensures assembly and stability of the functional kinetochore on CEN DNA.

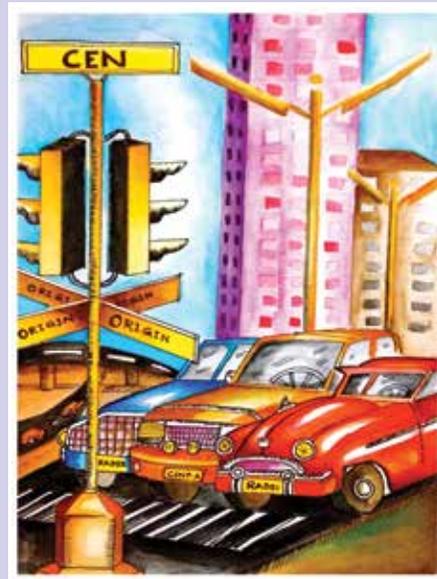


Fig.: Programmed stops bring CENP-A recruitment by the Rad51/Rad52 complex at *Candida albicans* centromere

OUR KEY AREAS OF INTEREST ARE

1. Mechanism of centromeric chromatin formation
2. Evolution of centromere structural elements
3. Epigenetic coding of the functional genome by histone H3 variants

KEY PUBLICATIONS

Mitra, et al., *PLoS Genetics*, (2014).

Thakur, et al., *Genome Research*, (2013).

Mechanisms Underlying Pathogenesis of Human Cerebral Malaria



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The patients infected with *Plasmodium falciparum* present with a range of outcomes from asymptomatic parasitemia to severe disease leading to death. The host and parasite factors that mediate the severity of the disease are poorly defined. Severe *falciparum* malaria leads mainly to cerebral, renal and pulmonary dysfunction. In India, severe *falciparum* malaria is mostly associated with renal and pulmonary complications rather than cerebral malaria. The genetic and molecular basis of this diversity remains unknown.

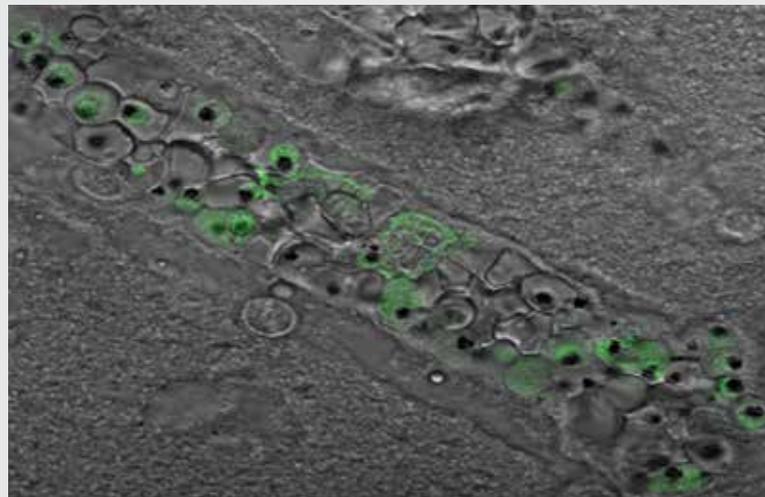


Fig.: SIM image of parasite specific protein in the brain blood vessels of a cerebral malaria patient

My research Group focuses on identifying the parasite factors responsible for virulence and host-pathogen interaction networks by 'Systems-Biology' and validating them by proteomics, cell biology, molecular biology, biochemical and genetic approaches.

Our efforts have led us to characterise molecules and pathways involved in signaling and intracellular trafficking required for parasite survival in cerebral malaria.

KEY PUBLICATION

Verma G & Surolia N. *Molecular and Biochemical Parasitology*, 192 (1), 21-29 (2013).

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



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Among the various HIV-1 genetic subtypes, subtype-C is the most predominant viral family causing half of the global infections. What makes subtype-C the super HIV? Its milder nature? For instance, we demonstrated that subtype-C is incapable of causing neuron death in the human brain primarily as a consequence of a single amino acid variation in the viral factor Tat. Our work makes it globally mandatory today that genetic diversity of HIV-1 families is considered when examining HIV neuro-pathogenesis.

Where is the HIV evolution headed, towards less pathogenic viral strains? We found that over the past decade, highly infectious HIV strains have originated in India, Brazil and South Africa and have been replacing the circulating viral strains at a rapid pace. The novel strains, though more infectious, may not be more pathogenic. With the help of 4 different clinics, we are all set to test this hypothesis.

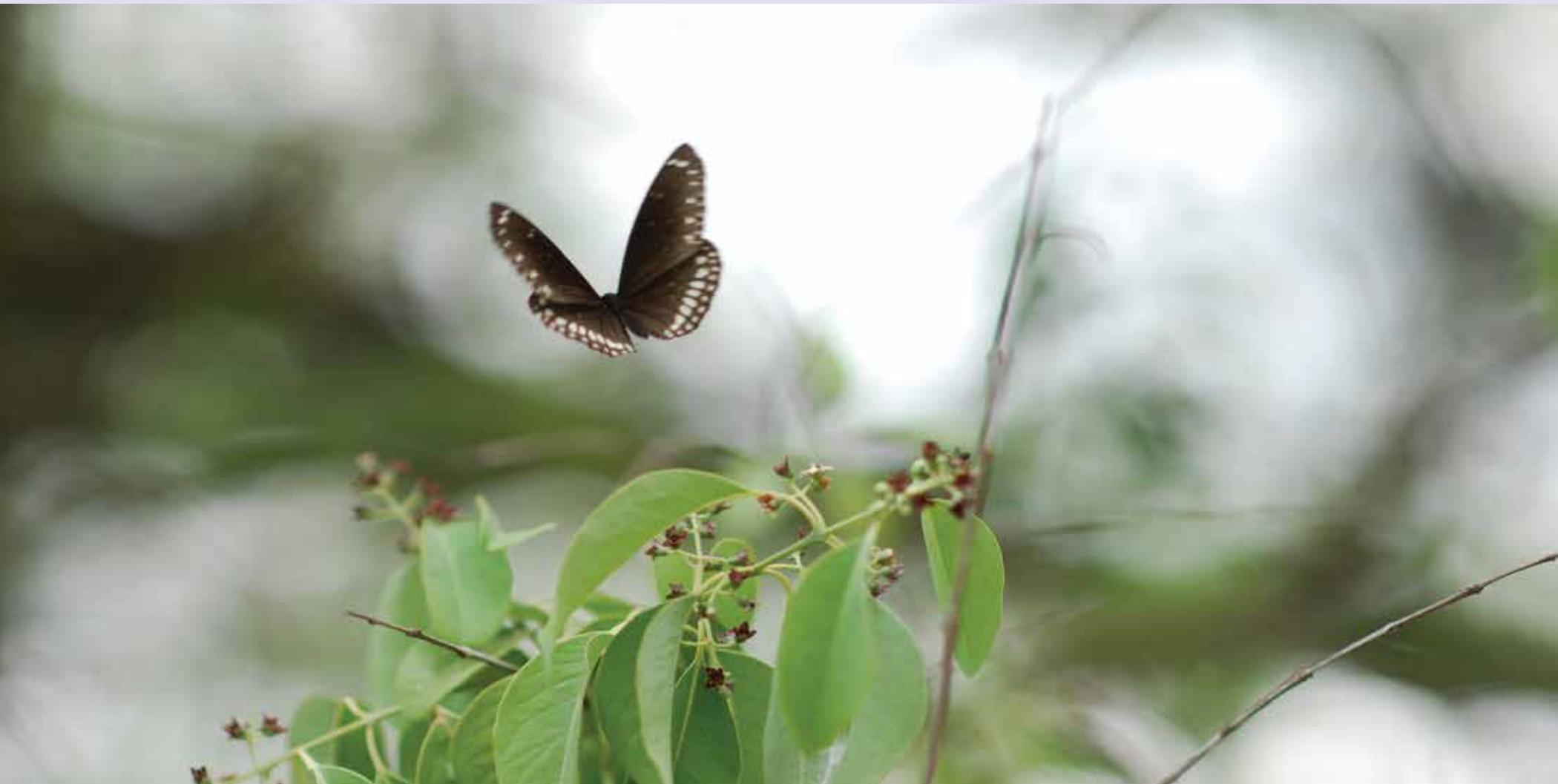
If HIV is smart, subtype-C is smarter. Everything about subtype-C is milder except the viral promoter, which is the strongest among all. Work in progress in our laboratory shows that subtype-C uses novel molecular circuits to efficiently regulate the establishment of viral latency and gene expression.

We desperately need a vaccine for HIV. More important, controlling chronic immune activation, which sets HIV infection in its own class, is the least understood and the most critical aspect that deserves attention. Can the alternative medicines of India offer a hope? In a pilot human clinical trial using a poly-herbal formulation in 61 subjects, we found a stabilized clinical profile in a study of 2 years. In a follow up study, we identified several potential immune markers that can serve as prognostic markers for future studies.

KEY PUBLICATIONS

M Asokan, et al., *Indian Journal of Medical Research*, 137, 69-85 (2013).

M Bachu, et al., *Journal of Biological Chemistry*, 287 (53), 44714-35 (2012).







NEUROSCIENCE UNIT

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FACULTY FELLOWS

James P Chelliah
Sheeba Vasu

ASSOCIATE FACULTY

Anuranjan Anand, FASc, FNASc
Narayan KS, FNASc, FASc

The field of Neuroscience is the academic pursuit of studies of the nervous system and its role in modulating behaviours and physiological processes in organisms.

The Neuroscience Unit was newly established in November 2014, the Silver Jubilee year of the Centre, becoming its youngest Department.

The field of Neuroscience is the academic pursuit of studies of the nervous system and its role in modulating behaviours and physiological processes in organisms. It is broad in its reach and extends from studies involved in understanding the unique molecular and biophysical properties of neuronal cells and their partners, as well as emergent properties of neuronal networks.

The fundamental theme of this Unit is to study the various aspects of nervous systems. Currently the research interests of the Unit include the study of synaptic function and its relationship with Intellectual Disability, neurogenetics of behavior in *Drosophila*, molecular and cellular mechanisms of human brain/mind disorders, developing biomaterials for interfacing sensory organs with soft analog devices and molecular neuro-oncology.

The diversity in individual research themes of the faculty also reflect the widely differing types of scientific approaches and methodologies used in understanding how the nervous system functions and determines various behaviours of organisms, including humans.

In the coming years, the Neuroscience Unit intends to expand its activities in the broad areas of computational neuroscience, cellular neuroscience and mammalian developmental neurobiology. The Unit is also looking towards building highly advanced imaging technologies to investigate not only synaptic function and morphology but also neuronal circuit function, which will have biomedical implications.

The unit will begin admitting students to the Ph D program from August 2015.

Molecular Pathways in Gliomagenesis



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Post-Doc: Baylor College of Medicine,
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Transcriptome profiling of primary and secondary GBM tumor samples had shown that the two transcription factors AEBP1 and ASCL1 are highly up regulated in primary and secondary GBM respectively.

We have now shown that AEBP1 is an anti apoptotic protein and is necessary for cellular growth and survival. Loss of function of AEBP1 leads to Caspase independent, but PAR and AIF dependent chromatinolysis in glioma cells. The biological function(s) of ASCL1 in glioma cells are now being investigated.

SynGAP1 in Neuronal Function and in Intellectual Disability



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A cardinal feature of human brain development is that sensory, cognitive and emotional experiences shape synapses and neural-circuit development. Several studies have shown that these parameters are altered in Intellectual Disability (ID) and Autism Spectrum Disorder (ASD), which affects ~3-4% of the population in the world. Mutations that cause ID and ASD are increasingly found in genes that encode for proteins that regulate synaptic function and/or structure. Heterozygous (het) mutations in SynGAP1, synaptic RasGAP, has been shown to cause ID and increase the risk for developing ASD in young children. We have recently demonstrated that in SynGAP1 heterozygous Knock-out (Het) mice, the net effect of SynGAP1 haploinsufficiency was to unleash dendritic spine synapse in the neonatal hippocampus during development, which drives excitatory/inhibitory (E/I) imbalance, seizures and various behavioural deficits. These early dendritic synaptic spine maturation is also linked to altered duration of critical period of plasticity that leads to life-long cognitive and social deficits. My lab is focused on understanding how SynGAP1 het mutation alters local neuronal circuit maturation and functional connectivity and alteration in synaptic function during learning and memory. These questions will be answered using patch clamp recordings, extracellular field recordings and confocal/2-photon imaging techniques.

KEY PUBLICATIONS

JP Clement, et al., *Journal of Neuroscience*, 25, 10447-52 (2013).

JP Clement, et al., *Cell*, 151, 709-723 (2012).

Neuronal Circuits in Fruit Flies



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My laboratory studies neuronal circuits that regulate rhythmic behaviours such as locomotor activity, sleep, adult-emergence, feeding and egg-laying in drosophilid flies. Genetic amenability of *Drosophila melanogaster* enables the manipulation of neuronal circuits in a spatio-temporal fashion. The nature of the neuronal network that modulates sleep/wake cycles by integrating circadian (daily clocks) and homeostatic control is of interest to us. We examine the role of temperature-sensitive ion channels dTRPA1 in modulating daily rhythms. We use the circadian neuronal circuit in fruit flies as a model to study progression of neurodegenerative Huntington's disease. We are also interested in studying the interaction between central and peripheral circadian oscillators that may control feeding and metabolic rhythms.

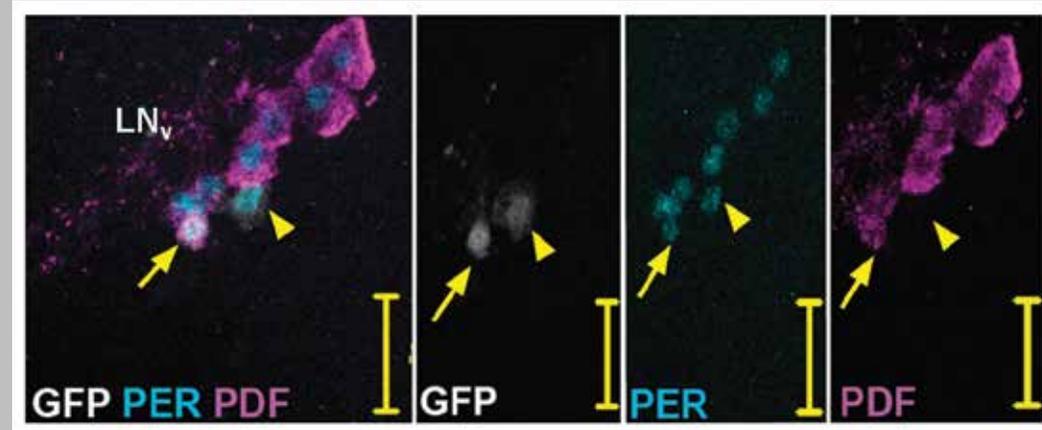
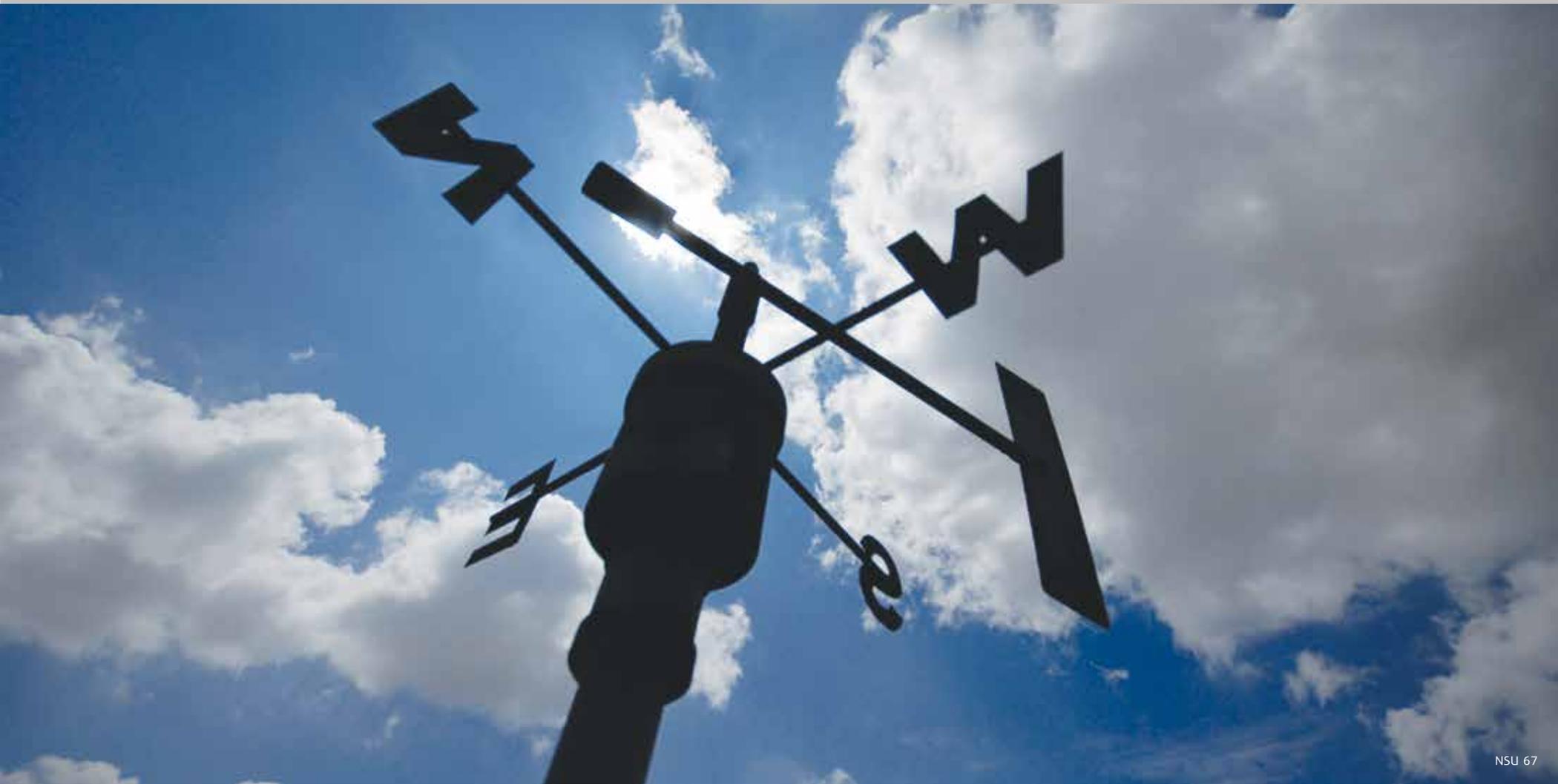


Fig.: Circadian neurons (PER and PDF) expressing TRPA1 ion channel (GFP-tagged) in adult *Drosophila* brain

KEY PUBLICATIONS

S Potdar, et al., *Journal of Neurogenetics*, 27, 23 (2013).
PM Prabhakaran, et al., *Journal of Experimental Biology*, 216, 4691 (2013).





NEW CHEMISTRY UNIT

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Hon FRSC, Hon F Inst P

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Sebastian C Peter
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**Jointly with ICMS

The research projects at New Chemistry Unit (NCU) deal with several interdisciplinary areas with interfaces in materials science and biology.

The New Chemistry Unit was created by the Jawaharlal Nehru Centre for Advanced Scientific Research as a part of the 11th Five Year Plan. This Unit is the brain child of Prof CNR Rao and the Unit works on the interdisciplinary aspects of chemical science.

The most important areas that are actively pursued are at the interface of chemical biology, chemical science and materials science. Some of the specific areas of research are solid state and materials chemistry, chemistry of metal chalcogenides, organic synthesis, biomaterials, supramolecular chemistry, antimicrobial therapeutics, drug delivery systems, patternable polymers, conducting polymers, semiconducting nanomaterials, renewable energy, liquid interfaces, multifunctional metal-organic hybrids, medicinal chemistry, theoretical chemistry, carbon and oxide based materials and catalysis.

The research projects involve new strategies for the synthesis of solid state materials that addresses the cotemporary energy issues and global environmental concerns. Synthesis of a host of nanomaterials including organic based zero-, one-, and two-dimensional materials are carried out with an aim to understand their electronic structure as well as applications in magnetic, optical, opto-electronic and electrical devices. Chemistry of carbon nanostructures constitutes one of the extensively studied systems within the Unit. Synthesis of extended designer solids for a range of applications including

metal-organic frameworks or porous coordination polymers, are being actively pursued.

Organic chemistry is an integral part of many research groups which involves the asymmetric synthesis, synthesis of functional organic materials, bio-organic chemistry, medicinal chemistry, polymers etc. Some of the specific areas are design and synthesis of peptide and protein based materials for biomedical applications, synthesis of antibacterial agents, developing new antibiotics, semi-conducting polymers/oligomers for organic electronics, supramolecular functional materials, organic inorganic hybrids.

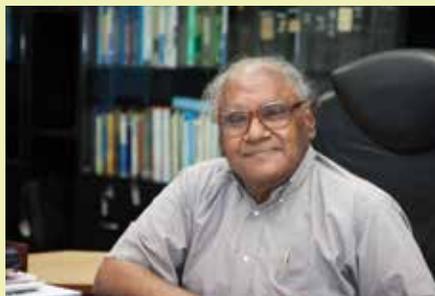
With the current energy crisis facing the world, more than half of the utilized energy is lost as heat. The Unit is involved in the research on alternative energy solutions such as thermoelectrics to open a new window to tackle the upcoming energy problems in near future. Additionally, the Unit is involved in developing materials for photovoltaic, lasers and phase change memory device applications by pursuing synthesizing single crystals of mixed valent rare earth materials. The Unit has developed various facilities for complete characterisation and analysis of various materials pursued here. The Unit also collaborates with various national and international research

centers to obtain access to state of art facilities like the synchrotron facility. In addition, the Unit has excellent facilities for computational and theoretical studies to complement the experimental research.

New Chemistry Unit is also actively involved in various academic activities of the Centre and offers various courses such as Ph D, Integrated Ph D in Chemical Science, MS-Ph D in Chemical Science and M.S by research in Chemical Science. The Unit is also actively involved in the teaching and training of students from various extension programmes like Summer Research Fellowship Programme (SRFP) and Project Oriented Chemical Education (POCE).

Special lectures and seminars constitute an important activity of the Centre. The Unit organizes Annual Chemistry Lectures regularly. In addition New Chemistry Unit is also actively involved in popularizing Chemistry to school children together with Education Technology Unit of the Centre.

Exciting New Chemistry



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In recent years, the discipline of chemistry has developed many exciting cross-disciplinary aspects. My research interests span solid state and structural chemistry, particularly the phenomena and properties exhibited by transition metal oxide systems, and materials chemistry, especially chemical synthesis and characterisation of designer solids, and nanomaterials with novel structures and properties.

The assembly of nanostructures is critical for device fabrication. Different types of aggregates of nanoparticles have been assembled, which show photoluminescence spectra different from the pristine nanocrystals, and are interpreted in terms of electronic coupling between the nanocrystals. In the area of carbon-based materials, besides finding new methods of preparing different kinds of carbon nanotubes and graphene, separation of metallic and semiconducting single-walled carbon nanotubes (SWNTs) using various chemical techniques have been investigated.

Graphene is a fascinating two-dimensional (2D) carbon material which is the parent of all graphitic carbon forms. There is considerable interest in investigating single-layer, two-layer and few-layer graphenes. Synthesis, characterisation, structure, functionalisation and properties of graphene are being carried out. Interestingly, molecular charge-transfer also markedly affects the electronic structure and properties of graphene. Doping graphene with boron (B) and nitrogen (N) as well as the search for graphene analogues have been investigated. In addition, the interaction of graphene with various organic and inorganic systems such as DNA nucleobases and nucleosides have been investigated. Other single-layered 2D structures such as BN and MoS₂ have been synthesized using novel chemical procedures. Functionalisation and solubilisation of inorganic and carbon nanostructures by employing various chemical reagents is an area of extensive research.

KEY PUBLICATIONS

CNR Rao, et al., *Chemical Physics Letters* (Frontiers article) 609, 172 (2014).
U Gupta, et al., *Applied Physics Letters* (Mater) 2, 092802 (2014).

Engineering Molecular Systems for Biological Applications



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Our lab is interested in engineering small molecules and programmable molecular materials to develop state-of-the-art imaging techniques and create novel sensing and therapeutic approaches (see Fig). We are translating concepts from synthetic

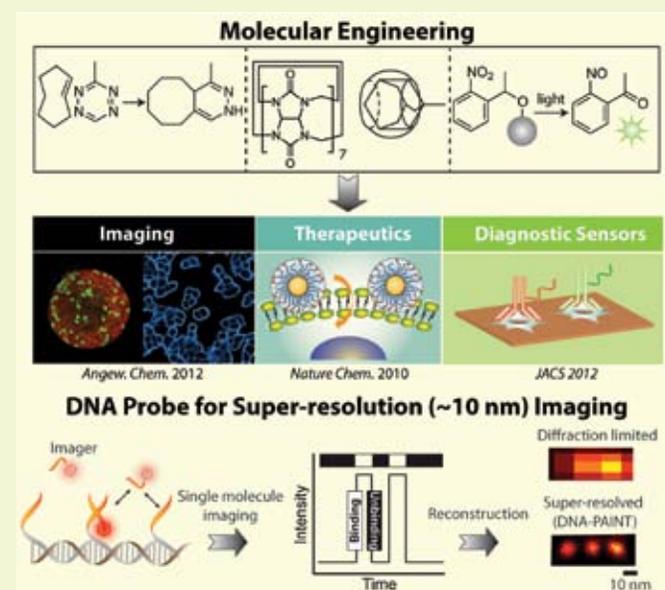


Fig.: Schematic showing the research activities in the lab.

chemistry into biological systems to develop novel chemical tools e.g. bioorthogonal chemistries for labeling and tracking specific biomolecules and therapeutics as they function *in vivo*. We are engineering small molecules and nanoparticle systems for performing selective chemistries in living system. Applications include selective assembly of small molecular components into distinct macromolecular structure for *in vivo* drug synthesis and barcoding. We are manipulating these systems using light to achieve spatiotemporally controlled regulation of biology at single cell or subcellular resolution.

The other focus of our lab is super-resolution imaging using programmable autonomous blinking of DNA probe (see Fig). This imaging technique accomplishes fluorescence ON/OFF switching for localisation-based super-resolution microscopy using transient DNA hybridisation. Employing this technique, we are addressing the current bottlenecks of *in situ* single-cell proteomic mapping, namely ultra-high multiplexing power (>100x) at ultra-resolution (~10 nm).

Thermoelectrics and Metal Chalcogenides



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Our research is directed towards the solid state chemistry; understanding structure–property relationship and electronic and phonon transport properties of metal chalcogenides. Main focus of our Group is to develop highly efficient thermoelectric materials which can directly convert waste heat to electrical energy and will have a significant role in future energy management. Recently, our Group discovered a new class of materials, cubic I–V–VI₂ (where I = Cu, Ag alkali metal; V = Sb, Bi; and VI = S, Se, Te) semiconductors, which can possess very low thermal conductivity, and thus can give rise to high thermoelectric performance. Biswas' Group has also been involved in the synthesis of rare kinetic or polytype metal

chalcogenide phases in the form of nanocrystals which can show fascinating electronic and phonon transport properties and phase transitions. Biswas' Group in NCU is actively involved in the solution based synthesis of two-dimensional ultrathin topological insulators, which are expected to show exotic electronic and phonon transport properties. We are also developing IR-detectors based on heavy metal based chalcogenides.

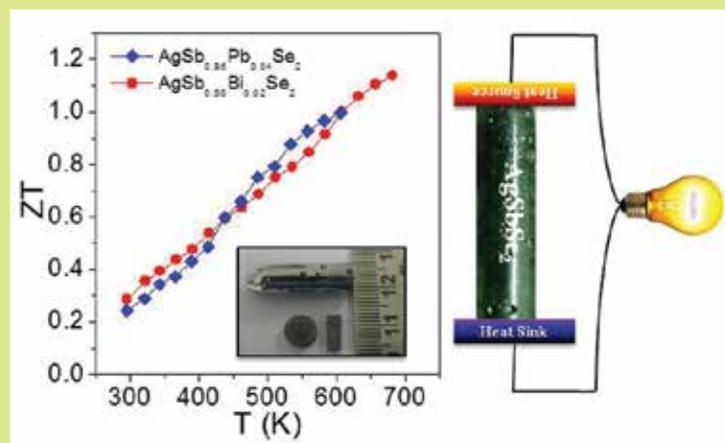


Fig.: High performance thermoelectrics (TE) based on AgSbSe₂. Schematic (right) shows TE power generation.

KEY PUBLICATIONS

SN Guin, et al., *Energy and Environmental Science*, 6, 2603 (2013).

SN Guin et al., *Chemistry of Materials*, 25, 3225 (2013).

Supramolecular Functional (Organic and Hybrid) Materials



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Post-Doc: Eindhoven University of Science and Technology, Netherlands

The underlying theme of our research lies at the interface between synthetic efforts on π -conjugated systems and the organisation of these molecules using supramolecular self-assembly principles, with the ultimate aim of developing novel

functional organic and hybrid materials. In our approach we target the electronic, optical, chiroptical and self-assembling properties of the π -conjugated backbone for the design of materials. Our Group has been working extensively on the mixed-stack charge-transfer assemblies for electronic and ferroelectric functionality and also to use them as reversible (stimuli responsive) supramolecular motif to control the functional properties like pore transport and adsorption properties of inorganic porous materials. We also design solution processable, luminescent organic-inorganic hybrids by the co-assembly ionic dyes and nanoclay particles. We also synthesize a variety of helical, dynamic assemblies of chromophores to study the mechanistic aspects of supramolecular polymerisation process, to use them as a chiroptical probe to monitor enzymatic kinetics and also for the amplification of circularly polarized luminescence.

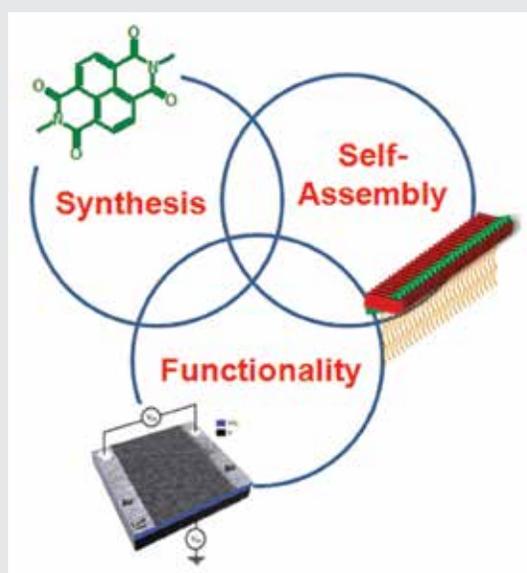


Fig.: Thematic illustration of the research activities in our Supramolecular Chemistry Laboratory

KEY PUBLICATIONS

APHJ Schenning and SJ George. *Nature Chemistry*, 6, 658–659 (2014).

M Kumar et al., *Nature Communications*, 2014, DOI: 10.1038/ncomms6793.

Bioorganic Chemistry



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Research is at the interface of chemistry and biology. His Group actively pursues the design and synthesis of small molecules, peptides, nucleic acids and their conjugates based biomimetic systems and materials through Nature-inspired molecular self-assembly approach. These biomimetic materials find applications as biomaterials, drug delivery systems, composites and in bioelectronics. They are undertaking the design and synthesis of a new class of smart-building blocks for metal directed assemblies for biosensor and smart materials applications.

His Group has established protocols to develop biomimetic noncovalent biopolymeric systems and materials through chiral transcription, amplification and retentive helical memory for use in chiral technology and to understand spontaneous deracemisation and amplification pathways for biological homochirality. They are presently working in the area of neurodegenerative diseases, global nucleic acid structure and functional analysis and bionanotechnology.

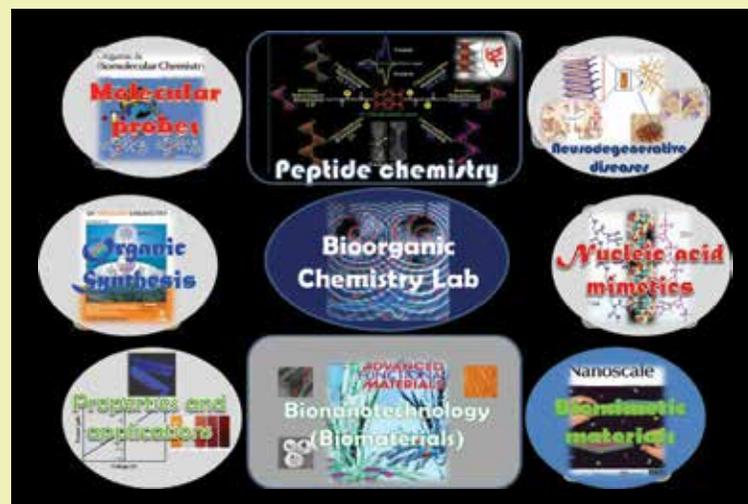


Fig.: Bioorganic Chemistry Lab

KEY PUBLICATIONS

K Rajasekhar, et al., *ChemPlusChem*, 79, 25–30 (2014).

MB Avinash, et al., *Advanced Materials*, 24, 3905–3922 (2012).

Chemical Biology and Medicinal Chemistry



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Infectious diseases remain a major threat to global health and are now the world's biggest killers, causing over 1.3 million deaths per year. The threat is compounded by the fact that an increasing percentage of pathogens are developing resistance against the available arsenal of drugs. Therefore there is an urgent need for a well-coordinated and integrated approach to tackle the threat of infectious diseases. Dr Halдар's research seeks to provide a platform to integrate organic chemistry and material science with biology to combat infectious diseases in a multipronged approach, namely, diagnosis, prevention and treatment. His research focuses on fundamental understanding of material-pathogen interaction and development of

innovative strategies that will provide solutions in tackling infections. His Group is involved in creating novel antimicrobial agents for the prevention and treatment of infectious diseases and combating the emergence of antimicrobial resistance. Additionally, his Group is interested in developing nanotechnology-based smart drug delivery systems for addressing nonspecific action and toxicity related issues of existing drugs for indications like infectious diseases and cancer.

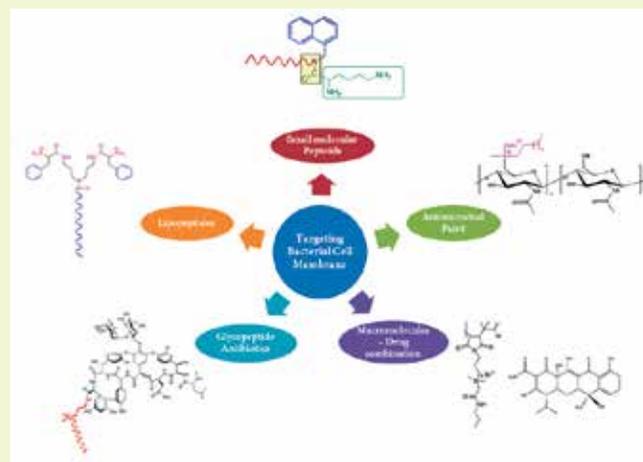


Fig.: Various Strategies to target bacterial cell membrane to combat drug resistance and infections

KEY PUBLICATIONS

V Yarlagadda, et al., *Journal of Medicinal Chemistry*, 57, 4558 (2014).

DSSM Uppu, et al., *Chemical Communications*, 49, 9389 (2013).

Designing New Ways to Small Molecule Heterocyclic Scaffolds



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Small molecule heterocycle ligands play an important role in drug discovery research and can exert powerful effects on the function of macrocycles that comprise living systems. Our Group has been involved for several years in the design and development of new, highly efficient general methods for synthesis of a large variety of structurally diverse and regiospecifically functionalized five/six membered heterocycles and their condensed analogs, which are structural components of a large number of pharmaceutical agents of considerable importance. Our diversity oriented synthesis of these molecules relies upon development of new class of three carbon 1,3-electrophilic organosulfur building blocks which are readily accessible in a one pot reaction from a wide range of cheap active methylene compounds. These new synthetic protocols are highly effective for heterocycle synthesis and elaboration of diverse substitution pattern for complexity generation on heterocyclic frameworks and are especially suitable in combinatorial chemistry for discovery and optimisation of new lead structures in drug discovery research.

Another area of our research interest revolves around design and development of new complexity generating multistep, one pot reactions such as domino reactions, multicomponent reactions for accelerating discovery process of new reagents and total synthesis of biologically important natural products. Most recently, we have been exploring transition metal catalyzed C-C and C-heteroatom bond forming reactions for construction of novel heterocyclic scaffolds.

KEY PUBLICATIONS

Ila Hiriya Kanavar, et al., *Chimia*, 67, 17 (2013).

Ila Hiriya Kanavar, et al., *Organic Letters*, 15, 5250 (2013).

Solid State Inorganic Chemistry



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The broad research interests of the Group are focused on the synthesis and properties of novel solid-state inorganic materials such as intermetallics, chalcogenides and polyoxometalates. The compounds are being synthesised by wide variety of techniques both in solid state and solution methods. We focus extensively on the growth of single crystal of interesting compounds using Bridgman, metal flux, hydrothermal and solution methods. Every compound synthesized will

be characterized in detail for their crystal structure by XRD and phase analysis using different microscopic and spectroscopic techniques. In intermetallics, special attention is given towards the compounds containing rare earths especially Ce, Eu and Yb because of the presence of an unstable electronic 4f-shell. Every new compound discovered displayed a novel situation in the physical properties such as magnetism, Kondo effect, heavy-Fermion and superconductivity. The intermetallic compounds in nano dimension are being developing as anode materials in fuel cells. We also focus on the design and synthesis of supramolecular inorganic-organic hybrids based on polyoxometalates for their potential applications in optical, bio and catalysis. The research in rare earth doped chalcogenide glasses focused on the applications in IR transmitter and other optical properties.

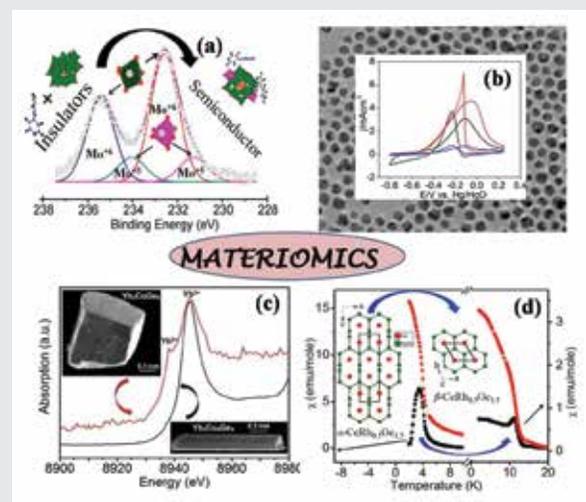


Fig.: a) Semiconductor hybrids (b) Fuel cell anode material (c) Yb valence (d) Spin glass behavior

KEY PUBLICATIONS

S Sarkar, et al., *Journal of Catalysis*, 318, 143 (2014).

U Subbarao, et al., *Inorganic Chemistry*, 52, 13631 (2013).

Semiconductor Nanocrystals: Electronic Structure Study



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The research in our Group is focused on the syntheses and study of electronic, optical and magnetic properties of semiconductor nanocrystals and nanoscale assemblies. We are currently involved in understanding the bulk and surface

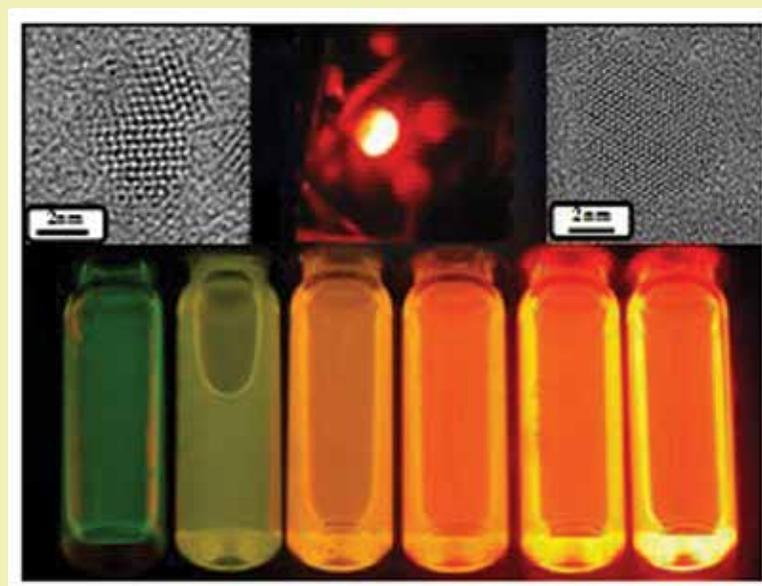


Fig.: Samples under UV-light illumination, TEM images and the LED emission from the same

electronic structure of quantum dots using novel techniques of copper doping as a nanosensor. More studies based on the contributions of long chain, short chain and inorganic ligands to the surface as well as the conduction band and valence band variation in core/shell structures is being carried out in the lab. We are also involved in understanding the electronic structure of nanocrystals and correlating their microstructure to the photophysical properties leading to near unity quantum yield and highly efficient light emitting devices. Studies of magnetic nanoparticles leading to novel new properties are also underway.

KEY PUBLICATIONS

A Saha, et al., *Journal of Physical Chemistry letters*, 4, 3544-3549 (2013)

GK Grandhi, et al., *ACS Nano*, 6, 9751-9763, (2012).







THEORETICAL SCIENCES UNIT

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Vidhyadhiraja NS

FACULTY FELLOW

Meher Prakash

HONORARY PROFESSOR AND SERB DISTINGUISHED FELLOW

Kalyan B Sinha, *FASc, FNA, FTWAS*

"It is the theory that decides what can be observed!", said Albert Einstein. Science without theory is unthinkable: theoreticians provide our fundamental understanding of how nature operates, and can also turn this knowledge into practical applications.

In the Theoretical Sciences Unit at JNCASR, we aim to address, explain and understand the rich diversity we observe in the physical world, be it in the properties of materials, the way in which matter responds to external stimuli, or the molecular processes in living organisms. We also use this understanding and theoretical framework in practical applications by predicting new phenomena or designing new materials. For this, we use the techniques of theoretical physics and chemistry in the context of interdisciplinary areas in materials science and biology.

The research in our Unit is inspired by two complementary approaches to the study of matter and life: the search for universality, and the exploration and explanation of diversity. 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 takes a form that is ultrahard as diamond or soft as graphite, ice contracts when it melts whereas copper expands, chewing gum stretches when stepped on whereas glass shatters, and most of life is multicellular and sexually reproducing, though these are ecologically expensive traits...why?? In order to understand this fascinating yet perplexing range of behaviour, we have to examine structures and properties at a fundamental level, and consider the complex consequences of having a large number of entities (be they electrons, atoms, molecules or living creatures) that interact strongly with one another. One fascinating aspect is that

even when the underlying natural laws are simple in form, complex behaviour is often manifested as system sizes increase.

Our faculty members have had their basic training in quantum many-body physics and chemistry, computational techniques and simulations, quantum density functional theory of fermions, statistical mechanics and mathematical physics. However, much of the work we currently pursue is interdisciplinary in nature. Accordingly, we also accept students who have undergraduate or graduate degrees in a variety of academic disciplines, such as chemistry, physics, engineering and computer science.

In addition to collaborating amongst ourselves on various problems, we have strong interactions with our experimental colleagues, both in JNCASR and outside. We use a mixture of analytical and computational techniques; in the latter, we are helped by the presence of excellent high-performance computational facilities at JNCASR.

The atmosphere in our Unit is vibrant, informal, liberal and interactive. Our faculty and students participate in a number of national and international conferences and workshops, we organize several

seminars and colloquia ourselves, and have a constant stream of distinguished visitors. Alumni of our Unit have excelled in their careers; several of them are now establishing their own groups at universities in India and abroad. We are always on the lookout for bright students who are curious about science and dedicated to research; we encourage them to contact us!

Theory and Simulations of Materials



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Starting with a quantum mechanical description of electronic motion in a given material, we derive a realistic model and analyze it to predict material-specific properties that arise from processes at many time and length scales. Our approach of multi-scale modelling and simulations allows us to connect macroscopic behavior of a material with its microscopic structure and chemistry. We work closely with experimentalists with goals to (a) understand unusual physical phenomena,

(b) complement experiment through determination of atomic-scale information of a material, and (c) predict novel materials and phenomena. Presently, our focus is on smart functional materials, topological insulators, strong light-weight metallic alloys and two-dimensional nano-materials with applications to energy and environment.

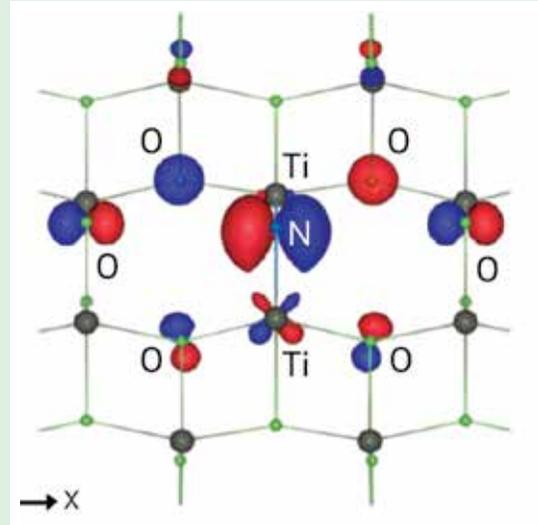


Fig.: Structure and iso-surface of a valence electronic state of nitrogen and fluorine substituted titanium dioxide

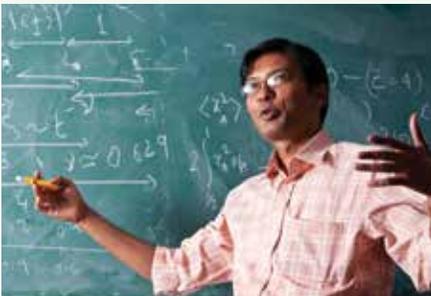
Specific ongoing projects in the group include (1) modelling and understanding mechanisms of shape-memory alloys, magnetoelastic and magnetoelectric effects in multi-ferroics, (2) prediction of new topological insulators with wide band-gap, (3) development of Ti and Mg alloys, (4) graphene, borocarbonitrides, molybdenum sulphide and related two-dimensional materials.

KEY PUBLICATIONS

Sharmila N Shirodkar and UV Waghmare, *Physical Review Letters* 112, 157601 (2014).

S Kouser, et al., *Physical Review B* 88, 064102 (2013).

Statistical Physics of Systems At and Away from Equilibrium



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Post-Doc: Johannes Gutenberg
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Primary research involvement of my Group has been in the statistical mechanics of phase transitions and related areas. In this broad area, we are interested in Phase Transition and Critical Phenomena, Kinetics of Phase Separation in Multicomponent

Mixtures, Structure and Dynamics in Confined Systems, Pattern Formation in Granular Material and Biological Systems, Structure and Dynamics in Supercooled Systems, Nucleation and Wetting Phenomena, Ageing Properties of Nonequilibrium Systems, Active Matter, etc. We are interested in investigation of systems both at and away from equilibrium, for which we use Monte Carlo, molecular dynamics and field theoretic continuum dynamical models. We investigate universality in apparently diverse systems.

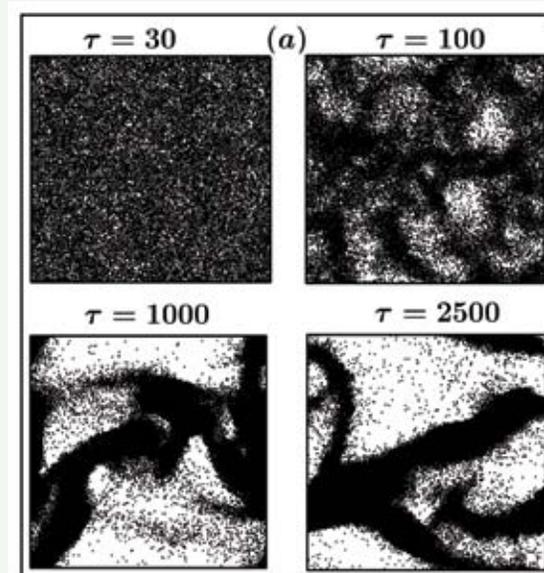


Fig.: Evolution of a granular gas of inelastic particles

KEY PUBLICATIONS

S Majumder and SK Das, *Physical Review Letters*, 111, 055503 (2013).

S Roy and SK Das, *Journal of Chemical Physics*, 139, 064505 (2013).

Nonequilibrium Phenomena in Physics and Biology



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Ph D: Tata Institute of Fundamental Research, Mumbai

Post-Doc: University of Cologne, Germany and Weizmann Institute of Science, Israel

I am interested in statistical physics and probability theory, and their application to interdisciplinary areas such as population genetics. During the last few years, my work has focused on modeling biological evolution and making experimentally testable predictions. I address the questions in these fields using analytical calculations and numerical simulations.

KEY PUBLICATIONS

S Seetharaman and K Jain, *Evolution*, 68, 965 (2014).

K Jain and A Nagar, *Evolution*, 67, 1143 (2013).

Computational Nanoscience



SHOBHANA NARASIMHAN

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Post-Doc: Brookhaven National Laboratory, Upton, New York and The Fritz-Haber-Institut, Berlin, Germany

We use theoretical and computational techniques to explore how physical and chemical properties change at the nanoscale; we then use this understanding to design novel nanomaterials for applications. The main tool we use for this is quantum mechanical density functional theory. Such *ab initio* calculations require no empirical input. Our work is related to pressing problems such as clean energy and device miniaturisation.

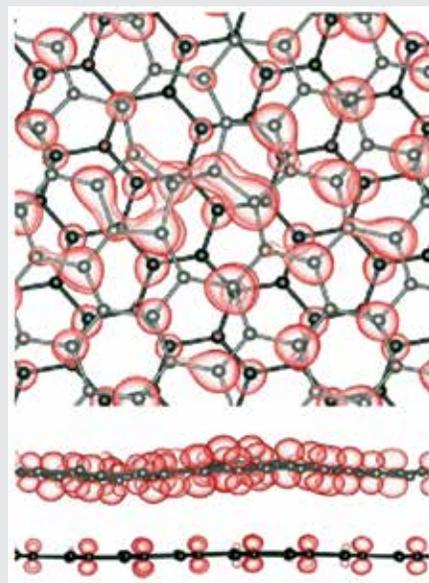


Fig.: Top and side views of charge density in twisted bilayer graphene with a Stone-Wales defect

Topics of current interest include nanomagnetism, molecular spintronics, surface alloys, two-dimensional materials such as graphene, van der Waals bonded nanostructures, materials for hydrogen and methane storage, and nanocatalysis.

As examples of recent successes of our research philosophy, we predicted that Fe and Au would form a two-dimensional surface alloy stabilized by magnetism, even though they are immiscible in the bulk; this was experimentally proved by our collaborators in the group of Rousset in Paris [*Physical Review Letters*, 105, 056101 (2010)]. We also predicted that the morphology of gold clusters could be switched from three-dimensional to planar by depositing them on an oxide doped with an electron donor [*Journal of the American Chemical Society*, 133, 2801 (2011)]; this prediction was subsequently verified in the group of Freund in Berlin. We have also proved that this improves their catalytic activity.

Advanced Quantum Theory: From Molecules to Materials



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Ph D: Indian Institute of Science, Bangalore

Post-Doc: University of California, Davis, USA and Northwestern University, Evanston, USA

The focus of research of Dr Pati's Group has been to understand the structure property relationships of a large class of systems, ranging from simple molecules to polymeric materials, where quantum effects give rise to many exotic phenomena. The goal is to design and model materials for microscopic understanding and applications purposes.

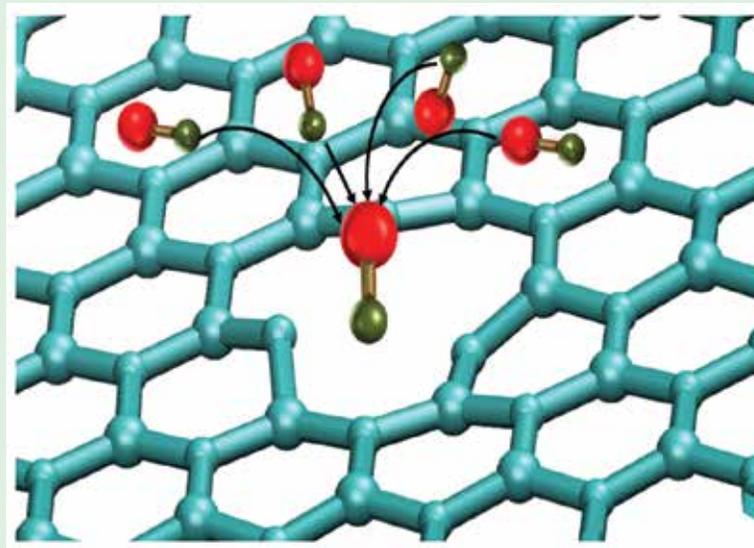


Fig.: An efficient hydrogen fluoride (HF) gas physisorber: N rich single vacant 2D Nanosheet - Ref: Journal of Physical Chemistry C 117, 21700 (2013).

The current areas of interest of the Group are: Quantum Magnetism, Electrical Transport through Molecules/quantum Dots, Nano-materials and New Carbon systems, Cold atom phenomena, Homogeneous and heterogeneous Catalysis, Optimisation of Li-ion battery components, Generalized Charge transfer in biological and bio-mimetic systems, Development of novel methods for studying diverse response phenomena arising from excited states.

KEY PUBLICATIONS

P Bothra and SK Pati, *Nanoscale* 6, 6738 (2014).
S Banerjee, et al., *Journal of Materials Chemistry, A* 2, 3856 (2014).

Computational Studies of Protein-Protein Interactions



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Post-Doc: ETH Zürich, Switzerland

Proteins perform many important cellular tasks, from transcription of genes, to defense in the form of antibodies. Some of these tasks can, in principle, be explained by knowing how proteins find and bind to their interaction partners. We use methods of theory and molecular dynamics simulations to study this finding and binding.

One of our interests is to understand how signals propagate in proteins. In several occasions, the activity level of a protein in one of its sites can be controlled by binding an additional ligand at a different site. While this concept of allostery is not new, there are several aspects that one can observe and study with newer developments in computer simulations. We are interested in understanding how the distal ligand affects the protein activity and how the signals propagate from the distal to the active site.

Another aspect of proteins that we work on is the intrinsic structural disorder. Several biologically fully functional and very important proteins have a structural disorder, which does not fit the common paradigm of structure-function relationship. We are interested in using theoretical methods to understanding what the underlying factors that differentiate these disordered proteins are.

KEY PUBLICATIONS

A Barducci, et al., *Proceedings of the National Academy of Sciences*, 110, E4708-E4713 (2013).
MK Prakash. *Journal of the American Chemical Society*, 133, 9976-9979 (2011).

Phase Transformations and Dynamics in Soft Matter



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Post-Doc: National Institutes of Health, Maryland, USA and Princeton University, Princeton, USA

My Group's research is in the area of statistical mechanics, with a focus on understanding a range of unusual and interesting properties of liquids and other disordered, typically fluid, substances, described generally as soft matter. Entropy plays a

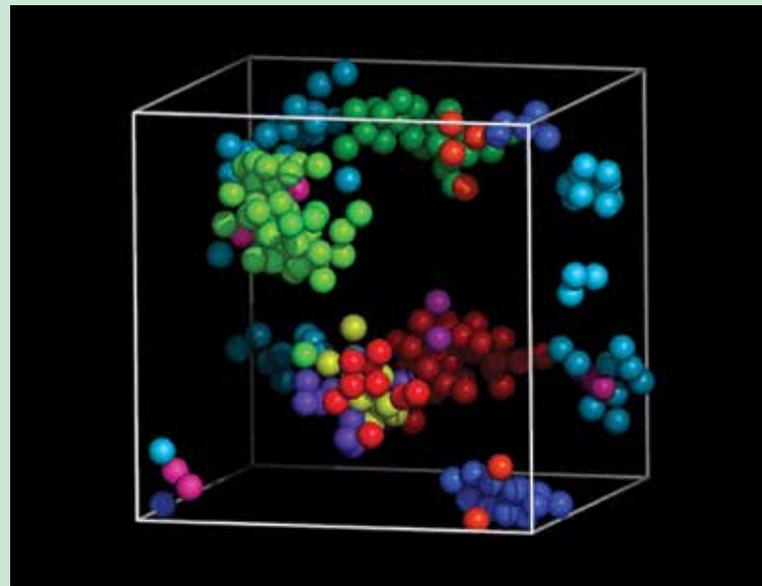


Fig.: Plastic rearrangements in an amorphous solid subjected to oscillatory deformation

large role in determining the properties of these systems. Such systems can exhibit rich phase behavior, complex microscopic dynamics, response to external perturbation and related time dependent phenomena. Inclusion of metastable states extends the time dependent phenomena of interest to the kinetics of phase transformations. Finally, understanding the full range of possible (history dependent) fates of such systems requires understanding of routes to structural arrest, exemplified by glass formation in dense liquids and jamming in sphere packing and granular matter. Amorphous solids formed by structural arrest exhibit interesting and not well understood memory effects and mechanical response. The properties and phenomena mentioned here form the scope of our research.

Non-Commutative Probability and Geometry: Mathematics of Quantum Mechanics



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Post-Doc: University of Geneva, Switzerland

The foundation of Quantum Mechanics has brought with it many new challenges to the mathematical community. It represents a whole new way of looking at spaces and functions as well as of assigning probabilities to hitherto non-compatible events, which is a truly non-Kolmogoroffian scenario.

One model of Non-commutative or Quantum Probability Theory was largely developed in the Delhi centre of the Indian Statistical Institute during the last two and a half decades. Besides being a new non-classical theory of probability and stochastic processes, it also 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 plays a crucial role.

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

Another area of contemporary research interest has been that of extending Krein's trace formula to multi-variable operator analysis. This is likely to have an impact on the computation of cyclic cohomology in non-commutative geometry.

KEY PUBLICATIONS

KB Sinha. *Journal of Indian Society of Agricultural Statistics*, 65 (1), 1-6 (2011).

KB Sinha. *Maths Newsletter*, Special ICM 2010 Issue 19(1), 195-203 (2010).

Correlated Electron Systems and Organic Electronics



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Post-Doc: Oxford University, UK

Materials for which a single-particle description of electronic properties fails, are defined as CORRELATED ELECTRON SYSTEMS. Interest in these QUANTUM MATERIALS derives from the wide range of phenomena they exhibit such as high temperature superconductivity in cuprates, heavy fermions in lanthanides/actinides, colossal magnetoresistance in manganites, and metal-insulator transitions in transition metal oxides. In recent years, there has been a resurgence of technological interest in these materials, which stems from the extraordinary sensitivity of transport and thermodynamic properties in these materials to external parameters such as temperature and pressure. Despite the decades of research in this area, enormous challenges remain for theoreticians and experimentalists.

Our Group employs diagrammatic perturbation theory-based techniques of quantum many body theory to understand these materials in the framework of simple models – the focus being to address issues relating to transport and thermodynamics, especially of heavy fermion systems and transition metal oxides. Most recently, we have developed a computational tool that integrates material-specific information with techniques in strong correlation physics, and thus equips us with predictive capabilities for strongly correlated electronic systems.

Concomitant to the 'blue skies science' explorations mentioned above, we also work on modelling opto-electronic devices based on organic polymers. These devices are emerging as inexpensive and efficient alternatives to traditional inorganic semiconductor-based devices. Modelling of such devices is challenging because of the inherent strong disorder in polymer thin films. We have developed discrete circuit level approaches as well as kinetic Monte Carlo-based simulations for investigating charge transport and device modeling. This work is being carried out in close collaboration with the Molecular Electronics lab in JNCASR.





CSIR COE CSIR CENTRE OF EXCELLENCE IN CHEMISTRY

LINUS PAULING RESEARCH PROFESSOR AND CHAIR

CNR Rao, FRS, FASc, FNA, FTWAS, Hon
FRSC, Hon F Inst P

In order to boost research interest in nanoscience, many academic activities such as courses in nanoscience, discussion meetings and symposia are being conducted.

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.

Developing new strategies for the synthesis, purification, functionalisation and solubilisation of novel carbon nanostructures such as, nanotubes (single-walled, double-walled and multi-walled), Y-junction nanotubes, metallic nanotubes, separation of metallic and semiconducting nanotubes from the mixture in a simple method to study the electrical transport, optical and other confinement properties. Synthesis of graphene nanoribbons by laser unzipping of nanotubes.

Graphene is one of the main areas of research in this laboratory. Synthesis of two to four layer graphene by arc-discharge of graphite in a hydrogen atmosphere. Besides providing clean graphene surfaces, this method allows for doping with boron and nitrogen. UV and laser irradiation of graphene oxide provides fairly good graphene samples, Raman spectroscopy is used to investigate the charge-transfer interactions of graphene with electron-donor and -acceptor molecules, as well as with nanoparticles of noble metals. Notable potential applications of the properties of graphene are low turn-on field emission and radiation detection. High temperature ferromagnetism is another intriguing feature of graphene. Incorporation of graphene improves the

mechanical properties of polymers, its incorporation with nanodiamond or carbon nanotubes exhibits extraordinary synergy.

After the synthesis and characterisation of graphene, serious attention is paid to other inorganic analogues of graphene. We have developed various chemical methods for the synthesis of layered transition metal dichalcogenides which includes MoS_2 , WS_2 , MoSe_2 , WSe_2 , NbS_2 and NbSe_2 . We are studying their applications in IR detectors, gas sensors, composites with polymers for mechanical properties and electrical properties, magnetic properties, and hydro-desulphurisation (HDS) catalysis. We have also used micromechanical cleavage method for obtaining the single-layers of MoS_2 , GaS and GaSe and studied their applications in transistors, detectors and sensors.

New method of synthesizing borocarbonitrides with significant surface area from low cost starting materials like urea, boric acid and activated charcoal has been discovered. Graphene-like $\text{B}_x\text{C}_y\text{N}_z$ samples with compositions close to BC_2N exhibit surface areas in the range 1500–1990 m^2/g , with the uptake values of CO_2 and CH_4 being in the ranges 97–128 wt % (at 195 K, 1 atm) and 7.5–17.3 wt % respectively. The CO_2 uptake in the case of the best BC_2N sample was 64 wt % at 298 K. The borocarbonitride samples show high uptake as well as selectivity of CO_2 over N_2 . The adsorptive characteristics of borocarbonitrides are comparable to or better than those of some of the MOFs

and other adsorbents reported in the recent literature. We have also prepared BC_xN where x varies between 1 and 2, by gas phase reaction of BBr_3 with ethylene and ammonia having nanocup-like morphology. Unlike borocarbonitrides prepared by urea method, gas phase synthesized BC_xN exhibit less surface area and gas adsorption properties.

Hydrogen is the ultimate clean and green source of energy. Only clean and environment friendly way to produce hydrogen is from water using natural energies such as sunlight. There have been several efforts to produce hydrogen via water splitting using electrolysis of water using solar cell, reforming biomass and photocatalytic and photoelectrochemical water splitting. Photocatalytic water splitting using powder catalyst dispersed in water by simply shining light is one of the most energy effective and easiest ways to obtain H_2 and O_2 . We are using spinel based photocatalysts containing "Mn₄O₄ cubane" like structure similar to that found in chlorophyll for oxidation water. Semiconductor based photocatalysts like N doped and N, F co-doped TiO_2 , solid solutions of InN-GaN-ZnO, layered MoS_2 etc are also being tried for H_2 evolution.

Multiferroic oxides are generally considered to be rare because magnetism and ferroelectricity mutually exclude each other as the microscopic origin of both these properties is different. Magnetism arises due to ordering of unpaired spins whereas ferroelectricity occurs due to





charge separation in the respective oxides. Magnetism (Spin-driven) induced ferroelectricity is one of the most effective routes which give rise to strong coupling between magnetism and ferroelectricity. Recent studies on ferrites of the general formula $\text{Al}_{1-x}\text{Ga}_x\text{FeO}_3$ ($x = 0, 0.5, 1$) shows multiferroic behaviour at low temperatures. All of them crystallize in the orthorhombic structure with the non-centrosymmetric space group $\text{Pna}2_1$. The crystal structure contains considerable amount of disorder among the cations and it is invariant with temperature. This family of ferrites are collinear ferrimagnetic ($T_N = 200\text{--}250\text{K}$) and exhibit spontaneous electric polarisation in the vicinity of $\sim 100\text{K}$

(below T_N) as obtained from pyroelectric current measurements. The appearance of polar state has been considered on the basis of non-centrosymmetric magnetic ordering arising from the inherent magnetic frustration and it was also evidenced from the studies of temperature dependent Raman spectroscopy. Application of magnetic field shows a considerable effect on the polarisation data and hence magnetoelectric effect. Therefore magnetically induced ferroelectric material can give rise to a new direction to design future room temperature multiferroic material which would find many new applications.



ACADEMIC ACTIVITIES

ACADEMIC PROGRAMMES

STUDENT LIFE

EXTENSION PROGRAMMES

LECTURES AND MEETINGS

RESEARCH & DEVELOPMENT

COUNCIL OF MANAGEMENT, ACADEMIC
ADVISORY COMMITTEE, PRESIDENTS,
HONORARY FELLOWS

ADMINISTRATION





ACADEMIC PROGRAMMES

It is a matter of great pride that from a student strength of two in 1994, to a strength of 291 in 2014.

Jawaharlal Nehru Centre for Advanced Scientific Research is a globally recognized research institution. The inspiration for creating this institution by our Founder, Prof CNR Rao, dates back to 1989. Although short term programmes commenced soon after, from an office in the Indian Institute of Science campus, the research programmes and other academic activities began in 1994 at the new campus in Jakkur. Faculty members were recruited and students were admitted to research programmes. The JNCASR community, comprising of the faculty and students, continue to work in diverse Units and multidisciplinary areas.

The first batch of Integrated Ph D students consisted of Mr Meciya Kalaiselvam and Mr R Srinivas Gopalan, who worked under the joint guidance of Prof CNR Rao and Prof GU Kulkarni. Mr R Srinivas Gopalan was awarded the first Ph D degree in 2001. Mr A Alagiriswamy and Ms Sheeba Vasu were the first students registered under the Ph D programme, who joined Prof KS Narayan and Prof Amitabh Joshi respectively. Until 2002, the degrees were

awarded by MAHE, Manipal. The Centre was recognized as a Deemed University in 2002 and Ms Vinmathi Vanitha, Ph D registrant under Prof CNR Rao, was the first student to receive JNCASR's Ph D degree. Master's degree programmes in Engineering and Research for engineers, doctors and biologists were introduced subsequently.

At present, Ph D, MS and Integrated Ph D degree programmes are offered each year by the Centre. Admission to the Centre's programmes is considered highly prestigious, and is extremely competitive – typically, less than 5% of students who apply are selected.

It is a matter of great pride that from a student strength of two in 1994, to a strength of 291 in 2014, JNCASR has indeed come a long way. The past decades have been a glorious journey of research and academics with many milestones. To date, students of the Centre have received 146 MS degrees and 179 Ph D degrees. 325 alumni of JNCASR are spread out across the world,

working in top notch universities and laboratories of international repute. Many of them have already set up their own research groups and have made a mark in the world of science.

Further information about the Academic activities of the Centre can be found at www.jncasr.ac.in/admit

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Blissfully and often, addictively out of phase with the world around us, we lead our bustling lives in a campus that is designed to enchant. - Keerthipriya, EOB

STUDENT LIFE

The student community in JNCASR is small by the standards of most universities, yet, it is diverse, with young people from across the country being enrolled in the many academic programmes offered. Graduate students are engaged in a variety of research problems, from aiming to develop new anti-malarial drugs or vaccines against HIV, as well as those who are interested in studying the physical and chemical properties of nano-materials. The campus offers myriad opportunities to listen to scientific talks and symposia from speakers of international repute from across the world, fuelling young minds with new ideas and exciting future possibilities. The Student's Residence located within the main campus is where majority of students reside and enjoy the comfort of adequately furnished, well-maintained single or double occupancy rooms that provide a clean and safe environment to relax after a hard day's work. The New Visiting Students Hostel, a separate unit that is adjacent to the main campus – is reserved for students in the first year and for summer-students and short-term visitors. The canteen facility within each hostel caters to the palate by providing nutritious, healthy and tasty meals and snacks. In addition, the Utility Store operates late into the night, enabling

one to buy food and drink or day-to-day commodities. Students can enjoy a variety of sports within the campus with – basketball, badminton, football and table tennis being hot favorites. For the fitness-conscious, the hostel has a modern, well-equipped gymnasium. The book-club and movie-club enjoy membership of a large number of students with a library holding books on a variety of topics. Come Friday evenings and the hostel comes alive with the screening of movies from the popular to the eclectic. You can also pick up a new hobby with dance, aerobics, yoga and classical music classes organized on-campus. The TV-lounge provides a place to watch sport, the latest soap or breaking-news in the company of friends. 'Dhwani', a student organisation hosts talks, screens documentaries and discussion meetings on a variety of topics. The 'Hostel day' and 'Fresher's Welcome' are two much awaited annual events that feature several sporting and artistic contests eagerly participated by students and faculty alike. Various festivals also see enthusiastic participation by students cutting across religion and language, which culminate in delicious feasts and colourful rituals. Our campus's most striking feature is the greenery provided by a variety of trees, bamboo

clumps and flowering plants playing home to many migratory and local birds and a variety of other fauna. Here, it is easy to be lost in one's own thoughts and experiments, insulated from the ceaseless bustle of life in the city.

With a great sense of pride, I can state that student life in JNC is largely free of extra burdens that can hinder one's intellectual progress; rather, all our basic needs are met, enabling one to pursue an academic career with focus and zeal. – Varun, CPMU

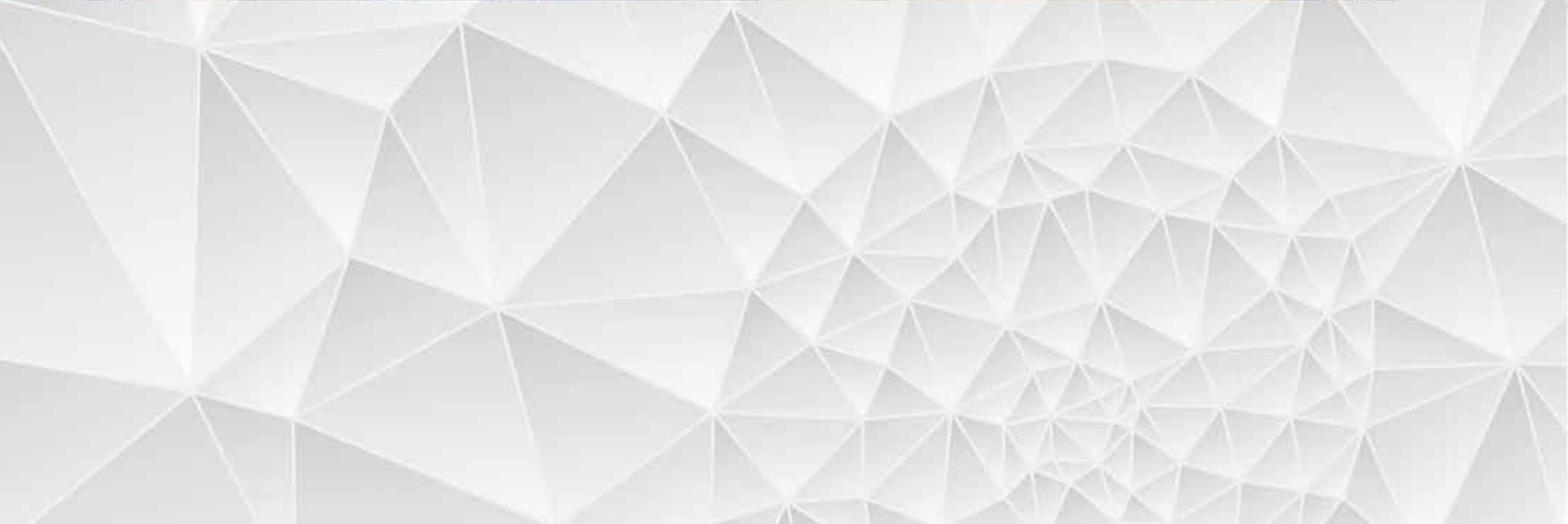


Spacious and nicely furnished single and double occupancy rooms, hygienic well-catered mess, TV rooms equipped with state-of-the-art plasma TVs, laundry service, and a utility store serving to the basic requirements of students, make the JNCASR hostel a perfect backdrop to a comfy, vibrant student life. -

Piyush, TSU



Over the years, I have had a strong bonding with the Centre and its members, creating a long lasting impression on me. I am proud to say that I am a JNCian, having the best moments of my life. - MB Avinash, NCU



EXTENSION PROGRAMMES

The Summer Research Fellowship Programme is one of the highly acclaimed programmes of the Centre, and the students are very appreciative of the benefits, enabling them to get inspired towards scientific research at a very early stage of their education.

In addition to pursuing research in various contemporary areas, Jawaharlal Nehru Centre for Advanced Scientific Research also conducts several Science Outreach and Fellowships Programmes. One such activity is the Summer Research Fellowship Programme for young students which was launched in 1991. Every year, around 70-100 fellowships are offered. This is one of the highly acclaimed programme of the Centre, and the students are very appreciative of the benefits, enabling them to get inspired towards scientific research at a very early stage of their education. Around 1700 students have benefitted from this programme since its inception in 1991. Several SRFP alumni have co-authored papers during their SRFP tenure.

There is an urgent need to sharpen the research skills of students from undergraduate level, and the Centre, tries in its own small way, to provide opportunities to a few bright undergraduate students in Chemistry and Biology with the opportunity of undergoing research training at our Centre. The Project Oriented Chemical Education (POCE) and the Project Oriented Biological Education (POBE) programmes have completed 10 and 8 years respectively. Ten meritorious students are selected from across the

country for each of these programmes. As part of this, students undertake small projects with faculty members of the Centre during their mid-semester breaks. They also attend special lectures and seminars at the Centre. On the successful completion of their training, which lasts for three summers, they are awarded a Diploma certificate in Chemistry or Biology. Till 2013, the Centre has awarded 46 Diplomas in Chemistry and 44 Diplomas in Biology. The programme has been highly successful and most of the POCE and POBE students have chosen research as their career. Several of them have found placements in top universities in Europe and America and some in reputed institutes in India.

The Centre offers Visiting Fellowships to research scientists from educational institutions and R & D laboratories to work with the faculty and honorary faculty of the Centre. This programme has been welcomed by many researchers as they get exposure to techniques not available in their own institutes.

The Centre and its faculty have been active in popularizing science at the school level, with a specific focus on targeting students between the age

of 13 to 18 years. The Centre organizes seminars, workshops, as well as faculty visits, to expose, both, teachers and students to current research in various fields of science.

The Centre through the Educational Technology Unit and Prof CNR Hall of Science, is actively involved in the concept, production and development of multimedia CD-ROMs especially for school students and teachers in various disciplines of science. Content has also been developed in vernacular languages. The aim is to direct its efforts towards popularizing science at the rural level and provide a rich source of supplementary reading material in science.

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RESEARCH AND DEVELOPMENT

As per the recent survey based on the standard performance-indicators, parameterized by the quality scientific publications, the Centre has been recognized as one of the foremost research institutes in the country.

Journey through various sections of this brochure will give an overview of the vast spectrum of research and development, education and training activities pursued at the Centre. As per the recent survey based on the standard performance-indicators, parameterized by the quality scientific publications, the Centre has been recognized as one of the foremost research institutes in the country. The Centre publishes more than 250 scientific papers annually in national and international peer reviewed journals with reasonably high impact factor.

The Centre provides a vibrant academic ambience with excellent state-of-the-art research facilities hosting highly intellectual and motivated faculty and research staff. Researchers at the Centre have been honoured with national and international recognitions for their outstanding contribution to the scientific world.

The Centre receives national and international grants. The public as well as industry funded projects are undertaken routinely for cutting edge research problems. Many initiatives have been taken to translate the excellence achieved in

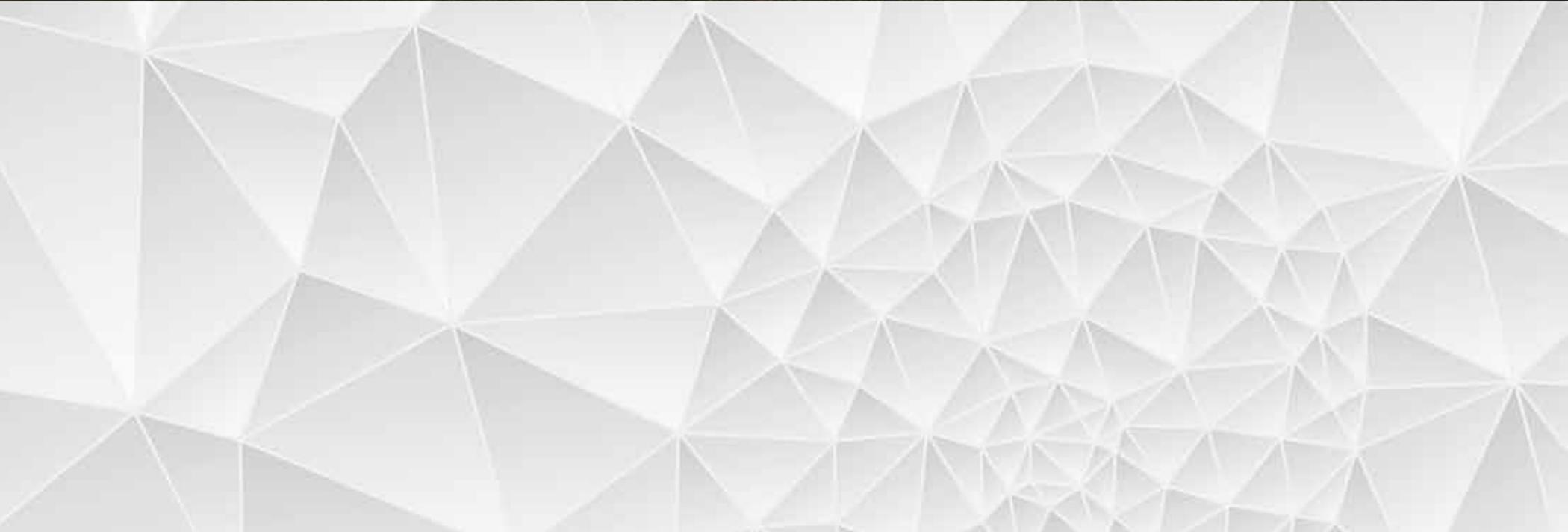
the academic endeavor for addressing problems in various sectors. It promotes interdisciplinary collaborations with various national and international leading research institutions across the globe and has led to periodic breakthroughs of technological relevance. Centre's inventions and solutions have been explored in the areas ranging from electronics-technology to manufacturing, and in pharmaceutical and health industries for disease-diagnostics and drug development.

The Centre has introduced the concept of encouraging faculty members to start and nurture for-profit, knowledge based Startup companies/Spin-offs which can maximize the success of translating research results (inventions/technologies/new knowledge/ideas).

In view of providing access to the wide array of scientific and engineering expertise available at the Centre and to encourage the national and multinational business entities, the Centre also extends consultancy services in the research areas pursued at the Centre. Some of our faculty are consultants for leading firms.

To explore the possibilities for collaborations, sponsored projects, contract, consultancy services and licensing the technologies, you are welcome to contact:

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INTELLECTUAL PROPERTY

The Academic and Research Institutions play an increasingly central role in the creation and implementation of the IP. Its strong bondage with enterprises enhances exploitation of research results through innovations and new technologies leading to affordable services/products/processes for the benefit of society.

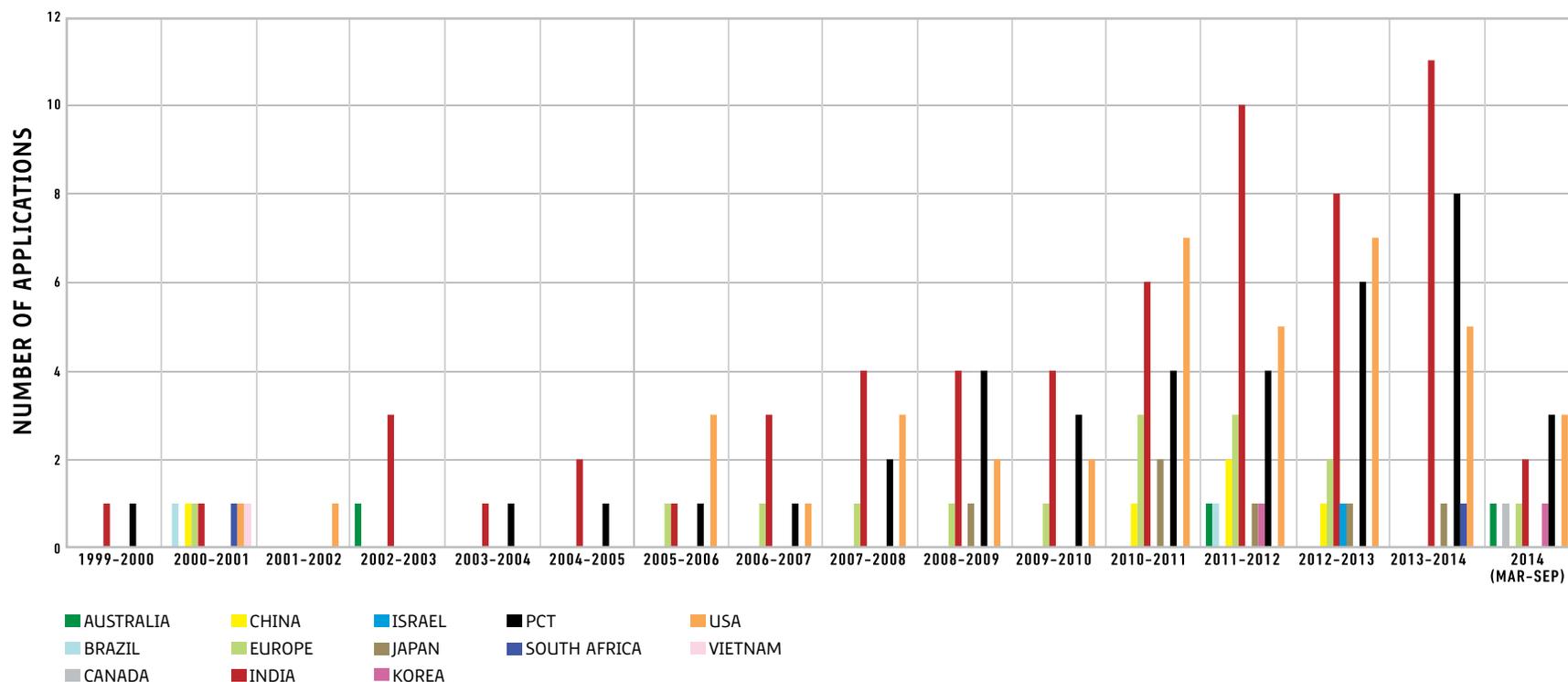
To encourage and facilitate the creation, development, management and protection of commercially exploitable IP and enforcement of IPR, the Centre has constituted an IP Management

Committee (IPMC) and framed an effective, efficient and enabling mechanism to achieve its mission. The Dean, R&D oversees the management of the IP Management Cell, which implements the recommendations/suggestions of the IPMC.

The multidisciplinary approach and extensive collaboration with public and private entities at national and international levels in solving challenging problems by our faculty has led to the generation of 64 inventions in the areas of

Nanotechnology, Biotechnology, Biomedicals, Diagnostics, Medicinal Chemistry, Photochemistry, Optoelectronics, Spectroscopy, Aeronautics, Electricity, Physics, Textiles/Paper, etc. for which 178 national and international patent applications have been filed. The Year-wise patent applications filed has been presented in the figure. To date, 38 patents have been issued and the rest are at various stages of prosecution. The Centre has successfully licensed 14 inventions and generated royalty.

NUMBER OF PATENT APPLICATIONS FILED (YEARWISE AND COUNTRYWISE)



Showcasing Inventions

The inventions generated have been showcased at JNCASR's website to explore the possibilities of identifying potential licensees. A few of the inventions have been showcased below.

Artificial Retina Concept

International Patent Application No.: PCT/IB2012/053711

Inventors: Prof Narayan KS, et al.

Reference Publication

Journal of the American Chemical Society, 133, 17942 - 17949 (2011)

Technology Background and specifications

- Colour Detection normally requires a filters or sub-pixels at the detector end to resolve. The finite area occupied by these standard color resolution in principle is a limiting factor to achieve the highest possible pixel density.
- The technology concept introduced at JNCASR provides a color-sensing device that relies on an interface of an electrolyte in contact bulk heterojunction semiconducting polymer layer on a transparent conducting substrate.
- The signals recorded upon photoexcitation with characteristic colour is in the form of a transient spike with the specific polarity and pulse properties. The use of polarity (positive and negative pulse corresponding to red and green respectively) in the response of the detector opens up a new paradigm in the color detection scheme. Additional colors are composites of these pulse responses and can be determined with a simple analysis.
- The color discrimination scheme resembles natural vision processes.

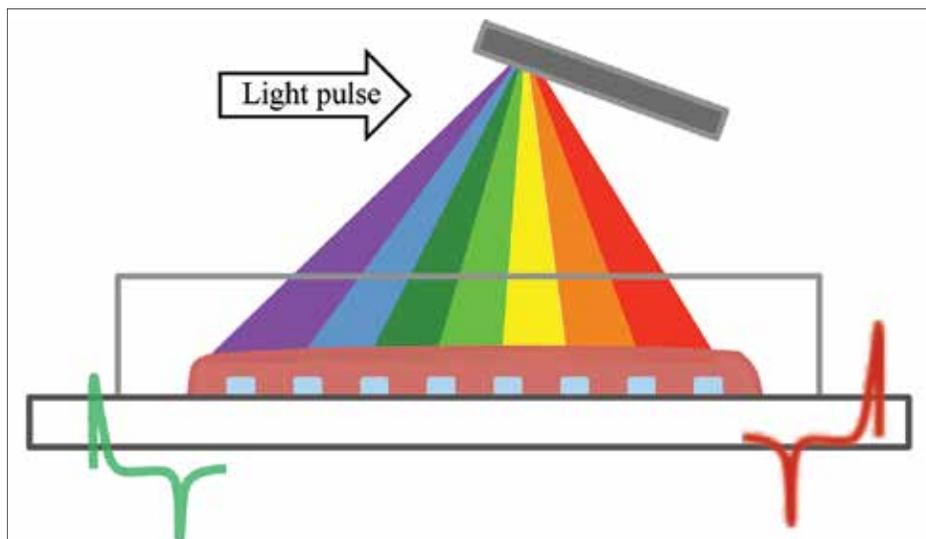


Fig.: Figure depicts a system for focusing various wavelengths of the visible spectrum across a multi-electrode array in accordance with an illustrative embodiment.

New Wings for Turboprop Aircraft

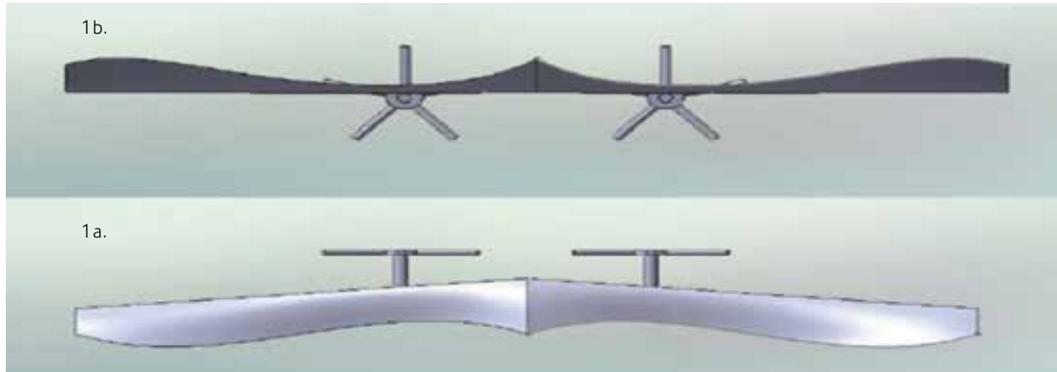


Fig. 1: Two views of a typical novel turboprop wing

1a: Shows the new plan-form.

1b: Is a view from behind the wing (wing twist magnified 20 times!); lower surface of the wing is coloured black to show how the trailing edge of the wing is twisted up along the span. At a wing lift coefficient of 0.27 the drag is about 8.7% lower than that of a typical current wing of same area and span.

Indian Patent Application No. : 1580/CHE/2009
 Industrial Design Regd. No. : 223622
 International Patent Application No.: PCT/IN2010/000448
 National Phase Applications filed : USA, Europe, Japan, China, Korea and Brazil
 Patent Issued : Korea No.10-2012-7002975, USA – Notice of Allowance received
 Inventors : Roddam Narasimha, SM Deshpande, Praveen Chandrashekarappa, Rakshith Belur Raghavan

Technology

This invention proposes novel wing plan-forms for aircraft driven by propellers mounted ahead of the wings, including in particular turboprops. Turboprops are inherently more fuel-efficient than turbojets or turbofans but are slower.

Advantages

The present aerodynamically more efficient wings can cut down fuel consumption further or increase flight speed or do bits of both. This development can thus make turboprops greener and/or faster and more productive.

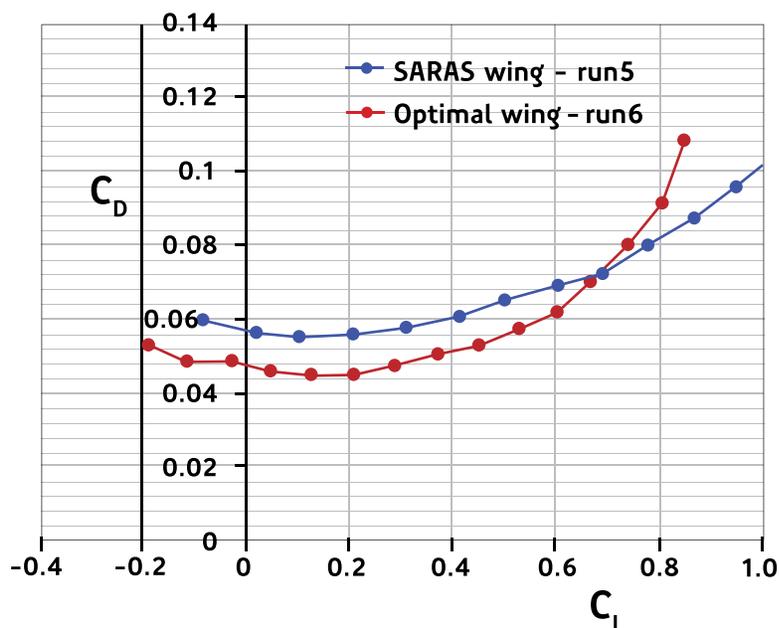
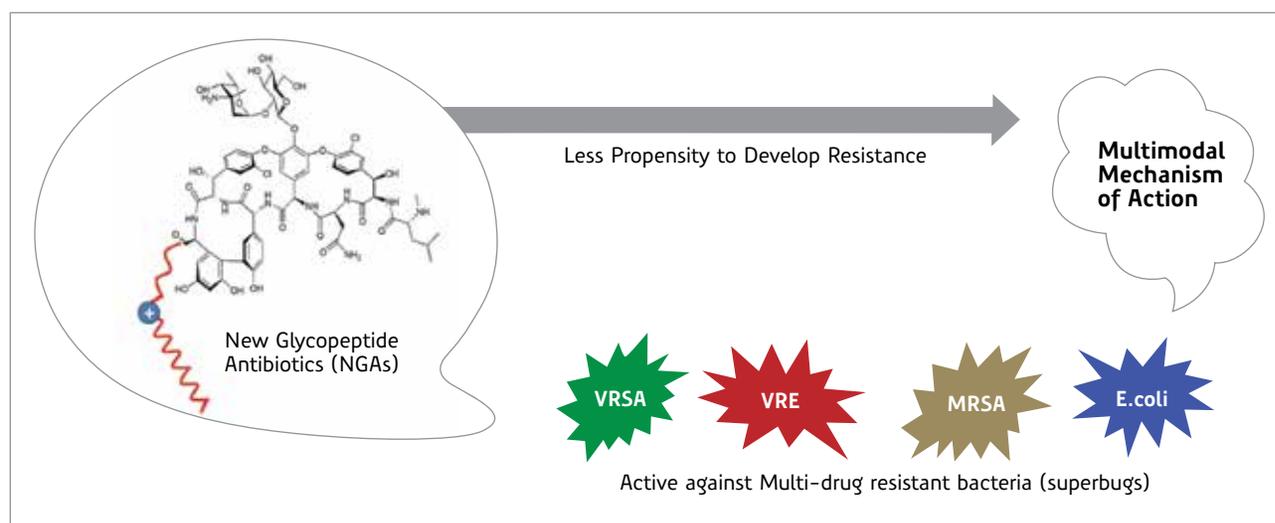


Fig. 2: Proof of concept by Wind tunnel test

Shows a proof of the concept from wind-tunnel test data on an aircraft model, in which the new wing brought down the total aircraft drag by 15% (red curve) relative to current design (black curve) at cruising speeds.

Development of a New Generation Antibiotic for the Treatment of Multidrug-resistant Bacterial Infections



Indian Patent Application No. : 3889/CHE/2011
 International Patent Application No.: PCT/IB2012/056373
 National Phase Applications filed : India, USA, Europe, Australia, Canada and Korea.
 Inventors : Jayanta Haldar, Venkateswarlu Yarlaagadda and Padma Akkapeddi

Invention

This invention offers new generation of antibiotics, NGAs for the treatment of infections plagued by drug-resistant bacterial pathogens. NGAs can revolutionize the antibiotic development as they curb bacterial resistance.

Advantages

Unlike existing antibiotics, NGAs stall the development of bacterial resistance and display multimodal mechanism of action against broad spectrum of bacteria with improved pharmacological properties.

Candidate	Lead optimisation	Validation of efficacy	Evaluation of safety in mice	Validation of efficacy in mice	Pharmacokinetics & Pharmacodynamics	Clinical trials
New Glycopeptide Antibiotic	→					

Copyright

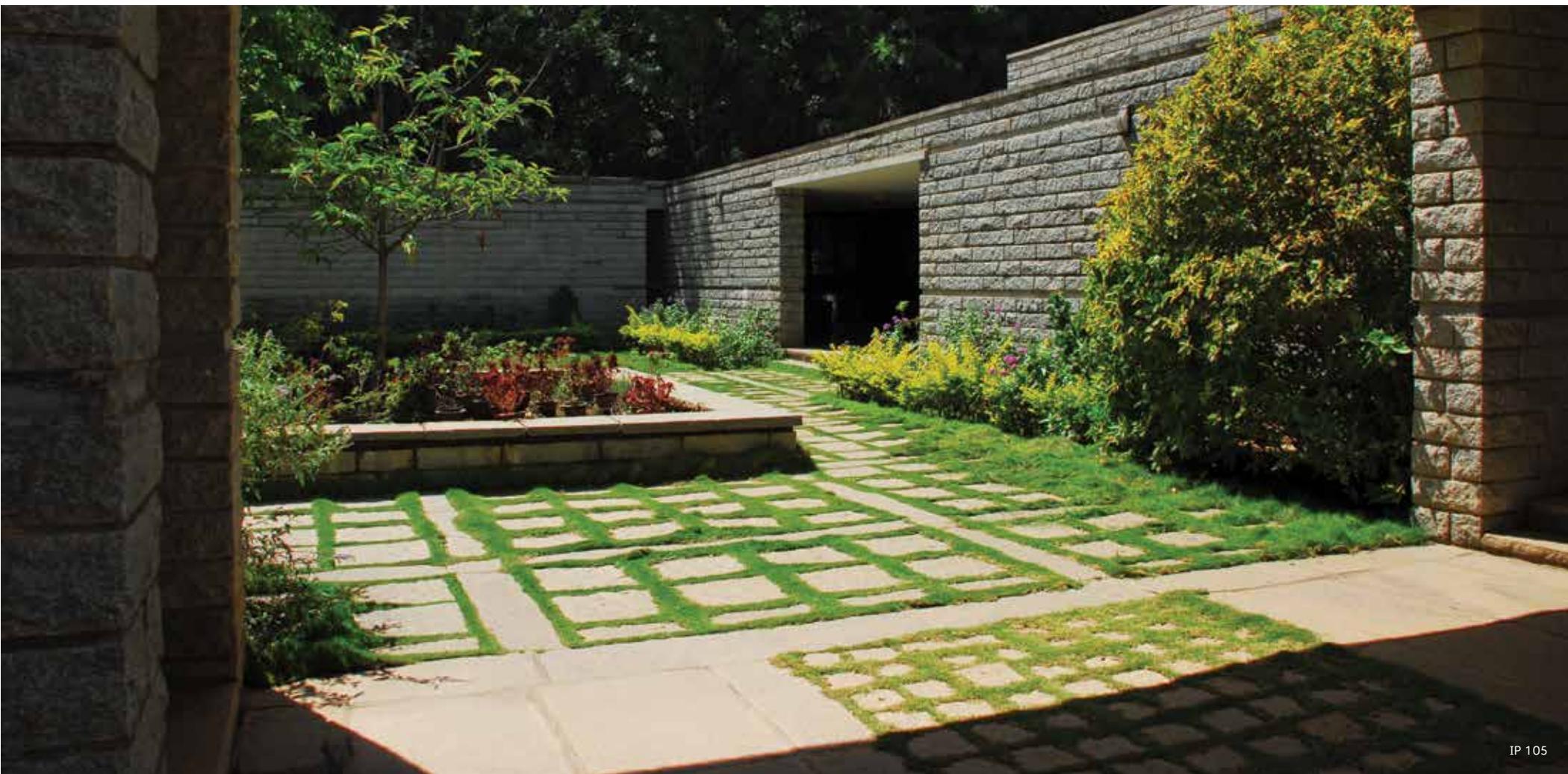
The Centre also holds copyright over a number of educational monographs and multimedia packages on interesting areas in science and technology.

Industrial Design

The Industrial Design for 'Wings for Propeller Driven Aircraft' developed by Roddam Narasimha, Madhusudan Deshpande, Praveen Chandrashekarappa and Rakshith Belur Raghavan has been registered.

Partner with us

The Centre's IP generation has strengthened its scientific and industrial acclaim and the activity is steadily growing. The Centre has been ranked in the top 10 Indian Applicants for Patent from Institutes and Universities by the Indian Patent Office for the year 2012-2013. The Centre is on a continuous look out for partners to enable and translate the inventions to commercialisation.





CENTRAL FACILITIES

Library

JNCASR Library has a core collection of books, journals, reference materials, conference proceedings and monographs. A comprehensive collection of online journals is subscribed in all areas of research being pursued at the Centre. We also meet the ever-growing needs for resources through inter-library resource sharing from institutions across India.

Quick facts

- Books: 8000+
- Online journals: 5000+
- Online databases: SciFinder, Web of Science
- Backfiles of journals: Elsevier, JSTOR, Science (AAAS), Nature Publications.
- Theses: 300+

To know more about Library, visit
<http://lib.jncasr.ac.in>
Write to us: library@jncasr.ac.in
Talk to us: +91 80 2208 2775/2713

Important links

JNCASR Institutional Repository:
<http://lib.jncasr.ac.in:9090/xmlui>
Online Catalogue:
<https://lib.jncasr.ac.in:8081>
Library Help Desk:
<http://lib.jncasr.ac.in/ddsticket>

Computer Laboratory

Computer Laboratory (CompLab) is responsible for establishment and maintenance of computer and network facilities at JNCASR, and its connectivity with the rest of the world through internet. Its goal is to continuously evolve the information technology (IT) resources at the Centre that meet the IT requirements of the highly heterogeneous community ranging from Administration, Scientists and Engineers, facilitating cooperation and collaborative interactions amongst them. It interfaces with every Unit and section at JNCASR, seeks inputs from a broad set of users in planning the IT infrastructure. This includes various servers, softwares, local area network (LAN), internet links, multi-media communication over internet and high performance computing (HPC) housed in the Central Facility. In addition, CompLab provides support and services to maintain computing resources in different groups at JNCASR, efficiently through an online ticketing system (www.jncasr.ac.in/complab).

CompLab hosts email, web, proxy and gateway servers of the Centre, Link-load-balancer, IronPortC150 (a spam-controller), a Firewall and maintains many other servers that cater to Purchase, Canteen and Library. An uninterrupted

LAN connectivity within the Centre is achieved at 1 Gbps with Optical Fiber Cable (OFC) backbone, CAT-6 network cables and a manageable chassis switch. The centre is connected to internet via 10 Mbps + 25 Mbps leased lines from BSNL & HCL Infotech, respectively. As a member of the National Knowledge Network, CompLab is expected to host a link at the band-width of 1 Gbps. CompLab maintains HPC resources at a moderate level, and has plans to expand them further. A centralized back-up facility via NAS/SAN helps store critical data from various servers as well as those from the Purchase and Accounts sections. Infrastructural support is given for Windows, Mac and Linux based machines across the Centre.

In addition to the Server and Cluster laboratories, CompLab maintains a 24-hour central computing facility of two terminal rooms with printers and several desktop Linux and Windows PCs running equipped with a wide range of the scientific softwares and databases.

Each member of JNCASR has a quota and access to free print-outs from CompLab's high-quality colour and monochrome printers.

In the near future, CompLab plans to further enhance the Email server, acquire Video (both Archival and Live) Streaming solutions.

Email: complab@jncasr.ac.in
Web: www.jncasr.ac.in/complab





Animal Facility

Situated in a secluded corner of the campus, Central Animal Facility (CAF) provides an excellent environment for animal care. The primary responsibility of the facility is supply, husbandry and quality control of animals used for various research programmes. The facility is equipped for studies on small animals and has a quarantine, breeding and experiment rooms for rodents and rabbits. The facility accommodates temperature and humidity regulated rooms with provision of clean air.

The facility has been registered for breeding and experimentation on laboratory animals under CPCSEA, Government of India (201/CPCSEA). An Institutional Animal Ethics Committee (IAEC) reviews the scientific projects before experiments are initiated and ensures compliance of animal research ethics guidelines during the course of the research work. Procurement of animals from other sources is regulated by the animal facility. Personnel working in the facility have been trained for proper handling of the laboratory animals and husbandry techniques involved.

Following strains of laboratory animals are available. Mice: BALB/c, C57BL/6, 129/ Svj, DBA/2J, Swiss albino, CD-1, Nude mice; Rat: Wistar Rats; Rabbit: New Zealand White.

CAF Convener: Prof Anuranjan Anand,
Veterinarian: Dr RG Prakash.



ENDOWED CHAIRS AND HONORARY FACULTY

Endowed Research Professors

CNR Rao (Linus Pauling Research Professor)
FRS, FASc, FNA, FTWAS, Hon FRSC, Hon F Inst P
MM Sharma (Kothari Chair/JNCASR/Mumbai)
Ila Hiriyakkanavar (Hindustan Lever Research Professor)

Members of Society

In addition to the Council of Management, following are the members of the society:

Ramachandran A (Bangalore)
Roddam Narasimha (Honorary Professor)

Honorary Professors

V Krishnan (JNCASR)
KS Valdiya (JNCASR)
Roddam Narasimha (JNCASR)
MRS Rao (JNCASR)
Kalyan B Sinha (JNCASR)
Bal Krishnan N (SERC/IISc)
Balaram P (Former Director, IISc)
Bhan MK (New Delhi)

Chandan Dasgupta (Physics/IISc)
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Sood AK (Physics/IISc)
Srinivasan J (ME/CAOS/IISc)
Suresh Das (KSCSTE/Thiruvananthapuram)
Varshney Umesh (MCB/IISc)
Vijay Raghavan K (Secretary, DBT)



PAULING BUILDING

COUNCIL OF MANAGEMENT, ACADEMIC ADVISORY COMMITTEE, PRESIDENTS, HONORARY FELLOWS

Council of Management

The following are the members of the Council:

Dr P Rama Rao Hyderabad	Chairman
President, JNCASR	Member (Ex-officio)
Prof CNR Rao Hon. President, JNCASR (JNC nominee)	Member
Prof Ashutosh Sharma Secretary, DST	Member (Ex-officio)
Shri JB Mohapatra Joint Secretary & Financial Adviser Department of Science & Technology	Member (Ex-officio)
Dr Baldev Raj Director, NIAS	Member
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Prof SK Joshi NPL, New Delhi (UGC nominee)	Member
Prof Anurag Kumar Director, IISc	Member (Ex-officio)
Mr AN Jayachandra Sr Administrative Officer, JNCASR	Secretary (Ex-officio)

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Prof KS Narayan

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Member

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Member

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IISER, Thiruvananthapuram

Member

Prof DD Sarma

SSCU, IISc

Member

Prof Devang V Khakhar

Director, IIT, Mumbai

Member (UGC Nominee)

Mr AN Jayachandra

Sr. Administrative Officer, JNCASR

Secretary (Ex-officio)

Presidents

2013 onwards: Prof KS Narayan (President In-charge)

2003 – 2013: Prof MRS Rao

2000 – 2003: Prof V Krishnan

1989 – 1999: Prof CNR Rao



Honorary Fellows

Ms Kiran Majumdar-Shaw	2015
Sheikh Saud Bin Saqr Al Quasimi	2013
Prof Antony K Cheetam	2012
Dr Manmohan Singh	2010
Dr Kapil Sibal	2010
Prof MS Swaminathan	2009
Prof S Varadarajan	2006
Prof Arcot Ramachandran	2005
Prof MM Sharma	2003
Prof CNR Rao	2000
Mr NR Narayana Murthy	1999
Prof C Subramaniam	1998
Prof Raja Ramanna	1995
Dr KR Narayanan, Former President of India	1995
Dr Ashok Ganguly	1995





ADMINISTRATION

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Dean, Academic Affairs	Shobhana Narasimhan
Dean, Fellowships and Extension Programmes	Maneesha S Inamdar
Dean, Research and Development	KS Narayan
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Associate Warden	Ranjani Vishwanatha
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Assistant Administrative Officer	CS Chitra
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Jr. Accounts Officer	Venkatesulu B
Sr. Stores & Purchase Officer	K Bhaskara Rao
Sr. Library-cum-Information Officer	Nabonita Guha
Sr. Secretary to President	A Srinivasan
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Project Engineer Gr.II (Civil)	Nadiger Nagaraj
Junior Engineer (Civil)	Veerasha NR
Junior Engineer (Elec.)	Sujeeth Kumar S
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Consulting Lady Medical Officers	Kavitha Sridhar
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Honorary Medical Officers	L Sharada
	C Satish Rao
	R Nirmala
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A lush green garden with a stone path, hedges, and trees. The path is made of large, flat, light-colored stones set in a grassy area. There are several hedges of varying heights and colors, including a prominent yellow-green one. Large trees with dense foliage surround the garden, and a white building is visible in the background.

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Dr Subi J George
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DESIGN

www.TheFool.in

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