# Annual Report 2012-13

Jawaharlal Nehru

**Centre For Advanced** 

**Scientific Research** 



Jakkur, Bangalore – 560 064 www.jncasr.ac.in



Linus Pauling Lecture : "The antimicrobial defense of Drosophila : A paradigm for innate immunity from liestohumans", speaker : Prof. Jules Hoffmann (Nobel Laureate), Institute of Molecular and Cellular Biology, University of Strasbourg, France, 12th October 2012



**5th Bangalore Nano Award** to Prof. G.U. Kulkarni, Chemistry & Physics of Materials Unit, 5-7 December 2012.



Atomic Layer Deposition System (ALD), TFS 200 installed at Sheikh Saqr Laboratory at International Centre for Materials Science.



Merck Millipore "India Innovation Award 2012" to Prof. Tapas Kumar Kundu, Transcription and Disease Laboratory, Molecular Biology & Genetic Unit.



ISRO Satish Dhawan Lecture : "Science for Musical Excellence of the Mridangam", Speakers : Vidhwan Umayalpuram Sivaraman & Dr. T. Ramasami, Secretary, DST, 16th October 2012.



Hindi translation of 'Chemistry Today' published and marketed by M/s Sastha Sahitya Mandal, New Delhi.



Special Lecture : "Recent trends in neurosurgery", speaker : Dr. D.V. Rajakumar, Consultant and Surgeon, Fortis Hospital, Bangalore, 11th April 2012.



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## THE CENTRE

### Foreword

I have great pleasure in presenting the Twenty Fourth Annual Report for the year 2012-13.

The Centre has been emerging as one of the leading institutions in the country for higher learning and research in frontier areas of science and engineering. The Centre has also been recognized as a Deemed to be University.

There is a steady increase in the number of research students in the Centre pursuing various academic programmes. The present student strength is 273. Forty two students joined the Centre during August 2012 admissions including seven students who joined during mid-year admission in January 2013. Sixteen students were awarded Ph D degrees, four with M S (Materials Science), seven with M S (Eng.), three with M S in Biological Sciences and one student was awarded M S in Chemical Sciences. In order to provide opportunities to teachers and others to obtain training and for carrying out science education projects, this Centre is offering a postgraduate diploma programme in science education. The academic, research, fellowship and extension programmes have been progressing as envisaged. The publication record is growing steadily. The faculty members have made significant scientific contributions. Prof. CNR Rao received the prestigious 2012 Award for International Cooperation by The Chinese Academy of Sciences. It is also a matter of great honour that Prof. Roddam Narasimha has been awarded the Padma Vibhusan, one of the most prestigious civilian awards of the country, Awards like India Innovation Award from Merck Millipore company to Prof. Tapas Kumar Kundu and his research team, India Citation Award 2012 from Thomson Reuters to Prof. Umesh Waghmare, CRSI Bronze Medal to Dr. Tapas Maji are the recognition earned by our faculty recently for their outstanding work in their respective fields. Adding a new dimension, the Federation of Indian Publishers have been given the Awards for Excellence in Publishing to the Kannada Book 'Nanoprapancha' authored by Prof. C.N.R. Rao and translated by Mrs. Indumati Rao.

The continuous recognition of our faculty members with several honours has reflected our standing within academic peers.

This year significant progress has been made in all spheres of academic activities at the Centre. A series of programmes were organized by Education Technology Unit (ETU) and Hall of Science toward the promotion of science education.

The C.N.R. Rao Hall of Science and Education Technology Unit has continued conducting the highly popular Teachers/students programs/workshops for students and teachers. In the POCE program for the year 2012, multimedia CD-ROM `NANOWORLD' was presented and a quiz was conducted from the CD-ROM `Understanding Chemistry' for the students followed by a visit to the `Chemistry of Materials Exposition' and Prof. C.N.R. Rao Archives. The book titled "Challenges and Opportunities in Science and Technology (Approach to an Action Plan)" was made ready by ETU for the Science Advisory Council to the Prime Minister. Outstanding Science Teacher Prize function and Lecture Program was organized to recognize outstanding science teachers in the country. Three-day Special Teacher Training Lecture Program was organised in Physics, Chemistry and Biology for PU teachers for which teachers from various Pre-University Colleges were deputed by The P.U. Board, Govt. of Karnataka.

During the financial year, 21 patent applications (Indian Provisional Application: 7, Indian Complete Application: 1, International Patent Application under PCT: 6, USA: 5, Europe: 1, China: 1) were filed and 4 US patents were granted.

The Centre maintains its vibrant academic activities through conferences, seminars, colloquia and discussion meetings.

The infrastructure is being constantly upgraded to meet the academic requirements and for scientific and student activities. All these developments would not have been possible without the continuous support from the Department of Science and Technology.

M R S RAO President

#### **INTRODUCTION**

The Jawaharlal Nehru Centre for Advanced Scientific Research (INCASR), Bangalore, a premier research institute in the country, was established in the year 1989, the birth centenary year of Pandit Jawaharlal Nehru, by the Department of Science and Technology. The objectives of the institute shall be to pursue and promote scientific research and training at the highest level in the frontier and interdisciplinary areas of science and engineering. The number of publications in international journals of repute and the filing of patents are steadily increasing year by year. The Centre, which is just twenty four years old, is creating news regularly in the scientific world with its breakthrough discoveries. The Centre has research collaborations with several national and international institutions. In recognition of the achievements of the Centre, the Ministry of Human Resource Development (GOI) has accorded the status of Deemed University, to enable the Centre to train quality manpower. The faculty members of the Centre have received national and international recognitions. Several faculty members of the Centre are Fellows of National and International science and engineering academies.

Prof C N R Rao, the founder of the Centre, held the office of President from 1989 to 1999. He is presently the Honorary President of the Centre and Chairman of the Scientific Advisory Council to the Prime Minister. Prof V Krishnan, who succeeded him, served as its President from 2000 to 2003. Prof M R S Rao is presently the President of the Centre.

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## **OBJECTIVES**

#### The objectives of the Centre are:

- To carry out front-line research in selected thrust areas of science and engineering;
- To promote collaborative research with scientists at the Indian Institute of Science and other institutions in the country;
- To provide a national and international forum for in-depth discussions on important scientific topics in areas of vital interest to scientists of the Centre and in the country at large;
- To organize periodic winter and summer schools in certain areas, where young talented scholars would be associated;
- To provide opportunities for talented young students to carry out research projects;
- To provide facilities to visiting scholars and faculty, from all over India and abroad, to work for extended periods with the faculty of the Centre;
- To publish monographs and reports on frontier and futuristic areas of science as well as monographs of educational value.

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# PROGRESS

The Centre has just completed 24 years encompassing several memorable and exciting moments. Following are the research units: Chemistry and Physics of Materials Unit, Educational Technology Unit, Evolutionary and Organismal Biology Unit, Engineering Mechanics Unit, Geodynamics Unit, Molecular Biology and Genetics Unit, and Theoretical Sciences Unit, the International Centre for Materials Science, New Chemistry Unit, and new Unit/Centre like the Thematic Unit of Excellence in Computational Materials Science is the newer in the lot. The new Nanoscience Centre is equipped with the state of the art facilities for advanced research in materials science.

The Centre is equipped with a good Library, an excellent computer support facility, Lecture Halls, a Chemical Education Laboratory, Conference and seminar halls, Faculty Offices and the Administrative Office. A seminar hall, a well-furnished accommodation for academic visitors and a Visitor House are also located at IISc campus.

During the year, forty two students joined the Centre during August 2012 admissions including seven students who joined during mid-year admission in January 2013. Sixteen students were awarded Ph D degrees, four with M S (Materials Science), seven with M S (Eng.), three with M S in Biological Sciences and one student was awarded M S in Chemical Sciences. Currently about 273 scholars are pursuing their research career. The research and training at the Centre has led to the award of 150 Ph D degrees, 41 M S (Engg.), 3 M S (research), 47 M S(of Int Ph.D) and 1 M Sc (by research) so far. The Centre has emerged as a place for interdisciplinary research, with effective interactions among scientists with backgrounds in biology, chemistry, engineering and physics. The JNC community has been working not only in pursuit of research, but also on dissemination of science-related activities reaching out to the common man.

Prof. CNR Rao received prestigious 2012 Award for International Cooperation by The Chinese Academy of Sciences. It is also a matter of great honour that Prof. Roddam Narasimha who has been awarded the Padma Vibhusan, one of the most prestigious civilian awards of the country. Faculty members have received several prestigious awards in their field like India Innovation Award from Merck Millipore company and Ranbaxy Research Award to Prof. Tapas Kumar Kundu, India Citation Award 2012 from Thomson Reuters to Prof. Umesh Waghmare, CRSI Bronze Medal to Dr. Tapas Kumar Maji, Bangalore National Nano Award to Prof. G.U. Kulkarni, Dr. Raja Ramanna Science and Technology Award for Science and Education from Karnataka State Council for Science & Technology - 2013 to Prof. S.M. Shivaprasad, TWAS Prize in Chemistry, 2012 to Prof. Swapan Kumar Pati, National Bioscience Award for Career Development 2012 to Prof. Kaustav Sanyal, and MRSI Medal, 2013 to Dr. Subi J. George. There are several prestigious fellowships which have been awarded to faculty members, such as Einstein Professor of Chinese Academy of Sciences 2012, Erudite Visiting Professorship from Mahatma Gandhi University, Kottayam and Academy Professor, Academy of Scientific & Innovative Research 2013 to Prof. C.N.R. Rao; Prof. P. Rama Rao has received Fellowship of National Academy of Engineering, USA; Honorary Visiting Professorship of Department of Biochemistry, I.I.Sc to Prof. M.R.S. Rao; Hon. Distinguished Professorship of ISRO and Academy Professor of Academy of Scientific and Innovative Research to Prof. Roddam Narasimha; Prof. K.B. Sinha elected as Emeritus Scientist of Indian Statistical Institute, Kolkata; Prof. Shobhana Narasimhan received Indo-Australia Senior Scientist Visiting Fellowship for the year 2012-2013 by INSA; Visiting Professorship Award (2013), by Yukawa Institute for Theoretical Physics, Kyoto University, Japan to Prof. Meheboob Alam; Sheikh Saqr Senior Fellow, 2012 to Prof. G.U. Kulkarni, DST J C Bose Fellowships to Prof. Swapan Kumar Pati and Prof. Umesh Waghamare; TWAS Young Affiliateship, 2012-2017 and Sheikh Saqr Fellow, 2012 to Prof. Tapas Kumar Maji; 2012-2013 Fulbright-Nehru fellowship for senior researchers to Prof. Ganesh Subramanian; DBT Wellcome Trust Fellowship to Dr. Ravi Manjithaya.

Several Ph.D. students have received awards and Best Poster prizes at national and international fora as a recognition to their contributions to science.

The Faculty members of the Centre have published around 300 scientific papers in reputed international journals during the year 2012-13, some of the journals are having high impact factor.

Many patent applications were filed for new inventions. Details are provided in a separate section on "Intellectual Property".

The interactions with academic institutions and universities globally have continued and the Centre is expanding

its formal ties in respect of collaborative research, exchange of graduate students and consultancy projects.

Honorary Faculty Members of the Centre have continued to play an important role in guiding academic and extension activities of the Centre.

Summer Research Fellowships, Project Oriented Chemical Education Programme, Project Oriented Biological Education Programme, Visiting Fellowships, Extension Programmes and Academic Exchange Programmes have attracted wide attention and have been highly successful.

For the Summer Research Fellowships programme, 73 students were selected and offered the fellowships this year. For POCE 2013-15, 10 meritorious students were offered the fellowship. Nine students of POCE-2010-12 were awarded Diploma in Chemistry. Under POBE 2013-15, 10 candidates joined the programme. Eight students of POBE 2010-12 batch received their Diploma in Biology certificates this summer on successful completion of their 3 year project training. Eight candidates have been selected to the Visiting Fellowships Programme 2012-13 under the Physical Sciences category and two under the Biological Sciences category. JNCASR-CICS Fellowship were awarded to 8 candidates from Nigeria, Yemen, Bangladesh and Armenia.

Since the beginning of the financial year 2012-13, ten Discussion Meetings, twenty four International Conferences, Workshops, and Schools were supported, either wholly or partially by the Centre. Around ninety nine seminars were held including nine Endowment Lectures and three General Lectures delivered by eminent scientists.

# HIGHLIGHTS OF RESEARCH AND OTHER ACTIVITIES

#### Research

#### **Chemistry and Physics of Materials Unit (CPMU)**

Clay-RGO hybrids have been prepared and their application in simultaneous adsorption of protein and DNA has been investigated. It was found that the water dispersible aminoclay is very efficient in dispersing the reduced grapheme oxide(RGO) in water at higher concentration. Hierarchical metal structures have been synthesized by a modified approach to nanoimprint lithography. A multi-state memory device has been realized based on electrically activated Pd oxide. Work had been undertaken towards understanding the formation of a) low carrier concentration InN thin films and its dependence on the kinetics of growth and surface modifications, and b) atomistic details of the wurtzite GaN nanorod and nanotubes formation on Al<sub>2</sub>O<sub>2</sub> substrates. The molecular features which govern the mechanism of supramolecular polymerization had been identified and delineated. It was discovered that density functional theory and empirical potential based MD simulations of liquid dimethyl carbonate, an environmentally benign solvent have shown clustering of conformers with high dipole moment. Two new families of multiferroic materials were investigated, namely  $RMO_3$  (M = Cr and Fe) and YMM'O<sub>3</sub> (M and M' are two different transition metals such as Cr, Mn and Fe). The Molecular Electronics lab carried out studies of photo-physical properties of semiconducting polymers, fabrication and device physics of organic solar cells and polymer based field effect transistors. Raman studies of RMO, (M = Cr, Fe, Mn) were carried out to understand the microscopic origin of multiferroicity in these compounds. Microscopic origin of gas adsorption in metal organic frameworks was investigated using Raman spectroscopy. First demonstration of SERS as a tool for determining small molecule binding to therapeutic proteins was demonstrated in the case of Felodipine and Aurora A.

#### **Education Technology Unit (ETU)**

The Education Technology Unit has been actively involved in the concept, development and production of multimedia CD-ROMs and books especially for school students and teachers in various disciplines of science, including resources in vernacular Indian languages. The C.N.R. Rao Hall of Science and Education Technology Unit has continued conducting the highly popular Teachers/students programs/workshops for students and teachers. These workshops/programs are conducted in different subjects like Physics, Chemistry and Biology. The Book `*Rasaayanshaastrada Arivu*' authored by Prof. C.N.R. Rao was translated by Mrs. Indumati Rao and produced by ETU for Karnataka Rajya Vijnana Parishath (KRVP).

In the POCE program for the year 2012, ETU presented the multimedia CD-ROM `*NANOWORLD*' and a quiz was conducted from the CD-ROM `*Understanding Chemistry*' for the students. A Webpage for the Hall of Science was a project taken up jointly by ETU & Complab.

The CNR Rao Hall of Science and ETU organized the Outstanding Science Teacher Prize function and Lecture Program on June 29, 2012. The awardees for the year 2011 are Shri. S.V. Burli and Smt. M. S. Rekha. A Special Teacher Training Three-day Lecture Program in Physics, Chemistry and Biology for PU teachers was organised.

ETU is engaged in producing a book for the Science Advisory Council to the Prime Minister titled *Science in India* (2004-2013)'.

#### **Engineering Mechanics Unit (EMU)**

*Prof. Roddam Narasimha's group*: in the area of Aerospace and Atmospheric Fluid Mechanics, the concept underlying a novel design of optimal wing planforms for turboprop aircraft, determined through special algorithms developed at JNC, have now been confirmed by wind tunnel tests conducted by NAL at IISc. Comprehensive simulations of a free shear layer in a vortex gas have been completed. It is shown that the vortex gas evolves to a stationary state characterizing a variant of Lundgren-Pointin equilibrium. In atmospheric fluid dynamics, entrainment measurements have been made in a transient diabatic jet for the first time.

In *Prof. K.R. Sreenivas's group*, results from the study of nocturnal atmospheric boundary layer has culminated in the publication of a set of three papers, two in Journal of Atmospheric Sciences and one in Quarterly Journal of Royal Meteorological Society. In this study an error was indentified in the flux-emissivity model for radiation widely used by many researchers in the atmospheric community. The error was responsible for spurious cooling

reported in many studies, and its effect extends all the way up to 1 km in the atmospheric boundary layer.

*Prof. Meheboob Alam's research group* was involved in experimental works on vertically vibrated binary granular mixtures which lead to exciting new results. A variety of phase-coexisting patterns was uncovered, characterized by the coexistence of patterns having different spatial and temporal symmetries.

Research group led by *Prof. Ganesh Subramanian* worked on concentration fluctuations in bacterial suspensions; bacterial suspension rheology; particle-level simulation; Vortex Rings Oscillations; sonic transition in viscoelastic flows; role of micro-scale inertia in multiphase heat-transfer.

#### Evolutionary & Organismal Biology Unit (EOBU)

The faculty of EOBU continued their research in the broad areas of animal behaviour /phylogeography, chronobiology, evolutionary genetics, neurogenetics, and population dynamics. Research in this unit had been in the areas of (a) biogeography of large mammals in the Western Ghats, (b) social organization in Asian elephants, (c) behavioural, neurogenetic and molecular bases of *Drosophila* circadian clocks, (d) evolution of adaptations to crowding, especially the interplay of food deprivation and waste buildup, (e) fruitflies as a model system for neurodegenerative disorders, (f) behavioural neurogenetics, (g) circadian entrainment by temperature cycles, (h) fruitfly metapopulation dynamics and stability.

#### Molecular Biology and Genetics Unit (MBGU)

MBGU currently has several research and training avenues in broad areas of biological sciences. Research in nine of its laboratories spans diverse areas of modern biology with emphasis on biomedicine.

*Autophagy Laboratory* studied autophagy and autophagy-related pathways. A new live cell assay have been designed to kinetically monitory general and selective autophagy pathways and have miniaturized it to suit the high throughput format.

*Molecular Mycology Laboratory* studied structure-function analysis of centromeres of several pathogenic yeasts: *Candida albicans, Candida dubliniensis, Candida tropicalis* and *Cryptococcus neoformans*. They observed that centromere DNA sequences are rapidly evolving when *C. albicans* and *C. dubliniensis* orthologous chromosomes were analyzed.

*Transcription and Disease Laboratory* aimed to understand the different aspects of chromatin functional dynamics which are responsible for the gene regulation and its link to cellular physiology and pathobiology. Two different diseases are being investigated in this context, namely cancer (oral cancer and breast cancer) and AIDS. It was found that human chromatin associated protein PC4, gets acetylated *in vivo* and possibly enriched in the transcriptionally active chromatin.

In *Vascular Biology Laboratory*, **o**ver the last year, significant progress was made in understanding mechanisms that maintain stem cell potency. The endosomal protein Asrij was identified as being essential for maintaining the balance between the pluripotent stem cell state and the differentiated state. Further it was showed that Asrij has a conserved function in maintaining stemness. A transcriptome analysis of rudhira mutants was performed and several key pathways were identified through which rudhira mediates its function.

*Human Molecular Genetics Laboratory*, in a study of over 750 families with non-syndromic hearing loss, has examined several deafness-causing genes (Cx26, Cx30, TMPRSS3, TMC1, HAR, CDH23, PDS and TMIE) and identified a large number of pathogenic mutations in these genes. This work has substantially extended allelic heterogeneity at these genes and provided a collection of mutant alleles for potential use in cell biological, biochemical and structure-function correlation studies. Another significant contribution made by the lab is the identification of a locus, DFNA59 for prelingual, profound, sensorineural hearing loss at chromosome 11p14.2-q12.3.

Research in one of the *Molecular Parasitology Laboratories* headed by Prof. Hemalatha Balaram has focused on understanding metabolism in the malaria parasite *Plasmodium falciparum*. Towards this end the enzymes involved in purine nucleotide metabolism in the parasite had been studied. Comparative structure-function analysis is also being carried out on the homologues from humans and archaea. Adenylosucinate synthetase from

*M. jannaschii* has been characterized biochemically. Another Parasitology lab in the unit headed by Prof. Namita Surolia is focusing its efforts on the role of *Plasmodium* kinases in host-pathogen interactions. This group has been focusing on understanding the molecular mechanism underlying the pathogenesis of cerebral malaria in Indian patients through a "Systems -Biology" approach. The group is also trying to decipher canonical and non-canonical intracellular trafficking pathways in Plasmodium falciparum, in the process they have found some novel proteins responsible for the development of the parasite. The group is also studying proteins involved in host-pathogen interactions.

In *Chromatin Biology Laboratory*, work in the chromatin TP2 is acetylated in vivo as detected by anti-acetylated lysine antibodies and mass spectrometric analysis. Recombinant TP2 is acetylated in vitro by p300 and PCAF. p300 acetylates TP2 in its C-terminal domain which is highly basic in nature possessing chromatin condensing properties. Molecular Parasitology Laboratory has focused on understanding metabolism in the malaria parasite Plasmodium falciparum. Towards this end the enzymes involved in purine nucleotide metabolism in the parasite are being studied.

#### New Chemistry Unit (NCU)

Several aspects of the chemistry of materials are being pursued by the research team led by *Prof. C.N.R. Rao.* These include transition metal oxides, nanomaterials and carbon materials. In transition metal oxides, multiferroic and magnetoelectric oxides are of interest. Work on inorganic nanomaterials includes synthesis, characterization, study of properties and phenomena. Carbon nanotubes and graphene are important areas being investigated.

*Dr. T. Govindaraju's* research activities were at the interface of chemistry and biology (*Organic synthesis, molecular probes, peptide chemistry, nucleic acid chemistry and bionanotechnology*). The design and synthesis of small molecules had been actively pursued including peptides, nucleic acids and their conjugates based biomimetic systems and materials possessing well defined nano-, meso- and micro-structures with properties similar to natural materials through Nature-inspired molecular self-assembly approach.

*Dr. Jayanta Haldar* had focused on infectious diseases in his research which continue to be one of the greatest health challenges worldwide and the threat is compounded by the fact that an increasing percentage of pathogens are developing resistance against the available drugs. The main focus of his research was towards the development of chemical and nanotechnology based innovative strategies to prevent the spread of infections and the development of new antimicrobial agents for the treatment of infectious diseases.

*Dr. Kanishka Biswas's research group* was focused on the synthesis and thermoelectric properties of cubic I-V-VI<sub>2</sub> (where I = Cu, Ag, or alkali metal; V = As, Sb, Bi; and VI = S, Se, Te) compounds both in bulk and nanocrystalline phases. Thermoelectric figure of merit, *ZT* of ~ 1.2 in lead free I-V-VI<sub>2</sub> compounds containing earth abundant Se in place of traditional rare and costly Te had been achieved, which has remarkable fundamental and technological importance.

The primary focus of research of *Dr. Ranjani Viswanatha's* research group was the synthesis and study of optical and magnetic properties of semiconductor nanocrystals. Towards that goal, her research group have been involved in the synthesis of Cu doped CdSe to use copper as a nanosensor to study the electronic structure and surface properties of CdSe.

*Dr. Sebastian C. Peter's research group* had focused on research in solid state inorganic materials such as intermetallics, chalcogenides and polyoxometalates from exploratory synthesis. They had discovered several new intermetallics, which are interest in terms of the structural diversity and physical properties.

The interface between synthetic efforts on  $\pi$ -conjugated systems and the organization of these molecules using supramolecular self-assembly principles, with the ultimate aim of developing novel functional materials was the underlying theme of research of *Dr. Subi Jacob George's research group*. In their approach, they targeted the electronic, optical and self-assembling properties of the  $\pi$ -conjugated backbone for the design of materials.

*Dr. Ujjal Gautam's research group* has investigated the possibility of C-H bond activation using metal peroxides with low decomposition temperatures. They had also investigated the efficient production of hydrogen fuel from

water by using semiconductor nanomaterials as catalysts.

*Prof. H lla's research group* had been involved for several years in design and development of new, highly efficient, innovative general methods for synthesis of a large variety of structurally diverse five/six membered heterocycles and their condensed analogs, which are structural components of a large number of pharmaceutical agents as pharmacophores of considerable importance. It was found that 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 rapid generation of combinatorial libraries for discovery and optimization of new lead structures in drug discovery research.

*Prof. Swapan K. Pati's research group* had worked on catalytic activities of a number of systems: Methane formation from hydrogenation of carbon dioxide on Ni (110) surface has already been studied.

*Prof. A. Sundaresan's research group* had investigated two new families of multiferroic materials, namely RMO<sub>3</sub> (M = Cr and Fe) and YMM'O<sub>3</sub> (M and M' are two different transition metals such as Cr, Mn and Fe).

*Prof.* M. Eswaramoorthy's reseach group had used aminoclay and laponite materials as scaffolds to organize organic chromophores and studied their light harvesting applications. It was discovered that these supramolecularly assembled, soft-hybrids are water-processable, showed high-transmittance and can be used for environmentally friendly, large-area-display fabrication.

*Dr. Sridhar Rajaram's reseach group* had explored perylene diimides as alternatives to fullerenes in organic solar cells. They showed that disrupting the planarity leads to a tenfold improvement of efficiency.

*Dr. Tapas Kumar Maji's research group* was actively involved in exploring various functional aspects of metalorganic frameworks (MOFs), covalent-organic frameworks (COFs) and conjugated microporous polymers (CMPs). Recently, They have synthesized a multi-chromophoric hybrid system where exciplex emission sensitized by energy transfer which is unprecedented.

#### Theoretical Sciences Unit (TSU)

*Prof. Umesh V. Waghmare's research group* worked in the area of multi-scale simulations of materials; fundamental Physics and Applications of Graphene; Materials with magnetoelectric coupling. Contributions were made to theory of electronic topological transitions, surfaces and interfaces.

*Dr. N. S. Vidhyadhiraja's research group* had pursued research in two directions: one is the development of a reliable and fast quantum many body technique for integration with band structure methods to be used for predictive modeling of strongly correlated electronic systems (SCES). The second direction is about investigations of heterogeneity in SCES.

*Dr. Subir K. Das's research group* has been actively involved in studies of equilibrium and nonequilibrium properties of various condensed matter systems.

*Dr. Kavita Jain* has worked in the area of adaptation dynamics of asexual populations in periodic selection regime; and evolution of mutation rates in adapted populations.

In *Prof. Swapan K. Pati's* group, research interests encompass a broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum systems. Methane formation from hydrogenation of carbon dioxide on Ni (110) surface has been studied.

#### **International Centre for Materials Science (ICMS)**

ICMS has expanded its infrastructure by installing sophisticated equipments like Superconducting Quantum Interference Device (SQUID), Inductively Coupled Plasma, Optical Emission Spectrometry (ICP-OES), UV Spectrometer, Photoluminescence Spectrometer (PL), etc. 9 scientists have visited ICMS under its short-term visitors' programme and. 2 have visited under the SSL project. It has also conducted several meeting and conferences during the financial year.

The Centre during the year has appointed Dr. Raju V. Ramanujan of Nanyang Technological University as Adjunct

Professor. RAK-CAM Sheikh Saqr Junior Fellowship has been awarded to Mr. Rana Saha and Ms. Sharvani S was awarded the Post Graduate Diploma in Materials Science.

*Prof. C.N. R. Rao's group* has initiated two major programmes on energy research: one related to artificial photosynthesis involving photocatalytic oxidation of water by nanoparticles of Mn and Co oxides and the other on photocatalytic  $H_2$  generation by hybrid nanostructures by using the Z-scheme. Synthesis, characterization and properties of anions substituted metal oxides where in oxygen is replaced by nitrogen and fluorine are being investigated.

Significant progress has been made on the formation and properties of nanomanifestations of III-nitride materials at *Prof. Shivaprasad's group*. Observation of magnetism at the apex of the nanowalls, coherent emission at the open screw dislocations and application as a versatile SERS substrate have been the highlights.

Aberration corrected atomic resolution imaging and quantification of oxygen atoms in ZnO has been performed by *Dr. Ranjan Datta's group*. Magnetic information from length scale as small as 5 nm from  $\text{CrO}_2$  in a TEM.

Research in the Soft Matter Lab of *Dr. Rajesh Ganapathy* mainly focused on two broad themes. The first was to understand the role of an external driving force on the dynamics of grain boundaries in sheared polycrystals. The second theme was to explore the role of particle shape anisotropy on glass transition dynamics and suspension rheology.

Perylene diimides were explored as alternatives to C70fullerenes in organic solar cells in the group of *Dr. Sreedhar Rajaram*. They showed that disrupting the planarity leads to a tenfold improvement of efficiency.

The primary focus of *Dr. Ranjani Vishwanatha's research group* is the synthesis and study of optical and magnetic properties of semiconductor nanocrystals. Towards that goal, they have been involved in the synthesis of Cu doped CdSe to use copper as a nanosensor to study the electronic structure and surface properties of CdSe.

#### Thematic Unit of Excellence in Computational Materials Science

The molecular features which govern the mechanism of supramolecular polymerization have been identified and delineated. Density functional theory and empirical potential based MD simulations of liquid dimethyl carbonate, an environmentally benign solvent have shown clustering of conformers with high dipole moment.

It was discovered, through density functional theory calculations, that doping the oxide substrate with an electron donor significantly reduces the barrier for oxygen dissociation on gold nanoparticles.

It has been shown that functionalizing graphene, either with various organic moieties on the edge, or by depositing various metal adatoms, significantly increases the binding of gases such as hydrogen and methane. This has implications for on-board vehicular storage applications.

It has been shown that the finding that magnetism drives surface alloy formation for FeAu/Ru(0001) does not hold for FeAu/Mo(110). This can be attributed primarily to the different nature of magnetic moments on substrate atoms in the two cases.

The electronic structure and energetics of defects in twisted bilayer graphene have been explored.

The effects of lead geometries on spin transport, spin spirals in surface alloy systems, photoswitching van der Waals crystals, and modification of surface work function by mixed SAMs.

A tri-lateral (India-UK-USA) grant was received to support research on solution of graphene and BN.

#### **Academic Activities**

During the year, forty two students joined the Centre during August 2012 admissions including seven students who joined during mid-year admission in January 2013. The present student strength is 273. Sixteen students were awarded Ph D degrees, four with M S (Materials Science), seven with M S (Eng.), three with M S in Biological Sciences and one student was awarded M S in Chemical Sciences.

#### Fellowships & Extension Programmes

For the Summer Research Fellowships programme, 73 students were selected and offered the fellowships this year. For POCE 2013-15, 10 meritorious students were offered the fellowship. Nine students of POCE-2010-12 were awarded Diploma in Chemistry. Under POBE 2013-15, 10 candidates joined the programme. Eight students of POBE 2010-12 batch received their Diploma in Biology certificates this summer on successful completion of their 3 year project training. Eight candidates have been selected to the Visiting Fellowships Programme 2012-13 under the Physical Sciences category and two under the Biological Sciences category. JNCASR-CICS Fellowship were awarded to 8 candidates from Nigeria, Yemen, Bangladesh and Armenia.

#### Reservation, Official Language and Implementation of the judgments/orders of the CAT

The Centre follows the national policy on reservation and official language as per rules and orders issued by the Government of India with necessary guidelines from the Council of Management from time to time. During the current year there were no cases pertaining to the Centre appeared before the CAT.

# **ACTIVITIES CHART**

# JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH





ANNUAL REPORT 2012-13

# THE ORGANISATION

## **Council of Management**

Administration and management of the affairs and finances of the Centre are conducted by the Council of Management. The Council of Management of the Centre meets twice a year.

The following are the members of the Council:

<b>Dr. P. Rama Rao</b> Hyderabad	Chairman
<b>Prof. M.R.S. Rao</b> President, JNCASR	Member
<b>Prof. C.N.R. Rao</b> Hon. President, JNCASR (JNC nominee)	Member
<b>Dr. T. Ramasami</b> Secretary, DST	Member
<b>Ms. Anuradha Mitra</b> (2011-14) Joint Secretary & Financial Adviser Department of Science & Technology	Member (Ex-officio)
<b>Dr. Baldev Raj</b> (2011-14) Director, IGCAR (DST nominee)	Member
<b>Prof. Chandan Dasgupta</b> (2011-14) IISc (IISc nominee)	Member
<b>Prof. S.K. Joshi</b> NPL, New Delhi (UGC nominee)	Member
<b>Prof. P. Balaram</b> Director, IISc	Member
<b>Mr. A.N. Jayachandra</b> Sr. Administrative Officer, INCASR	Secretary

## **The Finance Committee**

The Finance Committee of the Centre scrutinizes all financial proposals, and makes recommendations to the Council of Management.

The constitution of the Finance Committee is as follows:

<b>Prof. M.R.S. Rao</b> President, JNCASR	Chairman (Ex-officio)
<b>Prof. C.N.R. Rao</b> National Research Professor, JNCASR	Member
<b>Ms. Anuradha Mitra</b> Joint Secretary & Financial Adviser, DST	Member
<b>Shri. R.S. Gururaj</b> Sr. Accounts Officer, JNCASR	Member (Ex-officio)
<b>Prof. Chandan Dasgupta</b> Dean, Undergraduate Studies, IISc	Member
<b>Shri A.N. Jayachandra</b> Sr. Administrative Officer, JNCASR	Secretary (Ex-officio)

## **The Academic Advisory Committee**

The functions of the AAC include planning, execution and coordination of research and other academic activities of the Centre. It also regulates the courses of study, procedure for admission of students, examination, etc. It meets at least twice a year. The Committee makes its recommendations to the Council of Management on all academic matters.

The members of the Academic Advisory Committee are:

<b>Prof. M.R.S. Rao</b> President, JNCASR	Chairman (Ex-officio)
<b>Prof. K.B. Sinha</b> Dean, Faculty Affairs, JNCASR	Member (Ex-officio)
<b>Prof. G.U. Kulkarni</b> (2012-14) Dean, Academic Affairs, JNCASR	Member (Ex-officio)
<b>Prof. Namita Surolia</b> (2012-14) Dean, Fellowships and Extension Programmes, JNCASR	Member (Ex-officio)
<b>Prof. Chandrabhas Narayana</b> (2010-12) Dean, Fellowships and Extension Programmes, JNCASR	Member (Ex-officio)
<b>Prof. K.S. Narayan</b> (2012-14) Dean, R&D, JNCASR	Member (Ex-officio)
<b>Prof. Hemalatha Balaram</b> (2010-12) Dean, Academic Affairs, JNCASR	Member (Ex-officio)
<b>Prof. V. Nagaraja</b> (2012-14) Professor, MCB, IISc	Member
<b>Prof. U. Ramamurty</b> (2012-14) Professor, Mat. Engg., IISc	Member
<b>Prof. George K Thomas</b> (2012-14) IISER, Thiruvananthapuram	Member
<b>Prof. D.D. Sarma</b> SSCU, IISc	Member
<b>Prof. Devang V Khakhar</b> Director, IIT, Mumbai	Member (UGC Nominee)
<b>Mr. A N. Jayachandra</b> Sr. Administrative Officer, JNCASR	Secretary (Ex-officio)



## **Faculties**

All the faculty members are involved in various academic activities of the Centre and assist the Academic Advisory Committee in discharging its functions. The last Annual Faculty Meeting was held in November 2012 which included lectures by the faculty on the advances made in various research areas. Local faculty meetings were held in August 2012 and March 2013 to review the progress and provide inputs wherever required.

## Administration

President MRS Pao	$D = D (US_{c}) = A S_{c} = N A = N A S_{c} = AMS = TWAS$
	r II D (II3C), r A 3C, r IN A, r IN A 3C, rAM3, r I WA3
K B Sinha	Ph D (Univ. of Rochester), F A Sc, F N A, FTWAS
<b>Dean, Academic Affairs</b> G U Kulkarni	Ph D (IISc)
<b>Dean, Fellowships and Extension Pro</b> Namita Surolia	p <b>grammes</b> Ph D
<b>Dean, Research and Development</b> K S Narayan	Ph D (Ohio State Univ., USA), F N A Sc, F A Sc
Warden & Student Counsellor S.M. Shivaprasad	Ph D
<b>Associate Warden</b> Maneesha Inamdar	Ph D
<b>Sr. Administrative Officer</b> A N Jayachandra	B Com (Mysore), ICWA (Inter)
<b>Assistant Administrative Officer</b> C S Chitra	B Com (Bangalore)
Assistant Coordinator Princy Jaison Pereira	Ph D (Gujarat)
<b>Sr. Accounts Officer</b> R S Gururaj	B.Sc. (Mysore) M P Ed (Bangalore)
<b>Stores &amp; Purchase Officer</b> K Bhaskara Rao	M.Sc. (Hyderbad), M Phil (New Delhi)
<b>Library-cum-Information Officer</b> Nabonita Guha	MLIS (Varanasi)
Secretary to President A Srinivasan	B A (Hyderabad)
<b>Project Engineer</b> S Chikkappa	B E (Mysore)
<b>Junior Engineer (Civil)</b> Nadiger Nagaraj	DCE
<b>Junior Engineer (Elec.)</b> Sujeeth Kumar S	DEE

#### **Consulting Medical Officer**

B S Subba Rao

#### **Consulting Lady Medical Officers**

Kavitha Sridhar Archana, M L V HV Chandralekha

#### Physiotherapist

Y Yogesh

#### **Honorary Medical Officers**

G R Naghabhushan

- L Sharada
- C Satish Rao
- P K Raghupathy
- R Nirmala

#### **Honorary Security Officer**

M R Chandrasekhar

#### MBBS (Mysore)

MBBS (Bangalore) MBBS (Bangalore) MBBS

BPT - Mangalore

MBBS (Mysore), FCCP, FCGP, P G Dip in M&CH MBBS (DGO - Madras) MBBS (Mysore) MBBS (RGU) MBBS (Madras)

B Sc, LLB (Bangalore)

## UNITS, CENTRES, COMPUTER LABORATORY, LIBRARY AND ENDOWED RESEARCH PROFESSORS

## **Chemistry and Physics of Materials Unit**

Clay-RGO hybrids have been prepared and their application in simultaneous adsorption of protein and DNA has been investigated. The water dispersible aminoclay is very efficient in dispersing the reduced grapheme oxide(RGO) in water at higher concentration. The as-prepared clay-RGO hybrids show amphiphilic behavior and show good adsorption for DNA and proteins.

Hierarchical metal structures have been synthesized by a modified approach to nanoimprint lithography. A multistate memory device has been realized based on electrically activated Pd oxide.

Work has been undertaken towards understanding the formation of a) low carrier concentration InN thin films and its dependence on the kinetics of growth and surface modifications, and b) atomistic details of the wurtzite GaN nanorod and nanotubes formation on  $Al_2O_3$  substrates.

The molecular features which govern the mechanism of supramolecular polymerization have been identified and delineated. Density functional theory and empirical potential based MD simulations of liquid dimethyl carbonate, an environmentally benign solvent have shown clustering of conformers with high dipole moment.

Two new families of multiferroic materials were investigated, namely  $RMO_3$  (M = Cr and Fe) and  $YMM'O_3$  (M and M' are two different transition metals such as Cr, Mn and Fe). Although these materials have centrosymmetric structures they exhibit ferroelectricity at the magnetic ordering temperatures. The origin of ferroelectricity in  $RMO_3$  has been attributed to a combined effect of electric poling field and 3d-4f interactions. In the latter case, it is due to disorder at the B-site of the perovskite structure. Several other oxides were investigated for multiferroic properties.

The Molecular Electronics lab carried out studies of photo-physical properties of semiconducting polymers. Organic Photovoltaic and Field Effect Transistor devices had been fabricated and studied. The utility of conducting polymer interfaces for studying biophysical problems had been explored.

Raman studies of  $RMO_3$  (M = Cr, Fe, Mn) were carried out to understand the microscopic origin of multiferroicity in these compounds. Microscopic origin of gas adsorption in metal organic frameworks was investigated using Raman spectroscopy. First demonstration of SERS as a tool for determining small molecule binding to therapeutic proteins was demonstrated in the case of Felodipine and Aurora A.

#### New programme launched

High Pressure Brillouin Spectroscopic studies of topological insulators is being undertaken for the current academic year.

Following are the members of the Unit:

Chair	
S Balasubramanian	Ph D, F A Sc
Drofossors	
F101055015	
C. N. R. Rao	Ph D, D Sc, F A Sc, F N A, F R S, F T W A S, Hon. F R S C
S Balasubramanian	Ph D, F A Sc
K S Narayan	Ph D, F N A Sc, F A Sc.
G U Kulkarni	Ph D
S M Shivaprasad	Ph D
N Chandrabhas	Ph D, F N A Sc
Associate Professors	
Associate Trolessors	
A Sundaresan	Ph D
M Eswaramoorthy	Ph D

Tapas Kumar Maji Ph D

#### **Technical Officers**

V Sreenath (BE), S Srinivas (BE), Usha Govind Tumkurkar (M Phil)

#### **Research Students**

Partha Pratim Kundu, Narendra Kurra, Anshuman Jyothi Das, Sandeep Kumar Reddy, Satish Shetty, Venkata Srinu Bhadram, Jaya Ramulu Kolleboyina, Satyaprasad Premswarup Senanayak, Malleswararao Tangi, K.D. Mallikarjuna Rao, R. Bharath, K. Hima Nagamanasa, Ravichandran S, B.V.V.S Pavan Kumar, Gangaiah Mettela, Loukya Chowdary B, Rajdeep Singh Payal, Umesha Mogera, Amritroop Achari, Dhanya R, Gopalakrishnan K, Venkata Suresh M, B. Satyanarayana, Yelipeddy Sreedhar, S. Kiruthika, B. Karteek Kumar, A.Z. Ashar, Tarak Karmakar, Nivedita Sikdar, Devendra Singh Negi, Arpan De, Somnath Ghara, Sunita Dey, Sunil Walia, Sreedhara M.B, Sanjay Kumar Nayak, Amritha Rangarajan, Swathi, Papri Sutar, Dheeraj Kumar Singh, Ritu Gupta, Nitesh Kumar, Urmimala Maitra, Nisha Mariam Mammen, Soumik Siddhanta, Piyush Kumar Chaturbedy, Vini Gautam, Arpan Hazra, S.R.K. Chaitanya Sharma Y, Chidambar Kulkarni, Dileep Krishnan, Gayatri Kumari, M. Pandeeswar, Rana Saha, Sudeshna Sen, Varun Thakur, Dibyajyoti Ghosh, Anindita Chakraborty, Prashant Kumar, Ankush Kumar, Ram Kumar, Sisir Maity, Chandan Kumar, Chandan De, Anirban Mondal, Koushik Pal, Abhijit Sen, Rajib Sahu, Dipanwita Dutta, Sonu K.P., Kandula Neelima, Raaghesh A.V., Suchitra, Uttam Gupta, Sohini Bhattacharyya, Shantanu Aggarwal, Vikas Garg, Shivakumar D.T.

#### **Research Associate**

N Padmavathy

#### **Research Associate (Provisional)**

B E Prasad

**Technical Assistant** N R Selvi

R & D Assistants

Swati Chakraborty, Dhruv Joshi, Syamantak Roy, Sandheep P R

#### Junior R&D Assistant

Bhavya D R

#### Staff

Vijay Amirtharaj A, Ananda Raman

## **Education Technology Unit**

#### **Activities and Achievements**

The Education Technology Unit has been actively involved in the concept, development and production of multimedia CD-ROM's and books especially for school students and teachers in various disciplines of science since its inception. The Unit has been involved in developing and producing CD-ROMs and books in vernacular Indian languages.

The C.N.R. Rao Hall of Science and Education Technology Unit has continued conducting the highly popular Teachers/students programs/workshops for students and teachers. These workshops/programs are conducted in different subjects like Physics, Chemistry and Biology.

The Book `Rasaayanshaastrada Arivu' authored by Prof. C.N.R. Rao was translated by Mrs. Indumati Rao. It was edited, formatted and a print-ready copy was produced by ETU for Karnataka Rajya Vijnana Parishath (KRVP). The book sponsored by Vision Group on Science & Technology, Dept. of Science & Technology, Govt. of Karnataka to commemorate International Year of Chemistry-2011 was released at a function held at AMRL Conference Hall, JNCASR on March 12, 2012. Prof. P. Balaram, Director, IISc was the Chief Guest.

ETU has collated and produced a document titled `Science Outreach' listing all the Science Popularization 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. C.N.R. 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 in different subjects (Physics, Chemistry, Biology etc.) 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. These programs are sponsored by the CNR Rao Hall of Science and they are organized and conducted by CNR Rao Education Foundation and Prof. K.S. Valdiya.

In the POCE program for the year 2012, ETU presented the multimedia CD-ROM `NANOWORLD' and a quiz was conducted from the CD-ROM `Understanding Chemistry' for the students on May 25 & 30. A visit to the `Chemistry of Materials Exposition' and Prof. C.N.R. Rao Archives was conducted by ETU for the POCE students on June 11.

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'. Here the videos of the various lecture programs conducted at the Hall of Science for students and teachers 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 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.

ETU was given the task to format and design a book for the Science Advisory Council to the Prime Minister. The book layout was designed, formatted and the cover was designed by ETU. A print-ready copy of the book titled "Challenges and Opportunities in Science and Technology (Approach to an Action Plan)" was made ready and 10,000 copies were printed.

The CNR Rao Hall of Science Resource Persons meeting was organized on April 26, 2012 to chalk out the Teacher/student Workshops/ Programs to be conducted for the period June2012-December 2012. The meeting was chaired by Prof. C.N.R. Rao. Two Programs each in Physics, Chemistry and Biology were planned along with Special Teacher Training Lecture Programs (in all three subjects) for the benefit of Pre-University Teachers.

#### **Organisation of Programmes**

The Summer 2012 Science Outreach Programme sponsored by the CNR Rao Hall of Science, JNCASR was conducted in association with Himalayan Gram Vikas Samiti, Gangolihat by Prof. K.S. Valdiya on May 6-9, 2012. 148 Participants from 24 Govt. intermediate colleges attended the program which had lectures on topics in Science & Engineering from Eminent Scientists.

The CNR Rao Hall of Science and Education Technology Unit conducted 12 lecture programs for students and teachers during 2012. In addition to the planned programs, a program for the CNR Rao Hall of Science and ETU organized the Outstanding Science Teacher Prize function and Lecture Program on June 29, 2012. The awardees for the year 2011 are Shri. S.V. Burli and Smt. M. S. Rekha. In the lecture program that followed the award presentation function Prof. CNR Rao delivered the lecture `Celebration of Science' and Prof. Maneesha Inamdar gave a lecture on `Stem Cells and the Future of Medicine''. Around 225 students and teachers attended the program. Prof. C.N.R. Rao unveiled a portrait of Shri. Madan Mohan Malaviya at the CNR Rao Hall of Science. This was launched at the above function by Prof. M.R.S. Rao, President, JNCASR. In addition the special feature called `Lecture Videos' was also demonstrated. These are videos of the various lecture programs conducted at the Hall of Science. ETU organized and conducted a visit to the Chemistry of Materials Exposition and Prof. C.N.R. Rao Archives for the participants.

CNR Rao Hall of Science and ETU organized a Special Teacher Training Three-day Lecture Program in Physics, Chemistry and Biology for PU teachers. In all the three programs there were three lectures followed by a interactive Q&A Session. The P.U. Board, Govt. of Karnataka deputed teachers from various Pre-University Colleges.

In the Biology program, Prof. M.R.S. Rao, Prof. Jyotsna Dhawan and Prof. V. Nagaraja gave lectures. In the Chemistry Program Prof. S. Balasubramanian, Dr. Govindaraju & Dr. Ranjani Viswanatha gave lectures. Dr. Kavita Jain, Dr. Vidhyadhiraja & Prof. Umesh Waghmare gave lectures in the Physics program. Around 100-120 teachers attended these programs.

The Programs/workshops organised by the CNR Rao Hall of Science and ETU and conducted at the Madan Mohan Malaviya Amphitheatre were as follows:

29 June 2012 – Lecture Program (Science Teacher Award Function)

30 July 2012 – Program in Physics for students

6 August 2012 – Special Teacher Training Lecture Program (Program in Biology)

- 7 August 2012 Special Teacher Training Lecture Program (Program in Chemistry)
- 8 August 2012 Special Teacher Training Lecture Program (Program in Physics)
- 27 August 2012 Program in Biology for students
- 25 September 2012 Program in Chemistry for students
- 12 October 2012 Program in Physics for students
- 30 October 2012 INSPIRE Program
- 30 November 2012 Program in Biology for students
- 4 December 2012 Special Lecture Program
- 5 December 2012 Program in Chemistry for students

In each of the above programs over 200 students and teachers participated. All the above programs consisted of lectures and some demonstrations followed by an interactive Question and Answer session. All the above



programs were organized and conducted by CNR Rao Hall of Science & ETU under the auspices of the Science outreach program.

A special lecture program `INSPIRE program' was organized on October 30, 2012 by CNR Rao Hall of Science and ETU for students and teachers attending the INSPIRE-2012 Science Nurture Camp, Tumkur. The half-day lecture program had one lecture each in Physics, Chemistry and Biology.

The `Program in Biology for students' was conducted on November 30, 2012 by ETU & the CNR Rao Hall of Science. All the speakers were from NIMHANS, Bengaluru. On December 4, 2012 a special lecture program was conducted by ETU and the CNR Rao Hall of Science for the students participating in the Regional Children Science Congress organized by Jawahar Navodaya Vidyalayas. The half-day lecture program had a lecture each in Physics, Chemistry & Biology given by the faculty of the Centre. On December 5, 2012 a `Program in Chemistry for students' was organized in which lectures were delivered by Prof. E.W. (Bert) Meijer, Prof. Michael L.Klein and Prof. C.N.R. Rao. Around 225 students and teachers attended the program.

#### **On-going Projects and Future Plans**

The unit is engaged in bringing out a book "Pioneers in Chemistry" describing the achievements of eminent and famous scientists. It is planned to produce a book and CD-ROM in geography.

ETU is engaged in producing a book for the Science Advisory Council to the Prime Minister titled `Science in India (2004-2013)'.

As part of the Science Outreach Programs for students and teachers conducted annually in Uttarakhand, Prof. C.N.R. Rao will give the lecture `Nanoworld' (Nano ki duniya) with subtitles in Hindi. Mrs. Indumati Rao will present a 30-minutes Multimedia presentation of the Hindi version of excerpts from the CD-ROM titled `Nanoworld: An introduction to Nanoscience and Technology.

CNR Rao Hall of Science and Education Technology Unit will be organizing teachers/students workshops/programs in different subjects. The CNR Rao Hall of Science and ETU will conduct jointly with NCU two programs in Chemistry for students. It is planned to have a special lecture program called `Nano Day' with lectures, quiz etc. for students. It is proposed to have lectures and demonstrations with different themes in a particular subject. In the above programs faculty from JNCASR, IISc and other institutions will participate.

Following are the members of this Unit:

Chair Prof. V Krishnan	Ph D, F A Sc, F N A, F T W A S
<b>Coordinator (Hon)</b> Indumati Rao	M A, M S, C E
<b>Technical Officer</b> Jatinder Kaur	M Sc
<b>Multimedia Asst. (Hon.)</b> Sanjay Rao	B Sc, Cert. Multimedia

## **Engineering Mechanics Unit**

*Prof. Roddam Narasimha's group*: in the area of Aerospace and Atmospheric Fluid Mechanics, the concept underlying a novel design of optimal wing planforms for turboprop aircraft, determined through special algorithms developed at JNC, have now been confirmed by wind tunnel tests conducted by NAL at IISc. A study of multiple transitions between laminar and turbulent flow on a swept leading edge has been completed and published.

Comprehensive simulations of a free shear layer in a vortex gas have been completed. It is shown that the vortex gas evolves to a stationary state characterizing a variant of Lundgren-Pointin equilibrium. This evolution may be seen as a long process of relaxation, of which an early stage, lasting only a small fraction (appx.  $10^{-4}$ ) of the total relaxation period, corresponds to an explosive growth of the free shear layer. This explosive phase represents the classical turbulent fluid-dynamic regime. A method of desingularzing vortex sheet roll up has also been developed and is currently being analyzed.

In atmospheric fluid dynamics entrainment measurements have been made in a transient diabatic jet for the first time. These measurements exhibit large deviations in the values of the entrainment coefficient from those previously associated with steady jets and plumes: even the sign may differ. The first Navier-Stokes Boussineq solutions for a transient diabatic plume have also been obtained.

In *Prof. K.R. Sreenivas's group*, results from the study of nocturnal atmospheric boundary layer has culminated in the publication of a set of three papers, two in Journal of Atmospheric Sciences and one in Quarterly Journal of Royal Meteorological Society (expected to appear online by the end of February 2013). In this study an error was indentified in the flux-emissivity model for radiation widely used by many researchers in the atmospheric community. The error was responsible for spurious cooling reported in many studies, and its effect extends all the way up to 1 km in the atmospheric boundary layer. It was also showed that the codes based on this erroneous formulation showed unrealistic sensitivity to the ground emissivity. Related experimental work (both in laboratory and field) has helped to solve an eighty years old micro-meteorological mystery, lifted temperature minimum (LTM). It was identified that atmospheric aerosols are primarily responsible for this phenomenon and results have impact on the prediction of radiation-fog, and in prescribing the sensible-heat boundary condition for weather and climatic models.

On research related to the unsteady aero-dynamics of insect flight, preliminary measurements of lift forces during flapping flight were gathered. In a collaborative project with Dr. Santosh Ansumali, flow fields and force measurements were compared in the experimental studies with that predicted by 3-D numerical simulations.

In the coming academic year, apart from extending above research, his group is going to get involve in new research projects related to precision-agriculture, saving water and ways to extend agriculture into arid climates and the study of transport process in atmospheric boundary layers.

*Prof. Meheboob Alam's research group* was involved in experimental works on vertically vibrated binary granular mixtures which lead to exciting new results. A variety of phase-coexisting patterns was uncovered, characterized by the coexistence of patterns having different spatial and temporal symmetries. For example, a period-2 pattern can coexists with a period-1 pattern in a driven binary mixtures -- this finding is in stark contrast to related pattern formation scenario in mono-disperse granular system. It has been discovered that segregation (demixing) of different types of particles appears to be the key driving factor for the onset of phase-coexisting patterns. A simple recipe, based on the idea of non-equipartition of granular energy, has been identified to control these patterns.

In the field of Nonlinear Patterns, the research group has used a Landau-type order-parameter theory to understand patterns in three-dimensional sheared granular fluid. The onset of vorticity banding in sheared granular fluid has been explained as a bifurcation from its uniform shear base state. Interestingly, the nature of bifurcation (stationary or oscillatory) is found to depend on mean density and wave number. At moderate values of wave number, the bifurcation scenario, with increasing density, unfolds as: (i) supercritical pitchfork, (ii) subcritical pitchfork and finally to (iii) subcritical Hopf bifurcation. Our results agree with previously found vorticity-banded states in simulations of sheared granular fluid.

For three-dimensional perturbations, Prof. Alam's research group has found that multiple nonlinear states of both stationary and travelling waves can coexist for a given parameter combination of mean density and Couette gap. The vortical motion on the cross-stream plane has been characterized in terms of the fixed/critical points of the underlying flow-field: saddles, nodes (sources and sinks) and vortices have been identified. While the cross-stream velocity field for supercritical solutions in dilute flows contains nodes and saddles, the subcritical solutions are dominated by large-scale vortices in the background of saddle-node-type motions. The latter type of flow pattern also persists at moderate densities in the form of supercritical nonlinear solutions that originate from the dominant 2D instability modes for which the vortex appears to be driven by two nearby saddles. The location of this vortex is found to be correlated with the local maxima of the stream wise vorticity.

Research group led by Prof. Ganesh Subramanian worked on the below areas:

*Concentration fluctuations in bacterial suspensions:* A fluctuating hydrodynamics approach, together with an adaption of a formalism from classical inviscid hydrodynamic stability, has been used to analyse statistical correlations that develop in a bacterial suspension. In particular, the analysis aimed to understand the origin of the large concentration fluctuations predicted in such systems. (Collaborator: Prof. Donald L. Koch)

*Bacterial suspension rheology:* A singular perturbation approach, together with numerical solution of the governing advection-tumbling equation, has been used to characterize the rheology of a bacterial suspension, and the results will be compared to experiments (Student: Mr. Sankalp Nambiar).

A particle-level simulation has also been carried in order to verify earlier predictions for the instability of a swimmer suspension (Student: Mr. Deepak Krishnamurthy).

*Vortex Rings Oscillations:* Using the framework developed by a former student (Dr. Anubhab Roy), the spectrum of singular oscillations of a vortex ring was charaterised (Student: Mr. Shashikiran Reddy).

*Sonic transition in viscoelastic flows:* The nature of the flow field has been examined, in particular, the vorticity fluctuations induced by a sedimenting particle for finite Mach numbers (defined based on the speed of propagation of infinitesimal shear-stress fluctuations), and the change in the character of such fluctuations across a Mach number of unity (Student: Mr. Navaneeth K.M.).

*Role of micro-scale inertia in multiphase heat-transfer:* A model problem of a shearing flow around a neutrally buoyant drop was examined and a boundary-layer analysis was used to highlight the role played by closed-streamlines in the heat or mass transfer from the surface of the drop. The analysis aimed to calculate the Nusselt number as a function of the viscosity ratio (drop to ambient) and flow-type. (Student: Mr. Deepak Krishnamurthy).

The following are the members of the Unit:

Ph D, F N A, F A Sc, FTWAS
Ph D, F A Sc, F N A, F T W A S, F R S
Ph D, F N A, F A Sc
PhD, FASc, FNASc
Ph D
Ph D
Ph D
Ph D

#### Dhiraj Kumar Singh, Ponnulakshmi V.K., Ujjayan Paul, Mohammed Istafaul Haque Ansari, Shiwani Singh,

**CI**...

Saikishan Suryanarayanan, K. Siddharth, Lakshminarayana Reddy M.H., Vybhav G R, Shashank H J, Sunil V Bharadwaj, Manjusha Namburi N L D B, Rajesh Ranjan, Navaneeth K M, Rama krishna Rongali, Saikat Saha, Saunak Sengupta, Prasanth P, Dhake Milind Prakash, Sorathiya Shahajhan Hassanali, Thantanapally Chakradhar, Deepak Krishnamurthy, Kanwar Nain Singh, Rashmi Ramaadugu, Deepthi S, Sankalp Nambiar, Jumpal Shashikiran Reddy, Vicky Kumar Verma

#### **Research Associate**

Aarthi Sekaran

NBHM Post Doctoral Fellow Shailendra Kumar Singh

Research Associates (Provisional)

Sachin Yashavant Shinde, Virendra Kumar

#### **R&D** Assistants

Nakul Pande, Rayan Chatterjee

## **Evolutionary and Organismal Biology Unit**

The faculty of EOBU continued their research in the broad areas of animal behaviour /phylogeography, chronobiology, evolutionary genetics, neurogenetics, and population dynamics. Research in this unit had been in the areas of (a) biogeography of large mammals in the Western Ghats, (b) social organization in Asian elephants, (c) behavioural, neurogenetic and molecular bases of *Drosophila* circadian clocks, (d) evolution of adaptations to crowding, especially the interplay of food deprivation and waste buildup, (e) fruitflies as a model system for neurodegenerative disorders, (f) behavioural neurogenetics, (g) circadian entrainment by temperature cycles, (h) fruitfly metapopulation dynamics and stability. The Unit also continued to train personnel in the area of whole-organismal biology through the regular PhD, Integrated PhD and MS programmes, as well as through participation of faculty in POBE and SRFP programmes of the Centre as well as similar outreach programmes run by the three science academies and by DST and KVPY.

A few of the most salient research findings are summarized below.

- (a) Work on the social structure of female Asian elephants was continued and it was found that this social organization was more fluid than that of African savannah elephants.
- (b) While linear dominance hierarchies based on size or relatedness may be expected in elephants as they continue to grow throughout their lives and live in groups of related individuals, it was found that no linear dominance hierarchy exists between or within female Asian elephant groups, suggesting that resource dispersion was more important in influencing dominance relationships. However, there was also some effect of the age of an individual on the probability of initiating a dominance interaction.
- (c) Preliminary examination of Asian elephant male dominance relationships showed no linear dominance hierarchy although there was an effect of age here also. Male-male association networks were found, interestingly, to differ in the presence and absence of females.
- (d) Synchrony, precision and accuracy of circadian rhythms evolve in fruit fly populations as a correlated response to selection for emergence in a narrow window of time.
- (e) Genetic architecture underlying morning and evening emergence in *early* and *late* fruit fly populations is complex; while the genetic basis of circadian period is primarily autosomal and comprise additive interactions, those regulating phase of entrainment involve higher order dominance and epistatic interactions.
- (f) Temperature compensation mechanisms help fruit flies achieve strong (Type-0) phase resetting in their circadian clocks.
- (g) Unique patterns of adult emergence and activity/rest behaviours, not seen under laboratory conditions, become apparent when *D. melanogaster* are exposed to semi natural conditions A novel approach of studying rhythmic behaviours by visual observations of behaviours across the day and night revealed that the peaks in activity during dawn is likely to be related to courtship related behaviour, while the peak in the afternoon is a response to the high temperature and high light intensity experienced during thattime.
- (h) Circadian clocks evolve in *D. melanogaster* populations as a consequence of selection for faster pre-adult development.
- (I) Evidence was found for a role for the large ventral neurons of *D. melanogaster* in modulating levels of sleep in a photoperiod-dependent manner.
- (j) Evidence was found for the role of dTRPA1 an ion channel expressed by *D. melanogaster* in regulating mid-day inhibition of activity under warm-cold cycles. This was obtained using various genetic manipulations and environmental cycles in the laboratory and

under semi-natural conditions, and also by simulated natural conditions in the laboratory.

- (k) A study comparing daily activity/rest rhythms of four Drosophilid species under semi natural conditions across seasons revealed that species-specific preferences in the choice of zeitgebers among these closely related and sympatric species. A similar study which compared another important rhythmic behaviour, emergence of adults from pupal cases, was found to be less variable across species but more susceptible to change due to seasonal conditions.
- (l) Constant immigration of even a small number of individuals each generation into fruitfly populations has been shown to significantly reduce the magnitude of population size fluctuations and the likelihood of extinction. This simple, easy-to implement method for population stabilization works for both intrinsically unstable and relatively stable populations, albeit through differing mechanisms based on how migration affects the distribution of population size.
- (m) Detailed simulation studies reveal that the nature of migration (asymmetric versus symmetric) and the degree of instability of local subpopulation dynamics in two-patch metapopulations interact in bringing about stabilization of the local and global dynamics. In particular, contrary to earlier belief, asymmetric migration is not necessarily more stabilizing than symmetric migration, with the discordance between the gradients of instability and of net migration playing an important role in determining stability. Also, different zones of chaotic dynamics show differing sensitivity to the stabilizing effects of migration.
- (n) Typically, density (number of individuals per unit resource) has been used as a convenient descriptor of levels of crowding and is also used as the state variable in simple models of population growth and of density-dependent selection. It has now been shown experimentally that density is not necessarily a good surrogate for level of crowding, as fruitfly populations with identical larval density, but differing absolute amounts of food, exhibit differences in their pre-adult survivorship, development time and dry weight at eclosion. This work has led to the building up of an explanation of how food amounts and larval densities interact to alter the fitness consequences of inter-individual variation in larval feeding rate, urea tolerance and efficiency of food

conversion to biomass. Thus, the suite of traits that evolve in response to chronic larval crowding is likely to be determined by the ecology of the crowded culture in a complex manner that cannot be predicted simply from a knowledge of the larval density alone.

(o) Populations of fruitflies selected for rapid pre-adult development and early reproduction were shown to have evolved incipient reproductive isolation from their ancestral controlsafter about 400 generations of selection. One component of this isolation was due to the heavy mortality of selected line females after mating with control line males, possible mediated by the body size difference between selected and control lines. Further work has found evidence for body-size mediated male ability to harm their mates upon mating whereas female susceptibility to such harm does not appear to be mediated by body size. There is also evidence for body size independent components of male mating fitness, and some evidence for the correlated evolution of reduced levels of inter-locus sexual conflict in the faster developing lines.

The second batch of Integrated PhD students in the Unit successfully completed their two years coursework and, after one year of research, have submitted their MS theses.

In January 2013, the Unit also organized a two-day Symposium on Organismal Biology in memory of our founding Chair, Prof. M. K. Chandrashekaran. The faculty have also been active in delivering lectures at various meetings and workshops around India.

The following are the members of the Unit:

<b>Chair</b> Vijay Kumar Sharma	Ph D, F A Sc, F N A Sc
Professors	
Vijay Kumar Sharma	Ph D, F A Sc, F N A Sc, F N A Ph D, F A Sc, F N A Sc
Honorary Professors	
Raghavendra Gadagkar	Ph D, F A Sc, F N A, F T W A S
Mewa Singh	Ph D, F A Sc, F N A, F N A Sc
Vidyanand Nanjundiah	Ph D, F A Sc, F N A
DST Ramanujan Fellows	
T N C Vidya	Ph D
Sheeba Vasu	Ph D

#### **Research Students**

Pankaj Yadav, Priya M.P., Pavitra Prakash, Nandini R Shetty, Antara Das, Nikhil K.L., Keerthipriya P., Vishwanath Varma, Radhika Dilip Shindey, Hansraj Gautam, Anuj Menon, Manishi Srivastava, Singh Viveka Jagdish, Sheetal Potdar, Payel Ganguly, Joydeep De, Avani Mital, Manaswini Sarangi, Geetanjali Prabhakar Vaidya, Abhilash Lakshman, Manan Gupta

#### **Research Associates**

Koustubh M Vaze, Shahnaz Rahaman Lone

#### **R&D** Assistants

Subhankar Chakraborty, Sajith V S

## **Geodynamics Unit**

The Science Outreach Programme in Uttarakhand were sponsored and funded by C.N.R.Rao Hall of Science. Prof. Valdiya organised these programmes and had participated as a lecturing resource person. Following were the programmes:

- 1. In Someshwar, district Almora Science Outreach Programme was organised on November 1, 2012, which was attended by 445 student\* and 26 teachers from 7 colleges
- 2. In Gwaldam, district Chamoli, the programme was organised on November 2, 2012. This was attended by 250 students\* and 7 teachers from Central School.
- 3. In Bageshwar, district Bageshar, 600 students\* and 25 teachers had attended the programme from Countrywide Public School on November 3, 2012
- 4. At Rai Gyarsi, district Pithoragarh, 220 students from Primary School and village folks had participated in the programme on November 4, 2012
- 5. At Danya, district Almora, 386 students\* and 16 teachers had participated.

\*Pre-university students of Classes XI and XII

The themes of Prof. Valdiya's lectures were:

- (i) Earthquake and landslide hazards
- (ii) Grave water scarcity problem and recharging mountain springs
- (iii) Evolution of the Himalaya

#### **Research Paper Published**

Prof. K. S. Valdiya

1. Valdiya, K. S., The Saraswati was a Himalayan-born river. *Current Science* **2013** (January **10**), *104* (1), 42-52.

Following is the member of the Unit:

Chair

Ph D

# **Molecular Biology and Genetics Unit**

MBGU currently has several research and training avenues in broad areas of biological sciences. Research in nine of its laboratories spans diverse areas of modern biology with emphasis on biomedicine. These areas of research are: infectious diseases, cancer genomics, human genetics, mammalian stem cells, cardiovascular development, transcription regulation and mechanism of chromosome segregation. In the last two years there has been an active exchange of scientific ideas among this MBGU faculty and colleagues at the centre who are chemists, physicists and engineers. MBGU continues to attract some of the best students from all over the country. Students for the PhD, Integrated-PhD, MS-PhD, POBE and SRF programmes in MBGU are selected through competitive national-level selection process. Our academic programmes aim to provide training in a broad range of genetic, biochemical, cell and developmental biology approaches for basic and translational research. The essence of these programmes is to provide our students, ample flexibility and opportunity for pursuing a contemporary research theme. MBGU has 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. Certain important highlights of our work in this previous year are as follows:

#### Autophagy Laboratory

The laboratory studies autophagy and autophagy-related pathways. A new live cell assay have been designed to kinetically monitory general and selective autophagy pathways and have miniaturized it to suit the high throughput format. Through a genetic and a biochemical screening procedure, novel genes involved in these process have been identified. Future work will include performing a small molecule screening using the HTS and characterizing the mutants involved the autophagic processes.

#### Molecular Mycology Laboratory

This laboratory is studying structure-function analysis of centromeres of several pathogenic yeasts: *Candida albicans, Candida dubliniensis, Candida tropicalis* and *Cryptococcus neoformans*. They observed that centromere DNA sequences are rapidly evolving when *C. albicans* and *C. dubliniensis* orthologous chromosomes were analyzed. Centromeres of C. tropicalis have been recently identified. These centromere properties are different from those of *C. albicans* and *C. dubliniensis*. This laboratory also showed that kinetochore formation in C. albicans is a concerted process. Several members of the laboratory are now working to identify small molecules that can be used as inhibitors for a fungal specific protein complex present at the kinetochore.

#### Transcription and Disease Laboratory

Focus of this Laboratory was to understand the different aspects of chromatin functional dynamics which are responsible for the gene regulation and its link to cellular physiology and pathobiology. Two different diseases are being investigated in this context, namely cancer (oral cancer and breast cancer) and AIDS. It was found that human chromatin associated protein PC4, gets acetylated *in vivo* and possibly enriched in the transcriptionally active chromatin. PC4 knock down stable cell line was generated and was found that indeed it is involved in genome stability. Monoclonal antibodies have been generated against modified and unmodified NPM1, a chromatin interacting protein and a histone chaperone. It was shown that NPM1 does get overexpressed and hyperacetylated in oral cancer. These antibodies are in the process of commercialization. Also, the first of its kind natural and specific inhibitor of the lysine acetyltransferase- PCAF is discovered, and the role of PCAF mediated acetylation was elucidated in the process of muscle differentiation. It was also found that the anti-hypertensive drug, felodipine is a specific inhibitor of Aurora Kinase A by employing Surface Enhanced Raman Spectroscopy (SERS) and molecular dynamic technique, thus a new method of molecular level Drug-Protein interaction identification method was established.

#### Vascular Biology Laboratory

Over the last year, significant progress was made in understanding mechanisms that maintain stem cell potency. The endosomal protein Asrij was identified as being essential for maintaining the balance between the pluripotent stem cell state and the differentiated state. Further it was showed that Asrij has a conserved function
in maintaining stemness. In *drosophila hematopoiesis*, too Asrij is essential for maintaining the stem cell population. Asrij functions by actively modulating signalling at the level of endosomes. Thus, a novel mechanism was demonstrated that functions via endosomal regulation to achieve control on stem cell potency. It was an continued efforts to understand mechanism of cardiovascular development, by which the cytoskeletal protein rudhira was found to be essential for cell migration and angiogenic remodelling in vivo during mouse development. Rudhira null mutant embryos as well as conditional endothelial-specific knockouts die at midgestation due to vascular patterning defects. A transcriptome analysis of rudhira mutants was performed and several key pathways were identified through which rudhira mediates its function. Further analysis of these is in progress.

# Molecular Virology Laboratory

Recent analysis from the laboratory found that in India, over the past decade, the HIV-1 subtype C has acquired a stronger viral promoter and is expanding at a substantial rate, replacing the standard subtypeC strains. This is the first time that anyone identified divergent evolution in a major viral subtype of HIV-1. The newly emerging HIV-1 subtype C viruses containing a stronger viral promoter produce more viral particles and a higher viral load, probably providing an enhanced transmission advantage. This finding is perplexing because a stronger viral gene expression should also elicit enhanced immune activation that may be counterproductive to viral fitness. Some researchers believe that subtype C virus has a relatively higher degree of attenuation as compared to other subtypes and as a result is less pathogenic. Current results of this Laboratory propose that subtype C virus exploits a small window of opportunity to make higher viral load without eliciting a higher magnitude of immune activation. Future studies remain needed to further validate this notion. The laboratory is also credited with the most important finding that subtype-C Tat protein is a defective monocyte chemokine and proposed a hypothesis that the under representation of HIV-1 associated dementia in India is correlated to this important genetic difference. The laboratory undertook the evaluation of a polyherbal formulation of the Indian origin as a potential HIV-AIDS therapeutic strategy. The pilot clinical trial, the first of its kind, showed stabilized clinical profile in the study participants.

# Human Molecular Genetics Laboratory

This laboratory had examined molecular genetic basis of human neurological disorders: idiopathic generalized epilepsy (IGE), in particular, juvenile myoclonic epilepsy (IME) and a reflex/sensory form of epilepsy widely known as hot water epilepsy (HWE). In addition to examining the role of the known epilepsy-causing alleles in ion-channel genes, Prof. Anand has been exploring possible new molecular mechanisms in the causation of epilepsies. One of the recent findings from this lab comprises identification of an IGE locus and a gene at 3q13q21 (EIG8, OMIM-601199). A new epilepsy gene encoding CaSR (extracellular calcium-sensing receptor) at chromosome 3q13-q21 has been discovered by the nominee's laboratory CASR belongs to a family of G-protein coupled receptors. This is the first demonstration of *CaSR*'s function in the context of an epileptic disorder. The CASR protein is expressed in specific sub-regions of the human brain and that this protein 'measures' changes in extracellular calcium levels in the sub-regions and connects this information to intracellular signal transduction pathways in neurons. This contribution is well recognized in the field. Based on these findings, CaSR's biological role in the epilepsy/human brain and the consequences of its misregulation are being addressed in several laboratories abroad. CASR has a crucial role in regulating the growth of neuronal processes in the developing brain. The epilepsy-causing R898Q mutation detected by the laboratory has been investigated by a laboratory elsewhere and shown to be a gain-of-function allele that disrupts a critical arginine-rich retention motif of the CASR. This laboratory has gone on to examine this gene further and has identified several patient-specific CaSR mutations. On the basis of his studies of this gene in nearly 500 familial and sporadic cases of epilepsy, it appears that an overlapping genetic predisposition may underlie two seemingly distinct clinical entities, generalized and localized epilepsies. It is amply clear that CaSR's function in the human brain is crucial to maintaining normal neuronal excitability. Further studies on the role of CASR in neuronal signal transduction pathway may expand the pharmacological repertoire for seizure phenotypes.

#### Molecular Parasitology Laboratories

Research in these laboratories is focused on understanding metabolism in the malaria parasite *Plasmodium* falciparum. Towards this end the enzymes involved in purine nucleotide metabolism in the parasite are being studied. Comparative structure-function analysis is also being carried out on the homologues from humans and archaea. Adenylosucinate synthetase from M. jannaschii has been characterized biochemically. It is an archaeal enzyme that is 100 amino acids shorter than its counterparts from both eukaryotes and prokaryotes. This thermostable enzyme exhibits a biphasic Arrhenius plot with a switch in the rate-limiting step in catalysis contributing to the bend in the plot. GMP synthetase from *P. falciparum* has been kinetically characterized. Our studies show that the parasite enzyme exhibits different inhibition profile from that of the human counterpart suggesting its suitability as a drug target. Characterization of *P. falciparum* adenylosuccinate lyase indicated that the parasite enzyme has retained its specificity for both the substrates, SAMP and SAICAR. The presence of SAICAR specificity suggests that this is probably the only activity of the de novo purine biosynthetic pathway that is retained in the parasite. Active recombinant *P. falciparum* SIR2 has been successfully expressed and purified. Screening for modulators of Sir2 activity led to the identification of surfactin, a depsipeptide produced by Bacillus subtilis as a potent inhibitor of the parasite enzyme competing for the NAD<sup>+</sup> binding site. Another Parasitology lab in the unit is focusing its efforts on the role of *Plasmodium* kinases in host-pathogen interactions. Prof. Surolia's group has been focusing on understanding the molecular mechanism underlying the pathogenesis of cerebral malaria in Indian patients through a `Systems -Biology " approach. The group is also trying to decipher canonical and non-canonical intracellular trafficking pathways in Plasmodium falciparum, in the process they have found some novel proteins responsible for the development of the parasite. The group is also studying proteins involved in host-pathogen interactions.

#### Chromatin Biology Laboratory

Work in the chromatin TP2 is acetylated in vivo as detected by anti-acetylated lysine antibodies and mass spectrometric analysis. Recombinant TP2 is acetylated *in vitro* by p300 and PCAF. p300 acetylates TP2 in its Cterminal domain which is highly basic in nature possessing chromatin condensing properties. Mass spectrometric analysis showed that p300 acetylated 4 lysine residues in the C-terminal domain of TP2. Acetylation of TP2 leads to significant reduction of its DNA condensing property as studied by the CD and AFM analysis. Colocalization studies using GC-selective DNA binding dyes chromomycin A3 and 7-amino actinomycin D and AT selective dye DAPI indicate that TP2 is prefernitally localized to the GC-rich sequences. Interestingly, as spermatids mature, TP2 and GC rich DNA moves towards nuclear periphery and in the later stages of spermatid maturation TP2 is predominantly localized at the nuclear periphery. Another interesting observation is the mutually exclusive localization of GC and AT rich DNA in the elongating and elongated spermatids. A combined immunoflourescence experiment with anti-TP2 and anti-TP1 anbtibodies revealed several foci of overlapping localization indicating that TP1 and TP2 may have concerted function role during chromatin remodeling in mammalian spermiogenesis. Chromatin remodeling factor BRDT has been cloned and expressed in insect cells. The recombinant BRDT shows histone chaperone activity in vitro. Gene epxression perturbation following down regulation of mrhl RNA has been studied. Pathway construction has indicated that mrhl RNA plays an important role in the *wnt* signalling pathway.

Following are the members of the Unit:

Chair Anuranjan Anand	Ph D, F A Sc
Honorary Professors	
Dipankar Chatterji	Ph D, F N A Sc, F A Sc, F N A, FTWAS
H Sharat Chandra	Ph D, F A Sc, F N A, FTWAS
Professors	
Anuranjan Anand	Ph D, F A Sc
Hemalatha Balaram	Ph D, F A Sc
M R S Rao	Ph D, F A Sc, F N A, F N A Sc, FAMS, FTWAS
Namita Surolia	Ph D, F A Sc, F N A Sc
Ranga Udaykumar	Ph D

Tapas Kumar Kundu Maneesha Inamdar	Ph D, F A Sc, F N A Sc, F N Ph D
Associate Professor Kaustuv Sanyal	Ph D
<b>Faculty Fellow</b> Ravi Manjithaya	Ph D
<b>Technical Officer (Veterinary)</b> R G Prakash	B V Sc & A.H.

#### **Technical Staff**

Anand Kumar K, N Jeelan Basha, Prakash RG, Suma BS, Ushasree Pattamatta, V Mohan

#### **Research Students**

Abhishek Sinha, Laxmi Narayan Mishra, D. Karthigeyan, Sreyoshi Mitra, Manpreet Kaur, P.K. Raju Pedabaliyarasimhuni, Sanjeev Kumar, Sourav Roy, Nikhil Gupta, Shetty Ronak Kutty, Laxmi Shanker Rai, Gautam Chatterjee, Anjali Verma, Kalpita Rashmi Karan, Deeti K. Shetty, Kirthana M.V., Akhade Vijay Suresh, Khadilkar Rohan Jayant, Senapati Parijat Ramesh, Vijay J., Garima Verma, Shilpee, Malini Menon, Amrutha Swaminathan, Shukla Arpit Prakashkumar, Shalini Roy Choudhury, Simi Muraleedharan, Prabhu S. A., Amit Kumar Behera, Neha Varshney, Stephanie Kaypee, Piyush Mishra, Santosh S., Sutanuka Das, Sweta Sikder, Divyesh Joshi, Arnab Bose, Debosree Pal, Madhura D Joglekar, Palak Agrawal, Barve Gaurav Ramanand, T. Lakshmi Prasoona, Vikas, Shveta Jaishankar, Lakshmi Sreekumar, Surabhi Sudevan, R. Sunaina Singh, S. N. Suresh, Shreyas Sridhar, S Sundar Ram, Mariyam Abdullah Khorakiwala, Lakshmeesha K N, Pooja Barak, Saloni Sinha, Debanjan Mukherjee, Somya Bats, Meenakshi P., Arpitha A Suryavanshi, Alok Javali

A

#### **Research Associates**

Manjira Ghosh Kumar, Mamata Mishra, Sadhan Chandra Das, Sujata Kumari

#### **Research Associates (Provisional)**

Mahesh Bachu, Manoj Kumar

#### **R&D** Assistants

Vandhana Devi, Sourav Nayak, Saihitha Veerapaneni, Deepthi Sudarshan, Mahadeva Swamy M M, Asif Ahamad Bakshi, B K Viswanada Reddy, Sriram Kannan, Jasper Chrysolite Paul

#### Junior R&D Assistant

S Manu

# **New Chemistry Unit**

Several aspects of the chemistry of materials are being pursued by the research team led by Prof. C.N.R. Rao. These include transition metal oxides, nanomaterials and carbon materials. In transition metal oxides, multiferroic and magnetoelectric oxides are of interest. Work on inorganic nanomaterials includes synthesis, characterization, study of properties and phenomena. Carbon nanotubes and graphene are important areas being investigated.

Dr. T. Govindaraju's research activities were at the interface of chemistry and biology (*Organic synthesis, molecular probes, peptide chemistry, nucleic acid chemistry and bionanotechnology*). The design and synthesis of small molecules had been actively pursued including peptides, nucleic acids and their conjugates based biomimetic systems and materials possessing well defined nano-, meso- and micro-structures with properties similar to natural materials through Nature-inspired molecular self-assembly approach. These biomimetic materials find applications as biomaterials, drug delivery systems, composites and in bioelectronics. Dr. Govindaraju had been also involved in developing chiral unnatural amino acids and ligands as optical probes for sensing and bioimaging of variety of cations and anions through supramolecular host-guest interactions. The design and synthesis of new class of smart-building blocks for metal directed assemblies for biosensors and smart materials applications had been undertaken. In his laboratory, protocols had been established to develop biomimetic molecular self-assembly-based systems and materials through chiral transcription, amplication and retentive helical memory (studied by sergeants-and-soldiers method and majority rules) for use in chiral technology and to understand spontaneous deracemization and amplication pathways for biological homochirality. Dr. Govindaraju initiated new projects in the area of neurodegenerative diseases (Alzheimer's, Parkinson's, type 2 diabetes, Huntington and prion diseases) and nucleic acid chemistry).

Dr. Jayanta Haldar had focused on infectious diseases in his research which continue to be one of the greatest health challenges worldwide and the threat is compounded by the fact that an increasing percentage of pathogens are developing resistance against the available drugs. The main focus of his research was towards the development of chemical and nanotechnology based innovative strategies to prevent the spread of infections and the development of new antimicrobial agents for the treatment of infectious diseases. Recently, new generation polymeric biomaterials to make any surface antimicrobial had been engineered, which inactivate various pathogenic bacteria completely on contact. Towards therapeutic applications, novel Antimicrobial Peptides Mimics had been developed and was shown that they inactivate various wild-type and drug resistant pathogenic bacteria and are having no *in-vitro* and *in-vivo* toxicity. Recently, various analogues of vancomycin had also been developed that not only combat drug resistant Gram-positive bacterial (MRSA, VISA, VRSA, VRE) infections but also overcome inherent resistance of vancomycin towards Gram-negative bacteria.

Dr. Kanishka Biswas's research group was focused on the synthesis and thermoelectric properties of cubic I-V-VI<sub>2</sub> (where I = Cu, Ag, or alkali metal; V = As, Sb, Bi; and VI = S, Se, Te) compounds both in bulk and nanocrystalline phases. Thermoelectric figure of merit, *ZT* of ~ 1.2 in lead free I-V-VI<sub>2</sub> compounds containing earth abundant Se in place of traditional rare and costly Te had been achieved, which has remarkable fundamental and technological importance. His group was also involved in green ionothermal synthesis and thermoelectric property studies of ultrathin (2-4 layer) topological insulators such as  $Bi_2Se_3$ ,  $Bi_2Te_3$ ,  $Sb_2Te_3$  and solid solutions.

The primary focus of research of Dr. Ranjani Viswanatha's research group was the synthesis and study of optical and magnetic properties of semiconductor nanocrystals. Towards that goal, her research group have been involved in the synthesis of Cu doped CdSe to use copper as a nanosensor to study the electronic structure and surface properties of CdSe. They are also currently in the process of extending these studies to other II-VI semiconductors. The second area of research interest was to actively pursued the synthesis of particles of CdSe/CdS core shell systems that are defect free and hence obtain a near unity quantum yield. These particles are also cast into exploratory devices of light emitting diodes that were found to have efficiencies comparable to the world standards. They had also actively pursued the synthesis of CdTe and CdTe/CdS core shell systems to dope them with magnetic impurities like Fe, Co.

Dr. Sebastian C. Peter's research group had focused on research in solid state inorganic materials such as intermetallics, chalcogenides and polyoxometalates from exploratory synthesis. They had discovered several new intermetallics, which are interest in terms of the structural diversity and physical properties. The low dimensional intermetallic materials had been successfully used as good catalysts in selected chemical reactions.

Their objective of research on chalcogenide systems was to develop materials for photovoltaic and non-linear optical properties, and rare earth doped chalcogenide glass materials for lasers and phase change memory devices. The aim of their research in polyoxometalates was to look newer synthetic and self-assembly pathways and gaining a better insight in the mechanism of the interactions.

The interface between synthetic efforts on  $\pi$ -conjugated systems and the organization of these molecules using supramolecular self-assembly principles, with the ultimate aim of developing novel functional materials was the underlying theme of research of Dr. Subi Jacob George's research group. In their approach, they targeted the electronic, optical and self-assembling properties of the  $\pi$ -conjugated backbone for the design of materials. During the last year, they have initiated the design of solution processable, luminescent organic-inorganic hybrids by the co-assembly of ionic donor and acceptor dyes and laponite nanoclay particles. In addition, they have started a project on the synthesis of dipolar dyes for the design of self-assembled nanostructures with NLO and optical wave guiding functionalities. They had further extended their activities on supramolecular charge-transfer assemblies to impart them with novel properties like ferro-electricity.

Dr. Ujjal Gautam's research group has investigated the possibility of C-H bond activation using metal peroxides with low decomposition temperatures. They had also investigated the efficient production of hydrogen fuel from water by using semiconductor nanomaterials as catalysts. The self assembly of fullerene cocrystals in various solvents to understand the formation mechanisms of certain solvates had been studied which were promising for energy harvesting and electronics. By using their understanding, the use of solvates for separation of crucial solvents had been tried.

Prof. H. Ila's research group had been involved for several years in design and development of new, highly efficient, innovative general methods for synthesis of a large variety of structurally diverse five/six membered heterocycles and their condensed analogs, which are structural components of a large number of pharmaceutical agents as pharmacophores of considerable importance. Their diversity oriented synthesis of these molecules relies upon development of new class of organosulfur building block precursor pool, which are readily accessible in a one pot reaction from a wide range of cheap active methylene compounds. It was found that 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 rapid generation of combinatorial libraries for discovery and optimization of new lead structures in drug discovery research.

Another area of Prof. Ila's research interest revolves around design and development of new efficiency increasing one-pot reactions such as domino reactions, multicomponent reactions for accelerating discovery process. Recently, her research group has also explored transition metal which catalyzed C-C and C-heteroatom bond forming reactions for construction of novel heterocyclic scaffolds.

Prof. Swapan K. Pati's research group had worked on catalytic activities of a number of systems: Methane formation from hydrogenation of carbon dioxide on Ni (110) surface has already been studied. Propene to propene oxide on  $WO_3$  surface and doping of Ni(110) surface with Pd and Pt for the Methane formation had also been carried out. His research group has also studied electrochemical cells, with proper choice of Anode, Cathode and electrolyte solutions. Many biological systems, including DNA, G-qudruplexes and their metal-mediated properties had also been explored.

Prof. A. Sundaresan's research group had investigated two new families of multiferroic materials, namely  $RMO_3$  (M = Cr and Fe) and YMM'O<sub>3</sub> (M and M' are two different transition metals such as Cr, Mn and Fe). Although these materials have centrosymmetric structures, they exhibit ferroelectricity at the magnetic ordering temperatures. The origin of ferroelectricity in  $RMO_3$  has been attributed to a combined effect of electric poling field and 3d-4f interactions. In the latter case, it is due to disorder at the B-site of the perovskite structure. Several other oxides were investigated for multiferroic properties.

Prof. M. Eswaramoorthy's reseach group had used aminoclay and laponite materials as scaffolds to organize organic chromophores and studied their light harvesting applications. It was discovered that these supramolecularly assembled, soft-hybrids are water-processable, showed high-transmittance and can be used for environmentally friendly, large-area-display fabrication.

Dr. Sridhar Rajaram's reseach group had explored perylene diimides as alternatives to fullerenes in organic solar

cells. They showed that disrupting the planarity leads to a tenfold improvement of efficiency. In organocatalysis, it was proved that alkali metal ions engenders conformational stability and enhances selectivity. A mild synthesis of non-natural amino acids had been developed that avoids the use of toxic HCN.

Prof. Tapas Kumar Maji's research group was actively involved in exploring various functional aspects of metalorganic frameworks (MOFs), covalent-organic frameworks (COFs) and conjugated microporous polymers (CMPs). Recently, they have synthesized a multi-chromophoric hybrid system where exciplex emission sensitized by energy transfer which is unprecedented. Extensive work had been undertaken on nanoscale MOFs for different application like bioimaging, drug delivery and light harvesting. It was also shown that MOFs can act as precursors for synthesis of nanoporous carbon and borocabonitride materials and these carbon materials exhibit significant hydrogen and carbon dioxide storage capacity.

#### **Departmental Activities**

1. Dr. Kanishka Biswas has joined the Unit as DST Ramanujan Fellow.

2. The Second Annual Chemistry Lecture was delivered by Prof. Dongyuan Zhao, Department of Chemistry, Fudan University, Shanghai, China on "Hydrothermal Synthesis of Ordered Mesoporous Materials for Applications".

Following are the members of the Unit:

Chair		
C. N. R. Rao	Ph D, D Sc, F A Sc, F N A, F R S, F T W A S, Hon. F R S C	
Honorary Professor		
H. Ila	Ph D, F N A, F A Sc	
Faculty Fellows		
T. Govindaraju	Ph D	
Subi Jacob George	Ph D	
Jayanta Haldar (Ramanujan Fellow)	Ph D	
DST Ramanujan Fellows		
Sebastian C. Peter	Ph D	
Ujjal Gautam	Ph D	
Kanishka Biswas	Ph D	
Associate Faculty Members		
Swapan K. Pati (Professor)		
A. Sundaresan (Associate Professor)		
M. Eswaramoorthy (Associate Profess	or)	
A. Govindaraj (Honorary Associate Pro	ofessor)	
Tapas Kumar Maji (Associate Professor)		
Sridhar Rajaram (Faculty Fellow)		

#### **Research Students**

Avinash M.B., Debabrata Maity, Venkata Rao Kotagiri, Mohit Kumar, Ritesh Haldar, G. Ramana Reddy, Yarlagadda Venkateswaralu, Divakara SS Murthy Uppu, Bhawani N., S. Vijay Kumar, Nagarjun N., Chandradhish Ghosh, Sumanta Sarkar, Shivaprasad Manchineella, Pallavi Bothra, Arjun Kumar Chittoory, S. Yugandar, Udumula Subba Rao, Pramoda K., Ankit Jain, Moumita Rana, Swastika Banerjee, Lingampalli Srinivasa Rao, G. Krishnamurthy Grandhi, Anand Acharya, Avijit Saha, Jiaul Hoque, Satya Narayan Guin, Manoj Kumar Jana.

# **Research Associate**

Shridhar Ashok Malladi

#### **R&D** Assistant

Anand Raj

# Theoretical Sciences Unit

*Prof. Umesh V Waghmare's* research group worked in the following research areas: Multi-scale Simulations of Materials: Using first-principles effective Hamiltonian of  $PbTiO_3$  in MD simulations with a combination of constrained polarization and thermodynamic integration, a Ginzburg Landau theory derived[DOI: 10.1103/PhysRevB.87.024107], and a free energy landscape based analysis of ferroelectric transition, domain structure and associated dielectric response of  $PbTiO_3$  had been provided. This work has accomplished the following important findings: it (a) has determined the nature of the puzzling orthorhombic phase seen experimentally, (b) highlighted the contrast in the domain structures of  $BaTiO_3$  and  $PbTiO_3$ .

Fundamental Physics and Applications of Graphene: first-principles calculations has been used and a thorough analysis of topological defects in graphene had been carried out, identifying their electronic and vibrational spectroscopic signatures that can be used in experiments to characterize the defects in a non-invasive way. Secondly, a theoretical explanation had been given for the unusual ability of graphene to remove pesticides from water, seen experimentally by Pradeep et al, in terms of the water mediated interactions between graphene and pesticides including endosulfan [DOI: 10.1002/smll.201201125].

Materials with magnetoelectric coupling: A theoretical analysis of the multiferroic behavior in FeAlO<sub>3</sub> [DOI: 10.1016/j.ssc.2012.07.018] had been given, in terms of coupled phonons, spin and electronic charge degrees of freedom [DOI: 10.1103/Phys RevB.85. 134449]. It was proved that they specifically obtained first and second order coupling between spin and phonons in this class of materials.

There were other contributions to theory of electronic topological transitions, surfaces and interfaces.

*Dr. N. S. Vidhyadhiraja's* research group had pursued research in two directions: one is the development of a reliable and fast quantum many body technique for integration with band structure methods to be used for predictive modeling of strongly correlated electronic systems (SCES). Such a multi-orbital perturbation theory based solver is there in hand, that has been benchmarked extensively with continuous time quantum Monte Carlo. The research group is in the process of integrating it with a specific band-structure method, namely WIEN2K.

The second direction is about investigations of heterogeneity in SCES. In this context, programs have been implemented for investigating (a) layered structures, and (b) disordered systems. The latter has been done at three levels of increasing sophistication, namely the coherent potential approximation, the typical medium theory and the statistical dynamical mean field theory.

*Dr. Subir K Das's* research group has been actively involved in studies of equilibrium and nonequilibrium properties of various condensed matter systems. Significant new understanding has been obtained on the following basic problems:

- i. Hydrodynamic effects in kinetics of phase separation in bulk as well as confined systems.
- ii. Aging properties in kinetics involving solid-sold, liquid-liquid, vapor-liquid and paramagnetic to ferromagnetic transitions.
- iii. Phase behavior of systems containing active particles.
- iv. Effects of disorder in chemical reaction diffusion systems.
- v. Nucleation and growth of droplets in phase transitions.

During the last academic year, under his guidance, three students submitted theses. The details are given below:

- 1. Shaista Ahmad (jointly with Sanjay Puri); Ph.D. Thesis title: "Phase Transition Dynamics: From fluids to liquid crystals"; Degree will be awarded by Jawaharlal Nehru University.
- 2. Suman Majumder; Ph.D.Thesis title: "Nonequilibrium Dynamics in Some Phase Transitions: From finite to infinite length"; Degree will be awarded by JNCASR.
- 3. Saugata Patra; MS-Eng. Thesis title"Numerical Investigation of Pattern Dynamics in Complex Ginzburg-Landau Equation"; Degree will be awarded by JNCASR.

*Dr. Kavita Jain* has worked in the area of adaptation dynamics of asexual populations in periodic selection regime; and evolution of mutation rates in adapted populations.

In *Prof. Swapan K Pati's* group, research interests encompass a broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum systems. Methane formation from hydrogenation of carbon dioxide on Ni (110) surface has been studied. A large number of work involving various molecules (including fullerenes) over graphene, its B-N analogues and edge states in quantum dots have been studied. Novel electronic transport properties like negative differential conductance (NDC), spin filter, half-metallic, a number of new phenomena when light is shined on the device region have been studied in details. Kagome antiferromagnetic clusters with Dzyaloshinskii-Moriya interactions have been studied to understand magnetic behavior. Many biological systems, including DNA, G-quadruple and their metal-mediated properties have also been explored.

Prof. Swapan and his group plan to work on the following new topics:

(i) Quantum Dot Electronics using quantum many body methods.

(ii) Low dimensional interacting systems for various exotic phase transitions.

(iii) Electrochemical cells (Anode/Cathode/Electrolytes) optimizations.

Following are the members of the Unit:

<b>Chair</b> Umesh V Waghmare	Ph D, F A Sc, F N A Sc
Vikram Sarabhai Professor and I	lon. Professor
Kalyan B Sinha	Ph D (Univ. of Rochester), F A Sc, F N A, FTWAS
Professors	
Shobhana Narasimhan	Ph D, F N A Sc
Srikanth Sastry (on lien)	Ph D
Swapan K Pati	Ph D, F A Sc, F N A Sc
Umesh V Waghmare	Ph D, F A Sc, F N A Sc
Associate Professor	
N S Vidhyadhiraja	Ph D
Faculty Fellows	
Kavita Jain	Ph D
Subir Kumar Das	Ph D

#### **Research Students**

Madhura Marathe Pradeep, Arup Chattopadhyay, Suman Majumder, Sutapa Roy, Sananda Biswas, Pramod Kumar, Ulman Kanchan Ajit, Nagamalleswara Rao Dasari, Pralok Kumar Samanta, Shirodkar Sharmila Narendra, Kaushlendra Kumar, Alok Kumar Dixit, Summayya Kouser, Sarada S, Wasim Raja Mondal, Priyanka, Saugata Patra, Rukhsan Ul Haq, Sona John, Vasudevan M V, Ananthu James, Jiarul Midya, Subhajit Paul, Anjali Singh, Saikat Chakraborty, Naushad Ahamad Kamar, Vinay Ishwar Hegde, Meha Bhogra, Bradraj Pandey, Arpita Paul, Sukanya Ghosh, Debdipto Acharya, Rajdeep Banerjee

#### **Research Associate**

Himadri Barman

#### **Research Associate (Provisional)**

Shuvrajyoti Bhattacharjee

# **International Centre for Materials Science**

ICMS has expanded its infrastructure by installing sophisticated equipments like Superconducting Quantum Interference Device (SQUID), Inductively Coupled Plasma, Optical Emission Spectrometry (ICP-OES), UV Spectrometer, Photoluminescence Spectrometer (PL), etc. 9 scientists have visited ICMS under its short-term visitors' programme and. 2 have visited under the SSL project. It has also conducted several meeting and conferences such as: Winter School on "Chemistry and Physics of Materials" with University of Cambridge, UK, and RAK-CAM, December 3-8, 2012, ICMS-RMIT Conference on Smart functional materials, January 28-29, 2013, Indo-Israel Conference on Materials for Nanoscience, Biosensors and Energy, in collaboration with Weizmann University and Mahatma Gandhi University , February 4-5, 2013, Visit of Royal Society of Chemistry as a part of Road Show on February 6, 2013, IWAM 2013 at RAK-CAM during February 24-26, 2013.

The following lectures from distinguished speakers were organized by ICMS: The second Sheikh Saqr Materials Lecture was delivered by Prof. Claudia Felser, Director, Max Plank Institute Johannes Gutenberg University of Mainz, on December 3, 2012. The third Annual Materials Lecture was delivered by Prof. Prof. Ashutosh Sharma, IIT Kanpur, on April 8, 2013 and a talk was delivered by Prof. Veerabhadran Ramanathan, Distinguished Professor of Climate Sciences, Scripps Institution of Oceanography, University of California at San Diego,

The Centre during the year has appointed Dr. Raju V. Ramanujan of Nanyang Technological University as Adjunct Professor. RAK-CAM Sheikh Saqr Junior Fellowship has been awarded to Mr. Rana Saha and Ms. Sharvani S was awarded the Post Graduate Diploma in Materials Science.

# **Research Activities**

Professor C.N. R. Rao's group has initiated two major programmes on energy research: one related to artificial photosynthesis involving photocatalytic oxidation of water by nanoparticles of Mn and Co oxides and the other on photocatalytic H2 generation by hybrid nanostructures by using the Z-scheme. Synthesis, characterization and properties of anions substituted metal oxides where in oxygen is replaced by nitrogen and fluorine are being investigated. Multiferroics and magnetoelectrics continue to be investigated. A novel experimental set-up is being carried out, which involves examining products of electrical discharge of graphite and other materials in various liquid media including argon, nitrogen, water and organics.

Significant progress has been made on the formation and properties of nanomanifestations of III-nitride materials at Shivaprasad's group. Observation of magnetism at the apex of the nanowalls, coherent emission at the open screw dislocations and application as a versatile SERS substrate have been the highlights. High mobility in nano-GaN due to band tail states is being further probed for these materials. The band bending associated with the In top-layer formation has been observed and further experiments to find kinetic ways to form high quality, high mobility InN films are underway.

Aberration corrected atomic resolution imaging and quantification of oxygen atoms in ZnO has been performed by Dr. Ranjan Datta's group. Magnetic information from length scale as small as 5 nm from  $CrO_2$  in a TEM has been studied. ZnO crystal growth has been studied with Co, Mn, S, Li, N doping by PLD for device application.

Research in the Soft Matter Lab of Dr. Rajesh Ganapathy mainly focused on two broad themes. The first was to understand the role of an external driving force on the dynamics of grain boundaries in sheared polycrystals. Experiments were done using the confocal-rheometer, which allows us to track dynamics with single particle resolution under a well-defined shear. The problem is of relevance in numerous industrial processes that tune material performance by altering the spatio-temporal dynamics of grain boundaries. They found that shear introduces an anisotropy in the grain boundary mobilities and leads to directional grain growth. The second theme was to explore the role of particle shape anisotropy on glass transition dynamics and suspension rheology. The specific research problems which were embarked on were to explore reentrant glass dynamics in suspensions of colloidal ellipsoids and the shear-thickening behavior of suspensions of colloidal rods. A high-speed camera had been acquired that will be integrated with our rheometer for extensional rheology measurements on colloidal suspensions. Plans are there to investigate the role an oscillatory shear on the dynamics of colloidal glasses. Synthesis of novel colloidal particles are there in plan including clusters and flexible strings and to explore their role in colloidal self-assembly.

Perylene diimides were explored as alternatives to C70fullerenes in organic solar cells by Dr. Sreedhar Rajaram's research group. They showed that disrupting the planarity leads to a tenfold improvement of efficiency. 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 organocatalysis, they have shown that conformational rigidity can be enhanced using complexation with alkali metal ions. They have developed a synthesis of non-natural amino acids that avoids the use of toxic HCN.

The primary focus of Dr. Ranjani Vishwanatha's research group is the synthesis and study of optical and magnetic properties of semiconductor nanocrystals. Towards that goal, they have been involved in the synthesis of Cu doped CdSe to use copper as a nanosensor to study the electronic structure and surface properties of CdSe. They are also currently in the process of extending these studies to other II-VI semiconductors. The second area of interest that is actively pursued is to synthesize particles of CdSe/CdS core shell systems that are defect free and hence obtain a near unity quantum yield. These particles are also cast into exploratory devices of light emitting diodes that were found to have efficiencies comparable to the world standards. They have also actively pursued the synthesis of CdTe and CdTe/CdS core shell systems to dope them with magnetic impurities like Fe, Co. Electronic Structure study of nanoparticles using doping and study of magnetic properties of nanocrystals doped with magnetic impurities are underway.

Following are the members of the Unit:

#### Faculty

C.N.R. Rao, F.R.S., Hon. F. R. S.C., Hon. F. Inst. P., *Director* S. M. Shivaprasad, Ph.D. (Karnataka), *Professor*, jointly with CPMU Ranjan Datta, Ph. D (Cambridge), *Faculty Fellow* 

Rajesh Ganapathy, Ph. D (IISc.), *Faculty Fellow* Sridhar Rajaram, Ph. D (Univ. of Utah), *Faculty Fellow* Ranjani Viswanatha Ph.D. (IISc.), *Faculty Fellow* 

# **Honorary Faculty**

A. K. Sood, F. A. Sc., F. N. A., F. T. W. A. S. of IISc. A. Govindaraj, Ph.D. (Mysore), of SSCU, IISc U. Ramamurty, Ph.D. (Brown Univ.), of IISc

# **Adjunct Professors**

Timothy Fisher, Purdue (until Sep 2014) Vinayak Dravid, Northwestern University (until Sep 2014) Raju V. Ramanujan (June 2012 - June 2014)

# Fellow

Jay Ghatak

**ICMS Incharge Co-ordinator** Aruna V. Mahendarkar

# **Research Associates**

Mr. Chithaiah P -- SSL Mr. Nagaraja K K

#### **Technical Assistants**

Shivakumar K M, Prajwal D J, Kishor Upadhayaya

#### **Diploma Students**

Renu Tomar, St. Thomas college Ankit Kumar Sharma, Central University of Rajasthan Manju Unnikrishnan

#### **R & D Assistants**

Srishti Arora, Srikanth Revoju ---SSL,

Arnidom Chatterjee --SSL, Aloke Kumar Ghosh --- SSL

#### Graduated Students (Post Graduate Diploma Programme)

Bello Adedeji Abdulhakeem from Nigeria Dzade Nelson Yaw from Ghana S. Manjunath from Gulbarga University, Karnataka Arghya Bhowmik from Pohang University, South Korea Sharvani Shivaprasad, BVB College of Engineering Bolla Govinda Rao, Acharya Nagarjuna University

#### Junior Lab Assistant

Munegowda

#### **Visiting Scientists**

Dr. Mohd. Ikram, National Institute of Technology, India Dr. T. Nishimatsu, Tohoku University, Sendai Prof. Stefano Baroni, Italy Dr. Nacir Tit, UAE University, Al-Ain, UAE Mr. Jos Laurie Campbell, RMIT University, Australia Dr. Prashant Dubey, University of Allahabad, UP Mr. Felix Fabich, University Bergakademie Freiberg, Germany Dr. K. Sakthipandi, K S Rangasamy College of Technology, Tamilnadu Mr. Ushie Onumashi Afi, Federal University, Nigeria Mrs. Shruti Nambiar, University of Waterloo, Canada Dr. Jagaran Acharya, Tribhuvan University, Nepal Mr. Manjunath Chatti, ISSER, Kolkata Dr. Mrinmoy De, Northwestern University, USA

# Thematic Unit of Excellence in Computational Materials Science

(Formerly known as Centre for Computational Materials Science (CCMS)

# **Research Activities**

The molecular features which govern the mechanism of supramolecular polymerization have been identified and delineated. Density functional theory and empirical potential based MD simulations of liquid dimethyl carbonate, an environmentally benign solvent have shown clustering of conformers with high dipole moment.

It was discovered, through density functional theory calculations, that doping the oxide substrate with an electron donor significantly reduces the barrier for oxygen dissociation on gold nanoparticles. A new framework to understand these results, involving primarily the s and p bands of the gold nanoparticles, have been developed.

It has been shown that functionalizing graphene, either with various organic moieties on the edge, or by depositing various metal adatoms, significantly increases the binding of gases such as hydrogen and methane. This has implications for on-board vehicular storage applications.

It has been shown that the finding that magnetism drives surface alloy formation for FeAu/Ru(0001) does not hold for FeAu/Mo(110). This can be attributed primarily to the different nature of magnetic moments on substrate atoms in the two cases.

The electronic structure and energetics of defects in twisted bilayer graphene have been explored. It has been shown that these defects show clear signatures that can be picked up in STM images.

The effects of lead geometries on spin transport, spin spirals in surface alloy systems, photoswitching van der Waals crystals, and modification of surface work function by mixed SAMs.

Research interest encompasses a broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum systems. Methane formation from hydrogeneration of carbon dioxide on Ni (110) surface has been studied. A large number of work involving various molecules (including fullerenes) over graphene, its B-N analogues and edge states in quantum dots have been studied. Novel electronic transport properties like negative differential conductance (NDC), spin filter, half-metallicity and a number of new phenomena when light is signed on the device region have been studied in details. Kagome antiferromagnetic clusters with Dzyaloshinskii-Moriya interactions have been studied to understand magnetic behavior. Many biological systems, including DNA, G-quadruple and their metal-mediated properties have also been explored.

# Multi-scale Simulations of Materials

Using first-principles effective Hamiltonian of  $PbTiO_3$  in MD simulations with a combination of constrained polarization and thermodynamic integration, [http://dx.doi.org/10.1103/PhysRevB.87.024107] a Ginzburg Landau theory has been derived, and provided a free energy landscape based analysis of ferroelectric transition, domain structure and associated dielectric response of  $PbTiO_3$ . This work has accomplished the following important findings: it (a) has determined the nature of the puzzling orthorhombic phase seen experimentally; (b) highlighted the contrast in the domain structures of  $BaTiO_3$  and  $PbTiO_3$ .

# **Fundamental Physics and Applications of Graphene**

First-principles calculations were used and carried out a thorough analysis of topological defects in graphene, identifying their electronic and vibrational spectroscopic signatures that can be used in experiments to characterize the defects in a non-invasive way. Secondly, a theoretical explanation was given for the unusual ability of graphene to remove pesticides from water seen experimentally by Pradeep et al, in terms of the water mediated interactions between graphene and pesticides including endosulfan [http://dx.doi.org / 10.1002/smll.201201125].

# Materials with Magnetoelectric Coupling

A theoretical analysis of the multiferroic behavior in FeAlO<sub>3</sub> [http://dx.doi.org/ 10.1016/j.ssc.2012.07.018] has been provided, in terms of coupled phonons, spin and electronic charge degrees of freedom

[http://dx.doi.org/10.1103/PhysRevB.85.134449]. They specifically obtained first and second order coupling between spin and phonons in this class of materials.

Contributions to theory of electronic topological transitions, surfaces and interfaces.

#### New programmes launched during the year

Homogeneous as well as heterogeneous catalysis. Dynamical electronics processes. Organization of the India-UK Scientific Seminar at the University College, London. Received a tri-lateral (India-UK-USA) grant to support research on solution of graphene and BN.

Contribution to organization of Conferences/Schools:

- Cambridge-JNCASR Winter School on "Frontiers of Materials Science", JNCASR, Bangalore, December 3-8, 2012.
- Indo-US Workshop on "Advanced and Nano-Materials", JNCASR, Bangalore, January 21-22, 2012.
- Nano-India 2013, the National Meeting on Nano-Science, NIIST, Trivandrum, February 19-23, 2013.

Following are the members of the Unit:

#### Coordinator

Prof. Balasubramanian Sundaram

#### Members

Prof. Shobhana Narasimhan Prof. Srikanth Sastry Prof. Swapan Pati Prof. Umesh Waghmare

#### **Associate Members**

Prof. Amalendu Chandra, IIT Kanpur Prof. Sanjoy Bandyopadhyay, IIT Kharagpur Prof. Prabal K. Maiti IISc, Bangalore Prof. S. Yashonath IISc, Bangalore Prof. Tanusri Saha-Dasgupta, S.N. Bose National Centre for Basic Sciences, Kolkata Prof. Lavanya M. Ramaniah, Bhabha Atomic Research Centre, Mumbai Prof. P.B. Sunil Kumar, IIT Madras, Chennai Prof. K.P.N. Murthy, Indira Gandhi Centre for Atomic Research, Kalpakkam Prof. Charusita Chakravarty, IIT Delhi Prof. Surajit Sengupta, S.N. Bose National Centre for Basic Sciences, Kolkata Prof. Gautam Menon, Institute of Mathematical Sciences, Chennai Prof. B. Jayaram, IIT Delhi Prof. Rajendra Prasad, IIT Kanpur Prof. Dilip G. Kanhere, University of Pune Prof. G.P. Das, Indian Association for the Cultivation of Science, Kolkata Prof. Ganapathy Ayappa, IISc, Bangalore Prof. T.A. Abinandanan, IISc, Bangalore Prof. Indra Dasgupta, Indian Association for the Cultivation of Science, Kolkata Prof. Dilip Angom, Physics Research Laboratory, Ahmedabad Prof. Satyavani Vemparala, Institute of Mathematical Sciences, Chennai Prof. Indira Ghosh, University of Pune

#### **Programme Assistant**

Venkatesh K

#### Staff

Basavaraj T, Bharati Singh, Vijay Amirtharaj A

# **DST Unit on Nanoscience**

Conversion of inorganic carbonates to methane has been carried out using mixed metal carbonates as an alternative way to capture and convert the carbon dioxide, an important environmental problem. It was observed that presence of cobalt facilitate the complete conversion of carbonate to methane.

There has been significant work in the field of nanocarbons. Important contributions have been made in the area of carbon nanotubes as well as graphene, and some of the contributions in this area have received international attention. More importantly, in addition to the nanotubes and graphene made of carbon, graphene analogues of other inorganic layered materials have been synthesized and characterized.

Aminoclay is a layered magnesium organosilicate with the structure analogous to 2:1 trioctahedral smectites, such as talc but with covalently linked organosilicates in place of inorganic silicates, with an approximate composition  $R_8S_{88}Mg_6O_{16}$  (OH<sub>)4</sub> (R= alkylamine covalently linked to Si) This clay is easily exfoliable in water into nanosheets due to protonation of amino groups. These functional groups are very efficient in stabilizing metal nanoparticles to form clay-metal nanoparticles Composite film made with the aminoclay slabs and the polymer, polyvinylalcohol, showed enhanced strength without compromising its ductility, a problem commonly encountered in using inorganic filler with the polymer in macro composites. These composite film incorporated with Ag and Au metal could be used as food packaging materials.

Direct write methods have been developed which make use of a variety of metal-organic complexes as single source precursors to produce micro and nanoscale patterns of metals, oxides, sulfides, nitrides as well as of alloys. A desired interface can be easily obtained by exercising control over the chemical treatment. Based on this principle, a few devices such as strain sensor, have been produced. The direct methods not only cut down the number of process steps but also the cost and importantly, enable design of material interfaces which are beyond the conventional lithography.

Following are the members of the Unit:

# **Faculty members**

Prof. C. N. R. Rao Prof. G. U. Kulkarni Prof. K. S. Narayan Prof. Swapan K. Pati Prof. A. Sundaresan Prof. M. Eswaramoorthy Prof. A. Govindaraj

# **Technical Assistance**

Ms. N. R. Selvi

# **CSIR Centre of Excellence in Chemistry**

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.

New strategies have been developed for the synthesis, purification, functionalization and solubilization of novel carbon nanostructures such as, carbon quantum dots, graphene, single-walled nanohorns, carbon nanotubes, 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.

Graphene is one of the main areas of research in this laboratory. Synthesis of two to four layer graphene was carried out by arc-discharge of graphite in a hydrogen atmosphere as well as with other conditions. Besides providing clean graphene surfaces, this method allows for doping with boron and nitrogen. 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.

It was discovered that incorporation of graphene improved the mechanical properties of polymers, its incorporation with nanodiamond or carbon nanotubes exhibits extraordinary synergy. Hybrid nanocomposites of graphene oxide (GO) with zeolitic imidazolate frameworks (ZIF-8) as well as with porous graphene frameworks (PGFs) pillared by organic linkers exhibits interesting gas adsorption properties.

After the synthesis and characterization of graphene, serious attention is paid to other inorganic analogues of graphene. Various chemical methods have been developed for the synthesis of layered transition metal dichalcogendes which includes MoS<sub>2</sub>, WS<sub>2</sub>, MoSe<sub>2</sub>, WSe<sub>2</sub>, NbS<sub>2</sub> and NbSe<sub>2</sub>. Their applications in IR detectors, gas sensors, composites with polymers for mechanical properties and electrical properties, magnetic properties, and hydro-desulphurization (HDS) catalysis have been studied. Micromechanical cleavage method has been used for obtaining the single-layers of MoS<sub>2</sub>, GaS and GaSe and studied their applications in transistors, detectors and sensors.

The interaction of electron-donor and –acceptor organic molecules have been studied such as tetrathiafulvalene and tetracyanoethylene with different materials such as layered chalcogenides, as well as nanocrystals of ZnO and CdSe. The charge transfer from tetratiafulvalene to few layer  $MoS_2$  can be evidenced from optical measurements.

It was also discovered that nanosheets of transition metal oxides, such as  $MoO_3$  consisting of only a few-layers prepared by different methods exhibits enhanced photocatalytic activity. Also, it was established that in combination with a borocarbonitride, few-layer  $MoO_3$  composite shows good performance characteristics as a supercapacitor electrode.

High surface area borocarbonitrides were synthesized from low cost starting materials like urea, boric acid and activated charcoal. Graphene-like  $B_x C_y N_z$  samples exhibit surface areas in the range 1500-1990 m<sup>2</sup>/g, with the large uptake values of  $CO_2$  and shows good performance characteristics as supercapacitor electrode.

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<sub>2</sub> and O<sub>2</sub>. Spinel based photocatalysts have been used which contained "Mn<sub>4</sub>O<sub>4</sub> cubane" like structure similar to that found in chlorophyll for oxidation water. It was found that nanoparticles of Co, oxides like the spinel Li<sub>2</sub>Co<sub>2</sub>O<sub>4</sub> and the perovskite LaCoO<sub>3</sub> shows oxygen evolution in solution containing Ru(bpy)<sub>3</sub><sup>2+</sup>. Amongst the manganese oxides studies, Mn<sub>2</sub>O<sub>3</sub> with the bixbyite structure and LaMnO<sub>3</sub> with the perovskite structure containing Mn<sup>3+</sup>(t<sub>2</sub><sup>3</sup> e<sub>g</sub><sup>1</sup>) ions show high catalytic activity. N, F co-doped TiO<sub>2</sub> showed maximum hydrogen evolution of 400 moles/g of the catalyst with a rate of ~ 60 moles/g/h without the loading of any noble metal or other co-catalyst.

Multiferroic and magnetoelectric nature of  $Al_{1,x}Ga_xFeO_3$  (x=0, 0.5, 1) family of oxides all crystallizing in the orthorhombic structure, with a non-centrosymmetric space group (Pna2<sub>1</sub>), exhibits both multiferroic and magnetodielectric properties at low temperatures. Similarly  $GaFe_{1,x}Cr_x(Mn_x)O_3$  and  $Ga_{1,x}Cr_x(Mn_x)FeO_3$  are magnetoelectric as well as multiferroic.  $LnCr_{1,x}M_xO_3$  (Ln= Y, Lu; M = Fe, Cr, Mn) family of oxides showed spin-disorder induced ferroelectricity.



Following are the members of this Centre:

Chair Prof. C.N.R. Rao	FRS, FASc, FNA, FTWAS, Hon FRSC, Hon F Inst P
Hon. Associate Professor Prof. A. Govindaraj	Ph D

# **Computer Laboratory (CompLab)**

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 (http://www.jncasr.ac.in/complab).

CompLab hosts email, web, proxy and gateway servers of the Centre, Link-load-balancer, IronPortC150 (a spamcontroller), a Firewall and maintains many other servers that cater to Purchase, Canteen and Labrary. 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 chasis switch. The centre is connected to internet via 10 Mbps + 25Mbps 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 databses. Each member of JNCASR has a quota and access to free print-outs from CompLab's high-quality colour and monochrome printers.

In this financial year, CompLab has taken a number of steps to enhance the computing and other IT infrastructure of the Centre. Some of the important activities undertaken are:

- JNCASR users were facing bandwidth issues with the existing deep-root mail solution. This mail client was replaced with a Zimbra email solution, which is able to cope up with increased bandwidth in the campus.
- A new mail server '*Saturn*' has been installed to provide email services to alumni and temporary users of the Centre. This segregation of users into groups has allowed a better utilization of network resources.
- National Knowledge Network connectivity was enhanced to 200 MBPS from existing 100 MBPS line.
- An online system of printing has been installed in the campus. This has lead to better user experience as well as saving of space in the campus.
- A new colour printer and one poster printer have been installed for on-campus users. In-house poster printing facility has lead to substantial saving of time for JNCASR students.

Following are the members of CompLab:

# Head

Dr. Santosh Ansumali	Ph D
2 II O MII VO DITT III O MIII MII	

# Consultant

Vikas Mohan Bajpai

#### **R&D** Assistants

Vishnu Pradeep P V, Kiran Kumar, Divya Shivanna

# Library

The Library has a collection of over 8400 books and access to over 5000 scientific journals. Book exhibitions were also arranged. Several new journal titles subscribed. Journal articles were procured on request from faculty members and students from CSIR, DST and other neighboring libraries under document delivery service.

# **Overview of Collection**

Books			
Books procured during 2012-13	364		
Total books in collection	8408		
Journals			
Online journals subscribed	159		
Print journals subscribed	6		
Approx. price for newly subscribed journals	₹23,69,136.00		
Patent database (Derwent Patent Index) – from National Knowledge Resource Consortium	1		
Abstracting and Indexing database (Web of Science) – from National Knowledge Resource Consortium	Web of Science, SciFinder		
Online journals in collection (Subscription + consortium resources)	Over 5000		

# **Books Acquisition**

In the financial year 2012-13, 364 books worth ₹11,21,416/- (Rupees Eleven lakhs twenty one thousand four hundred and sixteen only ) were procured in the library based on the recommendations of JNCASR Faculty members.

# Journal Subscription and Consortium Resources

The total amount spent for the subscription of both print and online journals for the year 2012-13 is ₹ 90,71,482.00 (Rupees Ninety lakhs seventy one thousand four hundred and eighty two only). Thirty four new journals have been subscribed worth ₹23,69,196.00 (approx.).

Due to financial constraints, some key resources supported by National Knowledge Resource Consortium have been discontinued for 2013 such as journals from American Chemical Society, Springer, Springer Materials.

# **Document Delivery Service (DDS)**

Journal articles on requests from faculty and students were procured from libraries across the country and abroad under Document Delivery Service. Total 362 article requests have been fulfilled through inter-library cooperation. Twenty five articles were purchased online.

Following are the library staff members:

#### Library-Cum-Information Officer Nabonita Guha

- Senior Library cum Information Assistant Gr. I Nandakumari, E.
- Senior Library cum Information Assistant Gr. II Nagesh Hadimani
- Library cum Information Assistant Gr. II Senthil Kumar, N.

### Library Trainee

Kalpana S. (term ended on September 2012) Poornima Hosamani

R & D Assistant

N. M. Tara

Helper Rajeeva, J.

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# **ENDOWED RESEARCH PROFESSORS**

# Linus Pauling Research Professor

	<b>C N R Rao</b> Jawaharlal Nehru Centre for Adanced Scientific Research, Bangalore (Term: Life time)	F R S, D Sc, F A Sc, F N A, F R S, F T W A S, Hon F R S C
D S Koth	ari Chair	
	<b>M M Sharma</b> Emeritus Professor of Eminence, Mumbai University, Mumbai (Term: 01/01/1999 to 31/10/2013)	F R S, F A Sc, F N A
Hindusta	an Lever Chair	
	<b>S Chandrasekaran</b> Indian Institute of Technology, Madras (Term: 01/11/2011 to 31/10/2013)	F A Sc, F T W A S, F N A
Dr Vikra	m Sarabhai Research Professor	
	<b>Kalyan B Sinha</b> Jawaharlal Nehru Centre for Adanced Scientific Research, Bangalore (Term: 01/12/2011 to 02/06/2014)	F N A, F A Sc, F T W A S

# ACADEMIC PROGRAMMES

### Academic Activities

At JNCASR, research is carried out in six Units: Chemistry and Physics of Materials Unit (CPMU), Evolutionary and Organismal Biology Unit (EOBU), Engineering and Mechanics Unit (EMU), International Centre for Materials Science, Molecular Biology and Genetics Unit (MBGU), New Chemistry Unit (NCU) and Theoretical Sciences Unit (TSU). The research undertaken is inter-disciplinary in nature.

The Centre offers Ph. D, Integrated Ph. D, M.S (Research) and M.S Engg . degree programmes in Science and Engineering. Students are admitted to the Units mentioned above. The minimum academic qualification required to apply for the MS/Ph.D programmes of the Centre is M.Sc./B.E./B.Tech./M.E./M.Tech./MBBS degree/s. Candidates applying for M.S./Ph.D. programmes should have at least 50% in their highest University examination, and should also have qualified in GATE/UGC-CSIR-JRF/ICMR-JRF/DBT-JRF/JEST/equivalent examinations. Candidates applying for Integrated Ph.D. Programme of the Centre should have at least 55% marks in their Bachelor's degree in any area of Science or Statistics.

The Centre selects candidates on the basis of their academic record, performance in GATE /UGC-CSIR-JRF/ ICMR-JRF/ DBT-JRF/ JEST/ equivalent examination(s), recommendation from referees and performance in the interview. The selected candidates are offered course work, provided with research facilities for research and on successful completion offered with the degree.

#### **Research Admissions**

The present student strength is 273. Forty two students had joined the Centre during the August 2012 admissions. Seven students joined the Centre during January 2013 for the session of 2012-13. The advertisement for the regular admission to the Integrated Ph.D., Ph.D. and M.S. programmes 2013-14 session was released in all the prominent national and regional newspapers and announced on our web site.

#### **Degrees** Awarded

The Centre is a Deemed University, and awards Ph.D. and M.S. degrees. Following are the students who have been awarded degrees under the various degree programmes during April 2012- March 2013:

		Ph.D.	M.S. (Engineering)	
M	Aangaiarkarasi A.	Jitendra Thakur	Gangaiah Mettela	
K	C.S. Subrahmanyam	Surbhi Dhar	Sarada S	
B	Bharath S.	Jithesh K	Kaushlendra Kumar	
P	Prakash Kanoo	Pranab Mandal	Md Istafaul Haque	
H	Iimadri Barman	Shipra	Ansari	
S	nigdhadip Dey	Mighfar Imam	Gopalakrishnan K	
M	Aoumita Maiti	Sumesh P T	Nishit Srivastava	
M	Aanoj Kesaria	B Radha	Wasim Raja Mondal	
Master o	of Science (M S) in	Master of Science (M S) in	Master of Science (M S)	
Mate	erials Science	Biological Science	Chemical Science	
Anindita ( Darshana Dibyajyoti Prashant I	Chakraborty Joshi i Ghosh Kumar	V. Sivani Sheetal Potdar T. Lakshmi Prasoona	Ajmala Shireen P	

# Medal for the best thesis of the year 2011 – 12 in Physical and Biological Sciences categories each: Donated by Prof. CNR Rao

# **Physical Sciences Category**

Name	Research Supervisor	Thesis Title
B Radha	G.U. Kulkarni	Synthesis and Direct Patterning of Functional Nanostructures on Flat and Flexible Substrates towards Device Fabrication

# **Biological Sciences Category**

Name	Research Supervisor	Thesis Title
Jitendra Thakur	Kaustuv Sanyal	Genetic and Epigenetic Factors Determining Centromere Structure and Function in <i>Candida</i> Species

### Roddam Family Award for the Best Ph.D. Thesis in Engineering Mechanics :

Scroll and cash prize

# Ph.D. degree

Name	Research Supervisor	Thesis title
P.T. Sumesh	Rama Govindarajan	Statics and Dynamics of Drops on Solid Surfaces: Theory and Simulations

### **DISCUSSION MEETINGS**

The following discussion meetings were supported by the Centre. The meetings were organized by its faculty in association with faculty of other reputed research institutions in various areas of current interest.

- 1. Indian Society of Neuro-Oncology (ISNOCON 2012), Dr Vani Santhosh, April 6 8, 2012.
- 2. ACCMS Theme Meeting on 2D Nanostructures: Graphene and Beyond, Prof. Umesh V. Waghmare, JNCASR, July 29-30, 2012.
- 3. CFM 2012 Chemical Frontiers, Prof. R. Murugavel, IIT Bombay, August 14 16, 2012.
- 4. Discussion Meeting on Electronic, Optical and Magnetic Materials: experiment and Modeling, Prof. S. Ramasesha, IISc, November 25 28, 2012.
- 5. Meeting of Young Affiliates and Fellows of TWAS in Central & South Asia Region, November 15-17,2012.
- 6. Fourth International Advisory Board meeting, ICMS, December 3, 2012.
- 7. EOBU Symposium, January 9-10, 2013.
- 8. Indo-Israel Meeting, February 4-5, 2013.
- 9. Visit of Royal Society of Chemistry to ICMS as a part of Road Show on February 6, 2013.
- 10. Funding and Related Opportunities from ERC, Prof. Donald Dingwell, Secretary General, European Research Council Meeting, March 12, 2013.

#### **ENDOWMENT LECTURES**

**A.V. Rama Rao Foundation Lectures in Chemistry**: *Fluorescent Molecular Architectures with Exceptional Properties*, Dr A Ajay Ghosh, CSIR-Outstanding Scientist, Chemical Sciences & Technology Division, NIIST, Trivandrum and **Prize Lecture**: *Luminescent Nano Materials for Photonic Applications*, Dr Amitava Patra, Department of Materials Science, Indian Association for the Cultivation of Science, Kolkata, May 16, 2012.

**Prof. V. Ramalingaswami Memorial Lecture:** *Act of Observation and Cancer Biology*, Dr. R A Badwe, Director, Tata Memorial Centre & Hospital, Mumbai, July 9, 2012.

**Prof. C. N. R. Rao Oration Award Lecture:** *HIV says again - "In failure, I see my success",* Prof. Ranga Udaykumar, JNCASR, August 6, 2012.

**DAE - Raja Ramanna Lecture in Physics**: Novel Electronic Phenomena at Oxide Interfaces, Dr. Ramesh Chandra Budhani, NPL; Prize Lecture - Tweaking the magnetic domains and domain-walls in nanostructures: A prospective magnetic memory concept, Prof. Anil Kumar, IISc, September 28, 2012.

**Linus Pauling Lecture**: *The Antimicrobial Defense of Drosophila: a Paradigm for Innate Immunity from Flies to Humans,* Prof. Jules Hoffmann, Nobel Laureate, Institute of Molecular and Cellular Biology, University of Strasbourg, France, October 12, 2012.

**ISRO Satish Dhawan Lecture:** Science for Musical Excellence of the Mridangam, Dr. T. Ramasami, Secretary, Department of Science and Technology and Dr. Umayalpuram S. Sivaraman, October 16, 2012.

**Sheikh Saqr Materials Lecture:** *Heusler compounds: From semiconductors to spintronics,* Prof. Claudia Felser, Director, Max Plank Institute Johannes Gutenberg University of Mainz, Mainz, December 3, 2012.

**M.K. Chandrasekaran Memorial Lecture:** *Rhythms in time and space*, Prof. Anders Johnsson, Department of Physics, Faculty of Natural Science and Technology, Norwegian University of Science and Technology, Trondheim, Norway, January 9, 2013.

**IPR Lecture:** *Patent Laws and Its Importance to Scientific Research*, Prof. Srividhya Ragavan, Professor of Law, University of Oklahoma College of Law Norman, OU, USA, March 26, 2013.

#### **GENERAL LECTURE**

- 1. *Staff Orientation Lecture*, Dr. Anand Kumar, JNCASR, July 11, 2012.
- 2. *Handling Injuries An Interactive Session*, Dr. V. Yogesh, JNCASR, August 17, 2012.
- 3. *Paperless Office An experiment and experience*, Mr. M. N. Vidyashankar, Principal Secretary, Commerce & Industries Dept., Govt. of Karnataka on Monday, October 01, 2012

#### Lectures delivered at the Annual Faculty Meeting (November 2012)

- 1. Design of Molecules for Telomerase Inhibition, Prof. Santanu Bhattacharya
- 2. Organic Photovoltaics: Every Photon Counts, Prof. K. S. Narayan
- 3. *Warm cues for the fruitfly clock the role of a temperature sensitive ion channel in diurnal activity patterns,* Dr. Sheeba Vasu
- 4. Possible onset of Transient Universality in Fluid Turbulence, Dr. Santosh Ansumali
- 5. *"The richest don't take it all", Directional Grain Growth in Sheared Polycrystals: Evidence for a straintemperature equivalence,* Dr. Rajesh Ganapathy

#### CONFERENCES/WORKSHOPS/SYMPOSIA

- 1. International Conference on Networks in Biology, Social Science and Engineering, Prof. G. Rangarajan, IISc, July 12 14, 2012.
- 2. Recent Advances in Electrochemical Energy Materials and Devices, Prof. A. J. Bhattacharyya, July 24-27, 2012.
- 3. TSU In-House Symposium, August 4, 2012.
- 4. International Conference on Raman Spectroscopy (ICORS 2012), Prof. Chandrabhas Narayana, JNCASR and Prof. Umapati, IISc, August 12-17, 2012.
- 5. Indo-US workshop on Next Generation of Materials Using Neutrons, September 6-7, 2012, Convenor: Prof. G. U. Kulkarni
- 6. 9th Kannada Vignana Sammelana, Prof. K.I. Vasu, September 15 17, 2013.
- 7. Publishing Workshop, Institute of Physics, September 18, 2012
- 8. 8th JNC Research Conference on Chemistry of Materials, Dr. Subi Jacob George, JNCASR, September 30 October 2, 2012.
- 9. Indo-Japan Conference on New Functionalities in Electronic and Magnetic Materials, Prof. D. D. Sarma, October 18 20, 2012.
- 10. Two days Symposium on "National Mathematical Year NYM 2012", Shri Sasti Brata, Kabiraj, October 20 21, 2012.
- 11. Thematic Meeting on Lipid Protein Interactions in Membranes: Implications for Health and Diseases, Prof. Amitabha Chattopadhyay, November 1 5, 2012.
- 12. FCBS Workshop for Postgraduate Students and Lectures in Chemistry, Prof. M. V. George, NIIST, Trivandrum, November 8-10, 2012.
- 13. Indo-Taiwan Workshop on Nanodevices, November 26 27, 2012.

- 14. Winter School on "Chemistry and Physics of Materials" with University of Cambridge, UK, and RAK-CAM; Convenors: Prof. S. M. Shivaprasad and Prof. Umesh Waghmare; December 3-8, 2012.
- 15. International conference on Design of Biomaterials (BIND-12)", IISc, December 9-11, 2012
- 16. International conference on "Operator Algebras in Nonequilibrium Statistical Mechanics" at Bambolim Beach Resort, Bambolim, Goa, December 17-21, 2012
- 17. International Conference on Biomolecular Forms and Functions: A Celebration of 50 Years of the Ramachandran Map, Prof. Manju Bansal, January 8 11, 2013
- 18. International Conference on Quantum Information and Quantum Computing (ICQIQC), Prof. S. Raghuveer, IISc, January 9 11, 2013.
- 19. Annual Conference on Molecular Immunology Forum (MIF), Prof. Ranga Uday Kumar, JNCASR, January 17-19, 2013.
- 20. Indo-US Workshop on "Advanced and Nano-Structured Materials", JNCASR, January 21-22, 2013.
- 21. Workshop on SQUID magnetometry, Prof. A. Sundaresan, CPMU, JNCASR, Bangalore, January 23, 2013.
- 22. JNCASR-RMIT Workshop, January 28-29, 2013.
- 23. Indo-Australia Joint Workshop, January 28-29, 2013.
- 24. Indo-Israel Conference, January 30-31, 2013.
- 25. Indo-Canadian Symposium on Nano-Science and Technology ICSNST-2013, Mysore, February 20-22, 2013.

#### **SEMINARS / COLLOQUIA**

- 1. GTPases involved in Ribosome biogenesis, Prof Balaji Prakash, IIT, Kanpur, April 2, 2012.
- 2. *Research activities of St. Petersburg Electrotechnical University "LETI"*, Dr M Odit, St. Petersburg Electrotechnical University LETI, April 6, 2012.
- 3. *Gene networks in theory and practice*, Dr Mukund Thattai, Computational and Evolutionary Cell Biology, National Centre for Biological Sciences, Bangalore, April 12, 2012.
- 4. *T Cell Immunobiology in the lung: implications for pulmonary fibrosis*, Dr Sambuddho Mukherjee, Dept. of Cell Biology, Duke University Medical Center, USA, April 12, 2012.
- 5. *Genome Architecture and Disease*, Dr Tom Misteli, NIH and Editor-in-chief, Journal of Cell Biology, Bethesda, USA, April 13, 2012.
- 6. Lecture on LBM, Dr Santosh Ansumali, JNCASR, Bangalore, April 18, 2012.
- 7. *Quantum theory of materials: methods and applications*, Dr Manish Jain, Lawrence Berkeley National Laboratory, Department of Physics, University of California, Berkeley, May 1, 2012.
- 8. *Charge Separation and Recombination in Organic Photoconversion Systems*, Dr. Akshay Rao, Cambridge University, UK, May 2, 2012.
- 9. Science Outreach Programme Summer 2012, Prof K S Valdiya, JNCASR, May 6 9, 2012.
- 10. *Density controlled bio-functionalized nanostructures*, Dr Loredana Casalis, Sincrotrone Trieste S.C.P.A., Trieste, Italy, May 14, 2012.
- 11. *Non-normal and nonlinear instabilities in thermo-acoustic interactions*, Prof Sathesh Mariappan, Department of Aerospace Engineering, Indian Institute of Technology Madras, May 23, 2012.

- 12. *Biomaterials for neural tissue engineering*, Prof. Surya Mallapragada; *Pathogen mimicking nanoparticle for prevention and treatment of respiratory infectious disease*, Prof. Balaji Narasimhan, Department of Chemical and Biological Engineering, Iowa State University, June 14, 2012.
- 13. *Interplay of 4f-3d interaction and dynamical electrical transport in Sm based manganese oxides*, Prof. R. Mahendiran, Department of Physics, National University of Singapore, June 22, 2012.
- 14. *Theoretical studies for understanding a few observations on protein conformational dynamics*, Dr. Meher K. Prakash, Co-founder and C.E.O., Metaplastics SAGL, Lugano, Switzerland, June 22, 2012.
- 15. *Ultracold atoms in the presence of a synthetic gauge field*, Dr. Subhasis Sinha, Physical Sciences Division, Indian Institute of Science Education and Research, Kolkata, July 10, 2012.
- 16. *ICMS International Materials Lecture*, Prof. Chad Mirkin, Department of Chemistry and International Institute for Nanotechnology, Northwestern University, July 16, 2012.
- 17. *Molecular adaptation to cold temperatures and high pressure of a psychrophilic cellulase*, Dr. Nushin Aghajari, Senior Scientist, Institute for the Biology and Chemistry of Proteins, July 18, 2012.
- 18. Organic Nano-Electro-Mechanical-Sensor Systems for healthcare and Environmental Applications, Prof. V. Ramgopal Rao, IIT Bombay, July 19, 2012.
- 19. *Epigenetics of Human Gene Regulation, Steroid Hormone Signaling and Tumorigenesis*, Dr. Subhrangsu S. Mandal, Associate Professor, University of Texas, Arlington, August 3, 2012.
- 20. *Elephant conservation and human elephant conflict mitigation: playing blind man's buff?* Dr. Prithiviraj Fernando, Centre for Conservation and Research, Srilanka, August 7, 2012.
- 21. In search of some novel bimetallic homogeneous and heterogeneous catalysts: from molecular level to nanomaterials, Prof. Suresh Bhargava, Deputy Pro Vice Chancellor (Int) College of Science, Engineering and Health Head of Advanced materials & Industrial Chemistry School of Applied Sciences, RMIT University, August 10, 2012.
- 22. *Circadian clock protein Cryptochrome regulates the expression of pro-inflammatory cytokines*, Dr. Rajesh Narasimamurthy, Salk Institute for Biological Studies, USA, August 17, 2012.
- 23. Effective Hamiltonians for Excited States of Fluorescent Protein Chromophores, Prof. Ross H. McKenzie, University of Queensland, Brisbane, Australia, August 17, 2012.
- 24. *Magnesium Alloy Design: A perspective on multi-scale modeling*, Dr. Amitava Moitra, Fenske Laboratory Department of Chemical Engineering The Pennsylvania State University University Park, USA, August 21, 2012.
- 25. *Investigation of Local Structure in nano and disordered systems some recent XAFS results*, Dr. Debdutta Lahiri, High Pressure & Synchrotron Radiation Physics Division, BARC, Mumbai, August 24, 2012.
- 26. *Mesoscale methods for Extended hydrodynamics*, Dr. Santosh Ansumali, Faculty Fellow, Engineering Mechanics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India, September 4, 2012.
- 27. Next-Generation Genomics at C-CAMP Accelerating the Biological Research in India, Dr. Malali Gowda, Director, Next-Generation Genomics Facility, C-CAMP, NCBS, Bangalore, September 7, 2012.
- 28. *Non-local Stokesian hydrodynamics of active filaments*, Dr. Ronojoy Adhikari, The Institute of Mathematical Sciences, Chennai, September 10, 2012.
- 29. *Partial Decoherence in a Mesoscopic System*, Prof. Sushanta Dattagupta, VisvaBharati University, Shantiniketan, September 14, 2012.

- 30. *Viral latency and drug resistance in HIV-AIDS*, Dr. Amilkar Tanuri, Molecular Virology Laboratory, Institute of Biology Department of Genetics, UJRF, Reo de Janerio, Brazil, September 14, 2012.
- 31. *Predicting and explaining phenomena in carbon and boron nitride nanostructures*, Prof. Helio Chacham, Departamento de Fisica, ICEx, UFMG, Brazil, September 17, 2012.
- 32. *Nanotechnology based assays for detection of blood borne and biodefense pathogens*, Indira Hewlett, Chief, Laboratory of Molecular Virology, Division of Emerging and Transfusion Diseases, Office of Blood Research and Review, Center for Biologics Evaluation and Research (CBER), FDA, MD, September 18, 2012.
- 33. *Voltage gated ion channels*, Prof. Michael Klein, Institute for Computational Molecular Science, Temple University, Philadelphia, September 27, 2012.
- 34. *American Association for the Advancement of Science (AAAS) and Science Magazine*, Bill Moran, Global Director of International Collaboration and Custom Publishing, September 27, 2012.
- 35. Arora kinases beyond centrosomes: role of transcription factors' phosphorylation in gene expression and cell cycle, D. Karthigeyan, MBGU Colloquium, November 16, 2012.
- 36. *Chromosome Stability (JNCASR IISER, TVM) Meeting*, Prof. Kaustuv Sanyal, JNCASR, December 17 19, 2012.
- 37. *The use of Microfluidics in High-Throughput Single Cell Gene Expression*, Dr. Ramesh Ramakrishanan, Director of Molecular Biology at Fluidigm Corporation, San Francisco, US, October 3, 2012.
- 38. *Genetic, competitive and behavioural constraints on adaptation*, Prof. Deepa Agashe, NCBS, Bangalore, October 4, 2012.
- 39. *Modeling Transient Photovoltage Measurements*, Dr. Girish Lakhwani, University of Cambridge, October 5, 2012.
- 40. *Synthesis of Natural Products, Drugs, Agrochemicals and Materials by Multiple Pd-Catalyzed Transformations*, Prof. Lutz F. Tietze, Institute of Organic and Biomolecular Chemistry, Georg-August-University Gattingen, Tammannstr, Gattingen, Germany, October 5, 2012.
- 41. *Benefits of cooperation and communication in bacteria*, Professor Sandeep Krishna, Theory and Modelling of Biological Systems, National Centre for Biological Sciences, Bangalore, India, October 9, 2012.
- 42. *Inorganic nanotubes and fullerene-like nanoparticles*, Prof. Reshef Tenne and Prof. Alla Zak, Weizmann Institute, Israel, October 16, 2012.
- 43. Spin polarised transport via Dithienylethene molecule attached to magnetic nickel leads, Kanchan Ulman & Nisha Mariam, Ph. D Student, TSU, JNCASR, Jakkur Bangalore, October 16, 2012.
- 44. *Carbon fluids in the deep Earth: insight from ab initio simulations*, Dr. Leonardo Spanu, Shell Corporation, Bangalore, India, October 23, 2012.
- 45. Orientational Relaxation in an Ionic Liquid: An All-atom Simulation Study, Prof. Ranjit Biswas, SNBNCBS, Kolkata, October 26, 2012.
- 46. *Rotational wave packet imaging of molecules*, Dr. Ramakrishna Sesha Sankar, NorthWestern University, October 30, 2012.
- 47. *Hybrid quantum dot circuit: carbon nanotubes and ferromagnets*, Dr. Subhadeep Datta, Mesoscopic Physics Group, Laboratoire Pierre Aigrain, Ecole Normale Superieure, Paris, October 31, 2012.
- 48. *Computational-based Engineering and Vascular Devices and Disease*, Dr. Anamika Prasad, IIT-Patna, Assistant Professor (Adjunct), November 6, 2012.

- 49. Objects, space, and memory: how the hippocampal cognitive map comes together, Dr. Sachin Deshmukh, Assistant Research Scientist, Mind/Brain Institute, Johns Hopkins University, November 6, 2012.
- 50. *Mechanical Deformation of Amorphous Solids*, Professor Srikanth Sastry, TIFR Centre for Interdisciplinary Sciences, Hyderabad, November 6, 2012.
- 51. *Stable and accurate numerical methods for computational Cardiology*, Dr. Ishani Roy, King's College London, UK, November 6, 2012.
- 52. Are mosquitoes in disease "hot-spots" more efficient vectors? Insights on spatial variation in disease resistance and tolerance in a natural vector-parasite system, Dr. Guha Dharmarajan, Ramanujan Fellow, IISER Kolkata, November 8, 2012.
- 53. *The spatial and temporal dynamics of elephant social networks*, Dr. Shermin de Silva, Colorado State University, November 17, 2012.
- 54. *How do you publish in PRL? Why should you?*, Dr. Samindranath Mitra, Editor, Physical Review Letters, American Physical Society (APS), November 8, 2012.
- 55. *Guided Self-Assembly of Soft Matter Systems for Membrane Applications*, Manesh Gopinadhan, Yale University, November 23, 2012.
- 56. *Tissue Repair and Regeneration*, Prof. David Leavesley, Faculty of Health, Queensland University of Technology Australia, November 26, 2012.
- 57. *Thio-and selenocarbonyls: from Fundamentals to Functional Molecules*, Prof. Toshiaki Murai, Faculty of Engineering, Gifu University, Yanagido, Gifu, Japan, November 26, 2012.
- 58. *A Novel Regulatory Role of Protein S in Thrombosis and Hemophilia*, Dr. Rinku Majumdar, Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, USA, December 4, 2012.
- 59. New functions for BLM and RECQL4 helicases during neoplastic transformation, Dr. Sagar Sengupta, NII, New Delhi, December 6, 2012.
- 60. *Amyloid beta peptide oligomers in Alzheimer's disease*, Dr. Vijay Rangachari, University of Southern Mississippi, Hattiesburg, December 6, 2012.
- 61. *Journeys with Macrobicyclic Cryptands*, Prof. Parimal K. Bharadwaj, Department of Chemistry, IIT Kanpur, U.P., India, December 10, 2012.
- 62. Epigenomics of Cellular Differentiation: Discovering Fundamental Principles of Transcriptional Regulation, Dr. Vijay Tiwari, Institute of Molecular Biology gGmbH (IMB), Mainz, Germany, December 10, 2012.
- 63. *Epigenetic Mechanisms of Mitochondrial Retrograde Signaling and Regulation of Telomere Function*, Prof. Narayan G. Avadhani, Department of Animal Biology, University of Pennsylvania, December 12, 2012.
- 64. *Efflux pumps in clinical drug resistance, Prof. Rajendra Prasad, School of Life Sciences, Jawaharlal Nehru University, New Delhi, December 13, 2012.*
- 65. *Reentrant Glass Transition(s?) in Colloidal Ellipsoids and Directional Grain Growth in Sheared Polycrystals,* Dr. Rajesh Ganapathy, ICMS, JNCASR, Bangalore, December 18, 2012.
- 66. *Understanding Early Steps in DNA Mismatch Repair*, Prof. Eric Alani, Cornell University, USA, December 24, 2012.
- 67. *Taste detection and behavior in Drosophila*, Dr. Sunanda Marella, Stanford University, Stanford, USA, December 28, 2012.

- 68. Does nanotechnology really help, for higher thermal-electrical conversion efficiency, in thermoelectric materials?, Prabhakar Bandaru, Departments of Mechanical and Aerospace Engineering, Electrical Engineering, and Physics, at UC, San Diego, January 03, 2013.
- 69. Direct Synthesis of Carbon Based Nanostructures, Including Studies on the Physics and Chemistry of Fullerides, Prof. Dr. H. C. Martin Jansen, Max-Planck-Institute for Solid State Research, January 07, 2013.
- 70. *Alternative Methods of Gene Delivery in Various Animal Models*, Dr. Srinivas Rao, Chief, Laboratory Animal Medicine Vaccine Research Center, National Institute of Health, Bethesda, MD, USA, January 8, 2013.
- 71. *Role of G9a in differentiation and cell cycle exit of skeletal muscle cells*, Reshma Taneja, Associate Professor, Department of Physiology, University of Singapore, January 8, 2013.
- 72. Seismic imaging of the power spectrum of turbulent convection in the solar interior, Dr. Shravan Hanasoge, Department of Geosciences, Princeton University, Princeton, NJ, USA, January 08, 2013.
- 73. Onset of shear flow in confined soft amorphous materials, Dr. Pinaki Chaudhuri, University of Duesseldorf, Germany, January 09, 2013.
- 74. *Size-induced shifts in the thermodynamics of nanophase oxides and implications for materials science,* Geochemistry and Environmental Science, Prof. Alexandra Navrotsky, Peter A. Rock Thermochemistry Laboratory and NEAT ORU, UC Davis, January 09, 2013.
- 75. *Ternary diamond-like semiconductors for high performance thermoelectrics*, Prof. S.D. Mahanti, Department of Physics and Astronomy DOE Energy Frontier Research Center Michigan State University, East Lansing, Michigan, USA, January 15, 2013.
- 76. *Impact of the Dynamic Cytoskeleton on Intracellular Sub-Diffusion: A Local Motion Analysis*, Amitabha Nandi, University of Yale, January 17, 2013.
- 77. *Fluctuation and plasticity in foam-flow near jamming*, Dr. Vijayakumar Chikkadi, Weizmann Institute of Science, Israel, January 18, 2013.
- 78. *How pure water can unmix*?, Prof. Mikhail A. Anisimov, University of Maryland, USA, January 22, 2013.
- 79. *Mesoscale Solubilization in Aqueous Solutions of Hydrotropes*, Dr. Deepa Subramanian, University of Maryland, USA, January 22, 2013.
- 80. *Chromosomal movement and biased microtubule growth accelerate mitotic spindle assembly*, Prof. Raja Paul, Indian Association for the cultivation of science, Kolkata, January 30, 2013.
- 81. *Fluidics at Micro-Nanoscale: Soft Capillarity, Superoleophobicity, Bio-Electrohydrodynamics*, Dr. Siddhartha Das, Banting Postdoctoral Fellow, Department of Mechanical Engineering, University of Alberta, Canada, January 30, 2013.
- 82. *Quantum Phase Transition of Light: Cavity Quantum Electrodynamics*, Dr. Sujit Sarkar, Poorna Prajna Institute of Scientific Research, Bangalore, India, February 5, 2013.
- 83. Proteomic insights into the relationship between cellular iron homeostasis, Fe-S cluster assembly and tumorigenesis, Dr. Ajay Vashisht, Department of Biological Chemistry, David Geffen School of Medicine, University of California, Los Angeles, USA, February 8, 2013
- 84. Organic-based Magnets: New Chemistry and New Materials for this Millennium, Prof. Joel S Miller, Department of Chemistry, University of Utah, Salt Lake City, UT, USA, February 11, 2013.
- 85. *Correlation of charge extraction properties and short circuit current in various organic photovoltaic devices*, Dr. Th. Birendra Singh, Materials Science and Engineering Division, Commonwealth Scientific and Industrial Research Organisation (CSIRO), Clayton South, Victoria, Australia, February 12, 2013.
- 86. Climate Change From Science to Policy and Actions in the Field, Prof. Veerabhadran Ramanathan,

Distinguished Professor of Climate Sciences, Scripps Institution of Oceanography, University of California at San Diego, UNESCO Professor of Climate and Policy, TERI University, New Delhi, February 13, 2013.

- 87. *Cyclic conjugated chemical entities. From molecules to high-tech molecular devices,* Prof. Kamaljit Singh, Prof.. Kamaljit Singh Organic Synthesis Laboratory, Department of A p p l i e d Chemical Sciences & Technology, Guru Nanak Dev University, Amritsar, February 14, 2013.
- 88. *Pathogenic SYNGAP1 haploinsufficiency impairs cognitive development by disrupting the maturation of dendritic spine synapses*, Dr. James Chelliah, Department of Neuroscience, Scripps Research Institute, Florida, USA, February 19, 2013.
- 89. *Raman Spectroscopy and its applications in biology*, Prof. Chandrabhas Narayana, Chemistry and Physics of Materials Unit, JNCASR, February 19, 2013.
- 90. *Convection induced by radiative cooling in a layer of participating gas*, Dr. Prasanna Swaminathan, Department of Mechanical Engineering, IIT-Madras, February 20, 2013.
- 91. The role of a self-sustaining amyloidogenic protein in persistence of memory, Dr. Amitabha Majumdar, Stowers Institute for Medical Research, USA, February 21, 2013.
- 92. *Protein Analogous Micelles: Versatile, Modular Nanoparticles,* Prof. Matthew Tirrell, The Institute for Molecular Engineering, The University of Chicago, February 21, 2013.
- 93. *Exploring the function of integins in keratinocytes: A tail of 2 kindlins*, Dr. Srikala Raghavan, Institute for Stem Cell Biology and Regenerative Medicine (inStem), NCBS, Bangalore, February 22, 2013.
- 94. *Lamins and disease: Insights into stability of key proteins*, Dr. Veena Parnaik, Centre for Cellular and Molecular Biology, Hyderabad, February 26, 2013
- 95. *Mapping Confined Water Molecules to Design New Blockers Against the M2 Proton Channel of the Influenza Virus,* Dr. Giacomo Fiorin, Research Assistant Professor, College of Science & Technology, Institute for Computational Molecular Sciences, Philadelphia, March 05, 2013.
- 96. *Surprising complexity of human RNA polymerase III transcription*, Dr. Martin Teichmann, Universitae Bordeaux Segalen Institut European de Chimie et Biologie (IECB), March 08, 2013.
- 97. *Evolutionary Models of Late-Life Demography*, Prof. Laurence D. Mueller, Dept. of Ecology and Evolution, University of California, Irvine, March 20, 2013.
- 98. *Epigenetics and microRNAs in Inflammation and Diabetic Vascular Disease*, Dr. Rama Natarajan, Endowed Professor and Associate Chair, Department of Diabetes Director, Division of Molecular Diabetes Research Beckman Research Institute of City of Hope, CA, USA, March 26, 2013.
- 99. *Heterochromatin, epigenetics and age reprogramming,* Dr. Prim Singh, Division of Tumor Biology, Research Center Borstel, Germany, March 28, 2013.

# **FELLOWSHIPS AND EXTENSION ACTIVITIES**

# **Extension Programmes**

### Summer Research Fellowship (SRFP)

The advertisement for SRFP 2012 was released in eight major Indian newspapers and posted on JNCASR website. Out of 3015 applications received, 48 were selected and 40 joined this programme. Under this programme, the students receive a scholarship of Rs 6000 per month.

Category	No. of applications Received (for 2012)	No. of Fellowships offered in 2012	No of fellowships utilized in 2012
Life Sciences	850	17	14
Engineering Sciences	515	08	08
Atmospheric Sciences	80	03	03
Physical Sciences	565	08	04
Chemical Sciences	325	08	08
Mathematics	330	03	02
Materials Science	350	01	01
Total	3015	48	40

The advertisement for SRFP 2013 was also released in eight major Indian newspapers and announced on JNCASR website. Out of 1707 applications received, 73 students are selected and are being offered SRFP fellowships this year. The JNC faculty will be guiding 49 SRFP students; and 10 students by few faculty from NCBS and IISc . The remaining 14 are placed under various faculty of institutions outside Bangalore.

# **Project Oriented Chemical Education (POCE)**

Nineteen students of POCE batches of 2010(2010-12) & 2011(2011-13) had worked under different faculty members on various research projects. Nine students who had successfully completed POCE-2010-12 program were awarded Diploma in Chemistry.

Out of nine students who had completed POCE programme, one student- Promit Ray has joined JNCASR for the M.S.-Ph. D programme, two students are doing M.S. in U.S.A/ Germany, whereas six other students are pursuing their studies at institutions in India.

Mr. Promit Ray was awarded the "Best POCE-2010-12 student award". The award was donated by CNR Rao Education Foundation.

Ms. Amritha Rangarajan, student of the POCE batch of 2008 (2008-10) has joined JNCASR for M.S.(Engg.) programme.

Two students (of POCE-2012-14), during their winter vacation, have worked with faculty members.

Advertisement for the year 2013-15 program was released (in January) in 10 leading news papers of the country. 10 candidates have been selected. They are expected to join on 13 May 2013.

### Project Oriented Biological Education (POBE)

Advertisement for POBE-2013 was released in 10 newspapers and announced on our website. POBE batches of 2011 and 2012 will return for their training under EOBU and MBGU faculty of the Centre during May 2013 along with the fresh batch.

8 POBE students of 2010 batch received their Diploma certificates in Biology. Many of them are pursuing their MS at institutions in India and abroad. One student from the POBE batch of 2010 has joined JNCASR under the MS-Ph.D programme offered by the Evolutionary and Organismal Biology Unit.

Advertisement for the year 2013-15 program was released (in January) in 10 leading news papers of the country. 10 candidates have been selected. They are expected to join on 13 May 2013.

#### Visiting Fellowship Programme

Since 2006, 69 fellowships were offered of which and 52 have availed and completed the programme successfully. Eight candidates have been selected to the Visiting Fellowships Programme 2012-13 under the Physical Sciences category and two under the Biological Sciences category.

#### JNCASR-CICS (Centre for International Cooperation in Science) Fellowship

This Fellowship programme (earlier called as JNCASR-CCSTDS) has been renamed as is jointly instituted by the Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR) Bangalore and the Centre for International Co-operation in Science (CICS), Chennai to encourage mobility of scientists from developing countries. CICS is a Unit of the Indian National Science Academy (NISA), supported by the Department of Science & Technology, New Delhi. This programme aims to promote co-operation among developing regions.

Two Fellows selected for the year 2009-10 have been given certificates on successful completion of their 3 month training programme in India. 4 Fellows has been given certificates for the year 2010-11. 1Fellow has been awarded certificate for the year 2011-12.

The JNCASR-CICS Fellowship committee met during December 2012 for the selection of Fellowships for the year 2012-13. The Fellowships were awarded to 8 candidates from Nigeria, Yemen, Bangladesh and Armenia.

#### **National Science Day**

The Centre celebrated National Science Day on February 28, 2013. On this day, the Centre organized series of lectures for students and teachers from different schools from Bangalore at Prof CNR Rao Hall of Science. There was an overwhelming participation from around 200 students from 4 schools with teachers and students having an interactive session with the scientists after each lecture.

#### Science Outreach Programmes

CNR Rao Hall of Science-ETU-SOP had conducted *four* two -days workshops on, "Experiments using College Chemistry Kit" for the P. U. Sc. Students (of Govt. College, Brahmavar, Govt. P. U. College Udupi, S. V. P. U. Sc. College, Vidyanagar, Swami Vivekananda Rural P. U. College Aanekal, Swami Vivekananda Youth Movement, Mysore, Maharani Govt. College, Mysore). On completion of the workshop, one Chemistry Kit was donated to each college for future use.

# **INTELLECTUAL PROPERTY**

Innovation ecosystems have become more complex in recent times and are built on flow of ideas amongst innovation contributors from various sectors through national and international collaborations. Public Research Institutions have always played crucial role in providing platform technologies for translation into affordable services/products. To foster generation, protection and management of commercializable intellectual property, the Centre has framed an enabling mechanism through the Intellectual Property Management Committee [IPMC].

During the year, the IPMC reviewed a number of new inventions developed by its researchers and recommended filing of patent applications based on the commercial potential of the invention and the patentability criteria. The Committee approved filing of 21 patent applications (Indian Provisional Application:7, Indian Complete Application: 1, International Patent Application under PCT:6, USA:5, Europe:1, China:1) and obtained 4 US Patents. The details are listed below:

# **Patent Applications Filed**

# I. Indian Patent Applications

# (a) Provisional applications filed for the inventions of the following inventors:

- Jayanta Haldar, Divakara Siva Sathyanarayana Murthy Uppu, Akkapeddi Padma, Goutham Belagula Manjunath (Appl. No. 2747/CHE/2012, 6/7/2012)
- Ravi Ramchandra Manjithaya (Appl. No. 4080/CHE/2012, 28/9/2012)
- Tapas Kumar Kundu, Parijat Senapati, Gopinath Kodaganur Srinivasachar, Deepthi Sudarshan, Manjula Das, Smitha Pazhoor Kumaran, Manjunath Shivasangappa Devaraman, Ajithkumar Sumitrappa (Appl. No. 4084/CHE/2012, 28/9/2012)
- Chintamani Nagesa Ramachandra Rao, Ujjal Kamar Gautam, Srinivasa Rao Lingampalli (Appl. No. 4195/CHE/2012, 5/10/2012)
- Jayanta Haldar, Chandradhish Ghosh, Padma Akkapeddi (Appl. No. 5299/CHE/2012, 18/12/2012)
- Giridhar Udapi Rao Kulkarni, Kunala Durga Mallikarjuna Rao, Ritu Gupta, Boya Radha and Shanmugam Kiruthika (Appl. No. 954/CHE/2013, 5/3/2013)
- Ranjani Viswanatha, Avijit Saha, Kavassery Sureshwaran Narayan, Kishore Velichappattu Chellapan (Appl. No. 1163/CHE/2013, 18/3/2013)

# (b) Completed Application:

Hydrogen Sorbent Materials Inventors: Subi Jacob George, Kotagiri Venkata Rao Appl. No. 2287/CHE/2012, 7/6/2012

# II. International Patent Application under PCT

Manufacturing Strain Sensitive Sensors And/Or Strain Resistant Conduits From A Metal And Carbon Matrix Inventors: Kulkarni Giridhar Udapi Rao, BoyaRadha, Abhay A Sagade Appl. No. PCT/IB2012/052872, 7/6/2012

Artificial Retina Device (Bulk Heterojunction/Electrolyte Polymers As Novel Biocompatible Photoactive Multi Color-Sensing Technology) Inventors: Kavasssery Sureswaran Narayan, Vini Gautam, Monijit bag Appl. No. PCT/IB2012/053711, 20/7/2012

Polymer, Methods Of Obtaining The Polymer And Applications Thereof Inventors: Subi Jacob George, Kotagiri Venkata Rao Appl. No. PCT/IB2012/055021, 21/9/2012

A System And A Method To Detect Hydrogen Leakage Using Nano-Crystallised Palladium Gratings Inventors: Giridhar Udapi Rao Kulkarni, Ritu Gupta, Abhay A Sagade Appl. No. PCT/IB2012/055245, 1/10/2012



An Organic Solar Cell And Methods Thereof Inventors: Kavassery Sureswaran Narayan, Anshuman Jyothi Das Appl. No. PCT/IB2012/056338, 12/11/2012

Cationic Antibacterial Composition Inventors: Jayanta Haldar, Yarlagadda Venkateswarlu, Akkapeddi Padma Appl. No. PCT/IB2012/056373, 13/11/2012

# III. US Patent Applications

# (a) Provisional Application:

Solvent-Free Oxidation Of Toluene By Nanoparticles Of Cd And Zn Peroxides Under Favourable Operating Conditions Inventors: Chintamani Nagesa Ramachandra Rao, Ujjal Kamar Gautam, Srinivasa Rao Lingampalli Appl. No. 61/733,854,5/12/2012

# (b) Non-Provisional Applications:

Chromophores For Detection Of Volatile Organic Compounds Inventors: Subi Jacob George, Mohit Kumar Appl. No. 13/482,9876, 6/6/2012

Julolidine Conjugates And Methods For Their Preparation And Use Inventors: Govindaraju Thimmaiah, Debabrata Maity, Swapan Kumar Pati, Tapas Kumar Kundu, Arun Kumar Manna, Karthigeyan Dhanasekaran Appl. No. 13/597,323,9/8/2012

Graphene Ribbons And Methods For Their Preparation And Use Inventors: Giridhar Udapi Rao Kulkarni, Narendra Kurra, Abhay A Sagade Appl. No. 13/599,810, 30/8/2012

Vector, Vector Combinations, Methods And Kit Thereof Inventor: Ranga Udaykumar Appl. No. 13/809,758, 11/1/2013

# IV. European Patent Application

Vector, Vector Combinations, Methods And Kit Thereof Inventor: Ranga Udaykumar Appl. No. 11806381.7, 24/12/2012

# V. Chinese Patent Application

Inhibition Of Histone Acetyltransferases By CTK7A And Methods Thereof Inventors: Tapas Kumar Kundu, Mohammed Arif, Kempegowda Mantelingu, Gopinath Kodaganur Srinivasachar Appl. No. 201080045291.6, 6/4/2012

# **Patents Granted**

A Mirror Adapted In Microscope To Perform Surface Enhanced Raman Spectroscopy, A Microscope And Methods Thereof

Inventors: Chandrabhas Narayana, Pavan Kumar Gopalapura Venkataramu USA Patent No. 8,179,525 B2, Granted on 15/5/2012

A High Sensitivity Assay For Molecular Typing Of Biological Sample, Probes And A Kit Thereof Inventors: Ranga Udaykumar, Chandrabhas Narayana, Jayasuryan Narayana USA Patent No: 8227590, Granted on 24/7/12

Methods And Compositions For The Separation Of Single-Walled Carbon Nanotubes Inventors: Chintamani Nagesa Ramachandra Rao, Subi Jacob George, K Venkata Rao, Rakesh Voggu USA Patent No: 8246928, Granted on 21/8/12

A Template Free, Polymer Free Metal Nanosponge And A Process Thereof Inventors: Eswaramoorthy Muthusamy, Saikrishna Katla USA Patent No. 8404280, Granted on 26/3/13

# **RESEARCH PROGRAMMES**

# **Research Areas**

There are ongoing research programmes in several frontier, interdisciplinary areas of science and engineering. The main areas of research interest at present are:

- 1. Molecular modelling of materials
- 2. Nanomaterials and catalysis
- 3. Nanomaterials, nanofabrication, molecular crystals
- 4. Functional materials based on Metal-Organic Frameworks (MOFs)
- 5. Organic electronics: device physics & photophysics
- 6. Raman and Brillouin Spectroscopy, high pressure research in the study of materials
- 7. Chemistry of materials
- 8. Epitaxy and nanostructures
- 9. Magnetism, superconductivity and multiferroicity
- 10. Granular matter and other complex fluids
- 11. Mesoscale simulations and high performance computing
- 12. Instabilities and interfacial flows
- 13. Aerospace and atmospheric fluid mechanics
- 14. Fluid mechanics and heat transfer
- 15. Rheology of complex fluids, vortex dynamics, transport processes in the nocturnal boundary layer
- 16. Circadian rhythms in fruit flies and ants
- 17. Evolutionary genetics and population ecology
- 18. Neuronal circuits in fruitflies
- 19. Animal behaviour and sociogenetics
- 20. Neotectonics and environmental geology
- 21. Aberration corrected transmission electron microscopy
- 22. Soft materials
- 23. Physics of soft matter
- 24. Organic materials and organocatalysis
- 25. Physics and chemistry of nanomaterials
- 26. Functional organic and supramolecular materials
- 27. Organic synthesis, molecular probes, peptide and protein chemistry, nucleic acid chemistry, bionanotechnology
- 28. Bio-organic and medicinal chemistry
- 29. Designing new ways to small molecule heterocyclic scaffolds
- 30. Inorganic and solid state chemistry
- 31. Nanomaterials and renewable energy

- 32. Solid state inorganic chemistry
- 33. Molecular and cellular mechanisms of human genetic disorders
- 34. Molecular parasitology and molecular enzymology
- 35. Molecular, genetic and developmental analysis of the cardiovascular system
- 36. Transcription regulation and chromatin dynamics: implications in disease and potential therapeutics
- 37. Autophagy and autophagy related pathways
- 38. Chromatin biology and genomics
- 39. The HIV-1 subtype-c strain: success story of the fittest viral subtype
- 40. Genetic and epigenetic definition of Centromeres
- 41. Mechanisms underlying host-pathogen interactions in malaria
- 42. Materials theory
- 43. Statistical physics of equilibrium and non-equilibrium condensed matter systems
- 44. Mathematical models of biological evolution
- 45. Novel physics and chemistry at the nanoscale
- 46. Chemistry and physics of systems ranging from atoms to extended materials
- 47. Phase transformations and dynamics in soft condensed matter, and biological systems
- 48. Non-commutative probability and geometry: mathematics of quantum mechanics
- 49. Correlated electron systems and organic electronics
- 50. Chemical biology
- 51. Condensed matter theory
## **Research facilities**

(List of equipments procured during 2012 - 2013)

- 1. CLARUS 580 Gas chromatograph
- 2. Thermo Heraeus high-speed table top refrigerated centrifuge and accessories
- 3. Outdoor chiller unit Model OPC3-K
- 4. Nikon Trinocular Stereoscopic zoom microscope
- 5. Thin film deposition monitor
- 6. REVCO UXF freezer
- 7. High performance computing system
- 8. Millipore water purification system
- 9. Seebech Coefficient measuring apparatus
- 10. 1500deg.C tube furnace, Adapters, benchtop muffle furnace
- 11. LFA 457 Microflast laser apparatus
- 12. Electron beam power supply
- 13. 1500Deg. Box furnace, thermo couple assay
- 14. Imaging spectrometer and accessories
- 15. Spectroflurometer multimode reader
- 16. Emulsiflex high pressure homogenizer
- 17. K101 Control coater system and accessories
- 18. Mbraun Glove box
- 19. Versa Max TM microplate reader
- 20. Tata Elxsi HPC Clusters
- 21. Model VCS750 Ultrasonic processor with accessories
- 22. Hielscher ultrasonic Sonicator UP-100H
- 23. PPMS Evercool II system
- 24. FASTCAM SA4 Model 500k M2 mono high speed imaging system
- 25. Completely automatic anaerobic chamber
- 26. AMD Servers and accessories
- 27. Glove box simulators with accessories
- 28. Sheldon Anaerobic chamber and incubator
- 29. Absorption reflection spectrophotometer
- 30. Atomic Layer deposition system
- 31. Quantel lasers

- 32. Research grade Lambda 750 UV VIS NIR
- 33. Q2000 MDSC System
- 34. Rudolph Density Meter DDM2911
- 35. Vibration controller with accessories
- 36. Modular compact Rheometer MCR302 with PIV cell
- 37. MCOSM Multi gas incubator
- 38. Cryosystem 2000 with accessories
- 39. Empyrean Alpha-1 XRD System with accessories
- 40. HPC System
- 41. AMD Server with 6380CPU
- 42. AMD Server

S.No.	Project	Project Investigator	Funding Agency	Duration
1	Post doctoral fellowship in Nano-Science and Technology	Co-ordinated by JNCASR	DST	cont.
2	Unit on Nano-Science & Technology-UNANST - DST	Co-ordinated by JNCASR	DST	-
3	Training and research facility for human embryonic stem and human embroynic carcinoma cells	Prof. Manisha Inamdar & Prof.MM Panikar	DBT	-
4	DAE-SRC Outstanding Research Investigator Award to Prof. Anuranjan Anand. Project title "Whole Genome-based Studies to Identify Novel Molecular Genetic Pathways Causing Human Epilepsy Syndrome"	Prof. Anuranjan Anand	DAE	5 years
5	J.C. Bose Fellowship	Prof. M.R.S. Rao	DST, JCB	5 years
6	Delineating viral determinants of HAD using SCID mice	Prof. Ranga Uday Kumar	AECOM	cont.
7	Structure function analysis of Tumor suppressor, p53 interacting proteins: structural basis of p53 activation	Prof. Tapas Kumar Kundu	DBT	-
8	Development of triclosan for treating human malaria and inhibitors of fatty acid synthesis especially enoyI-ACP reeducates of as anti- malarial agents	Prof. Namita Surolia	DBT	4 years
9	Bhatnagar Fellowship -2005 Award to Prof. K.B. Sinha; Project title: "Quantum mechanics - a Mathematical tool to study non-equilibrium processes and dissipative systems in physical sciences, Geometry and information theory"	Prof. K.B. Sinha	CSIR	5 years
10	Investigation of Lift and Thrust in Asymmetric Fight	Prof. K.R. Srinivas	DST	-
11	Functional Genomics based approach to Novel anti-malarial targets and agents	Prof. Namita Surolia	ICMR	-

# **SPONSORED / ONGOING RESEARCH PROJECTS**

S.No.	Project	Project Investigator	Funding Agency	Duration
12	JNC-Brucker Sophisticated X-ray diffraction facilities	Co-ordinated by JNCASR	BRUKE R, AXS	-
13	NMITLY Project on "Mesoscale modeling for monsoon related weather predictions - Phase II"	Prof. Deshpande S.M.	CSIR	-
14	Swarnajayanthi Fellowship	Prof. S. Balasubramanian	DST	5 years
15	Development of TKFMG solver and its application to flutter prediction in turbo machines	Prof. Deshpande S.M.	GTRE	3 years
16	Density functional theory calculations	Prof. Umesh V. Wagmare	P&G	1 year
17	Chromatin Biology: Epigenomics of chromatin and chromatin remodelling during male germ cell differentiations and glioma progression	Prof. M.R.S. Rao	DBT	5 years
18	Ramanujan Fellowship	Dr. TNC Vidya	DST	5 years
19	India-Japan co-operative programme (DST-JST) 2007 - joint Project entitled "Feasibility study on the application of multiple order parameters in materials to information processing"	Dr. Sundaresan (Dr. Y. Tanka, - NIAIS, Japan)	DST-JST	3 years
20	ICPC NanoNet Coordination and support action	Prof. G.U. Kulkarni	ICPCNN	cont.
21	Swarnajayanthi Fellowship	Prof. Swapan K. Pati	DST	5 years
22	Numerical simulation of multiscale supersonic flows with low dissipative shock capturing schemes	Prof. S.M. Deshpande	DST	2 years
23	Bovine Mastitis: Unraveling molecular details of host microbe interaction and development of molecular diagnostic methods	Prof. Tapas Kumar Kundu	ICAR	3 years
24	Ramanujan Fellowship	Dr. Sheeba Vasu	DST	5 years

S.No.	Project	Project Investigator	Funding Agency	Duration
25	Extended applications of Highly Sensitive Nanometal Raman substrates, Paper based Nano Silver/Gold SERS Substrates (Plain Substrates, Au/Ag metal sponge based SERS Substrates), Specialised Substrates Bio-Chip, Nano silver - Antibacterial Products	Prof. G.U. Kulkarni, Prof. Hemalatha Balalaram, Prof. M. Eswaramoorthy	YNL	1 year
26	Ramanujan Fellowship	Dr. Santosh Ansumali	DST	5 years
27	DAE-SRC Outstanding Research Investigator Award for R/P "Multi scale modeling and simulations of functional Materials"	Prof. Umesh V. Waghmare	DAE	5 years
28	DAE-SRC Outstanding Research Investigator Award for R/P "Electronic, optoelectronics and photonic properties in soft matter and device exploration"	Prof. K.S. Narayan	DAE	5 years
29	MoU between BARC and JNCASR "Development of Test Facility for Thermal Hydraulics studies/Basic research Salt Water/FineHydrogen Bubble Test Facility for simulation of Hydrogen Transport - Management/ Fire safety behaviour/ Containment thermal hydraulics/pollution dispersion studies"	Prof. Meheboob Alam	BARC	3 years 5 months
30	Understanding pathogenesis of Malaria and strategies to treat it	Prof. Namita Surolia	DBT	3 years
31	Indo-Italian research Project: "Designing Novel Photosystems for Enhanced charge Transfer efficiency: A detailed theoretical modeling"	Prof. Swapan K. Pati, JNCASR; Prof. Anna Painelli, Univ. degli studi, ITALY	DST	3 years
32	Indo-US joint networked R&D centre on "Nanomaterials for Energy"	Co-ordinated by Prof. G.U. Kulkarni & Prof. Timothy S. Fisher, BNC, Purdue University, USA	IUSSTF	cont.

S.No.	Project	Project Investigator	Funding Agency	Duration
33	Indo-US joint Research Centre of Excellence in "Advanced Materials Research"	Co-ordinated by Prof. Swapan K. Pati & Vinayak P. Dravid, North- Western Univ., IL, USA	IUSSTF	3 years
34	Role of multifunction human histone chaperone NPMI in transcription and stress associated chromatin dynamics: Relevance in cancer manifestation	Prof. Tapas Kumar Kundu	DBT	3 years
35	IBM Faculty Award 2009	Prof. Umesh V. Waghmare	IBM	cont.
36	Indo-Italian Research Project:"Innovative catalytic patterns for nanowire growth"	Prof. G.U. Kulkarni	DST	3 years
37	India-European Union Research Project "MONAMI Modeling of Nano-scaled Advanced Materials Intelligently"	Prof. Srikanth Sastry	DST	3 years
38	Lineage specification and differentiation from single embryonic stem cells tracked by live cell imaging of reporter gene expression	Prof. Maneesha S. Inamdar	DBT	3 years
39	Optimization of the performance of DNA vaccine by engineering molecular strategies: use of HIV-1 tat as model antigen	Prof. Ranga Udaykumar	ICMR	3 years
40	Examination of the metabolic fate of fumarate a TCA cycle intermediate in Plasmodium falciparum	Prof. Hemalatha Balaram	DST	3 years
41	Analysis of conserved functions of rudhira in development, homeostasis and lifespan	Prof. Maneesha S. Inamdar	DBT	3 years
42	Structure-function studies on Plasmodium falciparum and Methanococcus jannaschii guanosine monophospate (GMP) synthetase:enzymes with ammonia channels	Prof. Hemalatha Balaram	DBT	3 years
43	Dominance Relationships in Female Asian Elephants	Dr. TNC Vidya	CSIR	3 years

S.No.	Project	Project Investigator	Funding Agency	Duration
44	National Bioscience Award for career development 2008; project entitled "Towards isolation of a novel gene for non-syndromic hearing loss at the 11p14.2-q12.1 locus"	Prof. Anuranjan Anand	DBT	3 years
45	Optimization of wing for RTA-70	Prof. R. Narasimha	NAL	1 year
46	INSA Senior Scientist	Prof. H. Ila	INSA	5 years
47	Vision Group on Science & Technology, Govt. of Karnataka	Co-ordinated by JNCASR	VGST	-
48	"Evaluation of molecular and immune status of the blood lymphocytes of subject who participated in the Siddha Clinical Trial CTRI/2008/091/000021" at JNCASR	Prof. Ranga Udaykumar	DST	1 year
49	Developing new synthetic routes for the preparation of unnatural amino acids and their use as metal (Bio-) sensors and chiral ligands in the asymmetric catalysis	Dr.T. Govindaraju	DST	3 years
50	Design, development and establishment of experimental facility at NPOL for studies on internal wake and wave fields generated by self propelled bodies in stratified water medium	Prof. K.R. Srinivas	NPOL	1 year
51	Experimental studies on the generation of internal wakes by the motion of self propelled under water bodies in stratified water medium and their characteristics: Observations measurements with visualization techniques and optical probes	Prof. K.R. Srinivas	NPOL	1 year
52	Evaluation of host immune responses to the Tat antigen of HIV-1 in the Indian clinical cohorts	Prof. Ranga Udaykumar, Co-PI: Dr. Suniti Solomon, Director, YRGC for AIDS, Res. And Edun., Chennai	DBT	3 years
53	Mechanisms of Chikungunya virus disease: mouse model, virulent and fitness determinants and the development of novel therapeutics	Prof. Ranga Udaykumar, JNCASR, Co PI: Prof. Shobha Broor, Dept. of Microbiology AIIMS, New Delhi	DBT	3 years
54	Ramanujan Fellowship	Dr. Rema Krishnaswamy	DST	5 years

S.No.	Project	Project Investigator	Funding Agency	Duration
55	Swedish Research Links Programme entitled "Computational studies of the electronic, magnetic and transport properties of interfaces for nanospintronics applications.	Prof. Shobhana Narasimhan	SRC	cont.
56	Targheed delivery of anti-retrovirals using stealth immunoliposomes	Prof. Ranga Udaykumar	ICMR	3 years
57	Indo-Spanish Joint Programme of cooperation in S&T entitled "Synthesis and properties of nitride- based nanomaterials"	Prof. A Sundaresan	DST	3 years
58	Analysis of asrij in Drosophila hematopoiesis and immunity	Prof. Maneesha S. Inamdar	DST	3 years
59	First-principles determination of thermal properties in nano-structured hexagonal solids with doping modifications for thermal energy harvesting	Prof. Umesh V Waghmare	AOARD	1 year
60	J C Bose Fellowship	Prof. Tapas Kumar Kundu	DST	5 years
61	Ramanujan Fellowship	Dr. Subir Kumar Das	DST	5 years
62	Ramanujan Fellowship	Dr. Jayanta Haldar	DST	5 years
63	Ramanujan Fellowship	Dr. Sebastian C Peter	DST	5 years
64	Development of Novel biodegradable surface coatings for biomedical application	Dr. Jayanta Haldar	DST	3 years
65	Development of Meshless Solver, Point Clouds and preprocessor in Computational Fluid Dynamics (CFD)	Prof. S.M. Deshpande	NAL	3 years
66	Study of conformation and conformational dynamics of some conducting polymers in their neutral and doped forms using vibrational spectroscopy and quantum chemical methods	Dr. Abhishek Kumar Mishra CCMS, JNCASR	DST	3 years
67	India-European Union (EU) research project entitled " ATHENA Advanced theories for functional oxides: New routes to handle the devices of future"	Prof. Umesh V Waghmare	DST	3 years

S.No.	Project	Project Investigator	Funding Agency	Duration
68	Plasfalsyn Structure/Function studies of plasmodium falciparum GMP synthetase	Prof. Hemalatha Balaram	DBT	3 years
69	Indo-Brazil Megaproject entitled " to decipher biological processes of organisms causing diseases of clinical importance in both the countries" (1) Profiling of FAS genes in populations of Plasmodium sp. In the Amazonian region Brazil; (2) Electron microscopy characterization of the intracellular traffic pathway of Apicoplast proteins in falciparum and Toxoplasma gondii and Relationship between the endoplasmic reticulum and the Anicoplast (3) Effect of drugs interfering with FAS biosynthesis pathway on Toxoplasma gondii, Trypanosoma cruzi and Leishmania	Prof. Namita Surolia	DST	3 years
70	Indo-Brazil Megaproject entitled " to decipher biological processes of organisms causing diseases of clinical importance in both the countries" (1) Determination of the structure of Plasmodium falciparum proteins involved in the purine nucleotide synthesis by X-ray crystallography	Prof. Hemalatha Balaram	DST	3 years
71	India-Japan research project: "Hematopoeitic Stem Cell Differentiation: Role of SAM Biosynthesis Arginine Methylation and p53	Prof. Tapas Kumar Kundu	DST	2 years
72	Advancing the Efficiency and Production Potential of Excitonic Solar cells (APEX)	Prof. K.S. Narayan	DST	3 years
73	DAE-SRCH Outstanding Research Investigator Award for the project titled "Dynamics and patterns in granular fluid: Theory and experiment"	Prof. Meheboob Alam	DAE	3 years
74	Synthetic Investigation Heterocyclic scaffolds	Prof. H. Ila	CSIR	3 years
75	Alloy development and mechanical behaviour	Prof. Umesh V Waghmare	GEGR	2 years
76	Swedish Research Links Programme: "Multiplexed immune and DNA-based diagnosis of tuberculosis"	Prof. Chandrabhas Narayana	SRL	3 years
77	INDO-IRAN Collaborative Programme in "Nano cience & Technology" at ICMS, JNCASR	Prof. C.N.R. Rao & Prof. G.U. Kulkarni	DST	3 years
78	India-South Africa thematic sub-project entitled "HIV Vaccine Immunogen Design: Identification of T-cell epitopes associated with control of viral replication in Indian and South African"	Prof. Ranga Udaykumar	DST	3 years

S.No.	Project	Project Investigator	Funding Agency	Duration
79	Understanding the Parasexual cycle of a hybrid formed between two asexual human pathogens candida albicans and Candida dubliniensis: A novel way to identify virulence factors	Dr. Kaustuv Sanyal	CSIR	3 years
80	Ramanujan Fellowship	Dr. Ujjal K Gautam	DST	5 years
81	Welcome Trust - DBT India Alliance award to Dr. Ravi Manjithaya; an Intermediate Fellowship entitles: Small molecule modulators of autophagy and autophagy related pathways	Dr. Ravi Manjithaya	WT-DBT	5 years
82	Identification of DNA replication origins and origin binding proteins of the human pathogen, Candida albicans	Prof. Kaustuv Sanya	] DBT	3 years
83	Theoretical Studies of molecular imprinted polymers for the detection of explosives and toxic gases	Prof. Balasubramanian S	NMRL- DRDC	3 years
84	Innovative Young Biotechnologists Award to Dr. T. Govidaraju; project entitles: "Development of Biomimetic Materials as substitutes for Natural Fibers using Designed Modular Peptides	Dr. T. Govindaraju	DBT	3 years
85	MoU between SHELL and JNCASR entitles: To develop and validate a predictive method for modelling physical properties of hydrocarbons	Prof. Balasburamanian S	SHELL	2 years
86	Indo-Finland collaboration on biotechnology titled: Innovative concept for infectious disease diagnostics	Prof. Ranga Uday Kumar, JNCASR & Dr. Swaminathan, RGP Lab.ICGEB, New Delhi	DBT	2 years
87	India-European Union (EU) research project Organic and Organic-Inorganic hybrid solar Cells: Optimization of Materials Properties, Bulk Heterojunction Morphology and Device Efficiencies (OISC/LARGECELLS)	Prof. G.U. Kulkarni	DST	3 years
88	Women Scientist Scheme A entitles: Computational studies on structural, mechanistic and spectroscopic characterization of lignocellulosic materials salvation and photosystem I charge/energy transfer processes	Dr. Ganga Periyasamy	DST	3 years
89	Studies on the physiological basis of maternal effects due rearing density in Drosophila melanogaster	Dr. B M Prakash	DST	3 years

S.No.	Project	Project Investigator	Funding Agency	Duration
90	Programme support on chromatin and disease (Chromatin dynamics and transcription regulations: Implications in disease and therapeutics	Prof. Tapas Kumar Kundu Co-PI: Prof. Ranga Udaykumar	DBT	5 years
91	MoU between JNCASR and NCI (Nippon Chemical Industrial Co. Ltd.) on project "Develop inorganic nanomaterials for drug release"	Prof. M Eswaramoorthy	NCI	-
92	"Targeting protein lysine acetylation in oral cancer and neurodegenerative disorders using nanomaterials"	Prof. Tapas Kumar Kundu & Prof. Eswaramoorthy M	DBT	3 years
93	Analysis of conserved pathways involved in maintaining homeostasis and survival in mammals and Drosophila	Prof. Maneesha S Inamdar	WT	3 years
94	Thematic Unit of Excellence on Nanochemistry at JNCASR	Coordinated by Prof. G.U. Kulkarni	DST	5 years
95	Estimating the lift in flapping flight for the design of Entompter/MAV	Prof. K.R. Sreeenivas	ADE	3 years
96	Numerical Simulation of cloud flow and mixing layers	Prof. R. Narasimha	INTEL	1 year
97	Aerodynamic shape optimization	Prof. S.M. Deshpande	INTEL	1 year
98	Grid-based libraries	Dr. Santosh Ansumali	INTEL	1 year
99	MoU between JNCASR & Raja Ramanna Centre for Advanced Technology on " High Pressure XRD Measurement System"	Prof. N. Chandrabhas	RRCAT	1 year
100	J.C. Bose Fellowship	Prof. Amitabh Joshi	SERB	5 years
101	Ramanjujan Fellowship	Dr. Kanishka Biswas	SERB	5 years
102	Thematic Unit of Excellence on "Computational Materials Science" at JNCASR	Proj. Co-ordiator Prof. S. Balasubramanian	DST	5 years
103	Development and evaluation of active polymer nanocomposite packaging materials for food contact applications	Prof. G.U. Kulkarni	DFRL	1 year
104	Indo-Brazil S&T Cooperation of Joint Project: Pathogenic and molecular characterization of HIV-1 from diverse tissues and body fluids of subjects characterized with HIV associated dementia and other neurologic manifestations	Prof. Ranga Udaykumar	DST	5 years

S. No.	Project	Project Investigator	Funding Agency	Duration
105	"Structure-property relations in RE2TGe3 (RE=rare earths; T=transition metals) compounds (CRS-M-166)"	Dr. Sebastian C Peter	UGC	3 years
106	Rare earth doped chalcogenide glasses for optical and photonic applications	Dr. Sebastian C Peter	SERB	3 years
107	Regulation of Chromatin Associated proteins by miRNAs: Implications in Breast Cancer	Prof. Tapas Kumar Kundu	DBT	3 years
108	Structure-function analysis of centromeres of a pathogenic budding yeast candida tropicali	Prof. Kaustav Sanyal	DBT	3 years
109	Pulsed Laser Desposition (PLD) growth of ZnO BCN and study their properties from atomic scale imaging and spectroscopic techniques	Dr. Ranjan Datta	SERB	3 years
110	Indo-Italian Project entitled: From Small Molecules to Advanced Molecular Materials: Transport and Transfer Properties	Prof. Swapan K Pati	DST	3 years
111	MoU between AOARD, USA & JNCASR "The Feasibility of producing field effect transistor structures by utilizing the effect of donor/acceptor organic molecules when they are physisorbed onto a graphene surface and modulation of the electronic properties of graphene by various metal and semiconducting nanoclusters"	Prof. Swapan K Pati	AOARD	2 years
112	"Numerical Investigations of Unsteady aerodynamics in insect Flight"	Prof. Sunderesan A	ADE	3 years
113	Reprogramming somatic cells to model cardiovascular differentiation for research and therapeutic potential	Prof. Maneesha Inamdar	DBT	3 years
114	Analysis of factors regulating self renewal and differentiation to aid generation of lineage restricted stem cells/progenitors for cell replacement therapy	Prof. Maneesha Inamdar & Prof. He- malatha Balaram	DBT	3 years
115	MoU between JNCASR & HPCL "Development of Microbial catalysts (Biocatalysts) for Fermentative Butanol Production"	Dr. Ravi Manjithaya	HPCL	2 years
116	"Mechanisms of Lysine acetyltransferase (KAT/HAT) activation by small molecule activators and use thereof in memory"	Prof. Tapas Kumar Kundu	IFCPAR	3 years
117	CSIR Centre of Excellence in Chemistry at JNCASR	Prof. C.N.R. Rao	CSIR	5 years
118	Collaborative projects between JNCASR/ICMS & DST	Prof. C.N.R. Rao	DST	-

S.No.	Project	Project Investigator	Funding Agency	Duration
119	DNS of Turbo-Machinery Blading	Prof. Roddam Narasimha	GTRE	2 years
120	Collaboratitve Programme between DRDO and JNCASR	Prof. C.N.R. Rao	DRDO	5 years

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## **PUBLICATIONS**

The Centre has registered a very good progress in its publications. A chart showing the year-wise publication and the impact factor thereof is appended below:



## **Chemistry and Physics of Materials Unit**

- Kumar, P.; Tangi, M.; Shetty, S.; Kesaria, M.; Shivaprasad, S. M., Growth of aligned wurtzite GaN nanorods on Si(111): Role of Silicon nitride intermediate layer. *MRS Online Proceedings Library* 2012 1411, mrsf11-1411-ee09-24, http://dx.doi.org/ 10.1557/opl.2012.760
- Bera, S.; Dhara, S.; Milekhin, A.; Chu, M. W.; Shivaprasad, S. M., Editorial: Spectroscopic and Structural Insight into the Size-Dependent Behavior of the Nanophase. *International Journal of Spectroscopy* 2012 (2012), 197064 http://dx.doi.org/ 10.1155/2012/197064
- 3. Galkin, K. N.; Chusovitin, E. A.; Kumar, M.; Shivaprasad, S. M.; Galkin, N. G.; Goroshko, D. L., The study of Si(5 5 12) cleaning in the ultra-high vacuum conditions. *Physics Procedia* **2012** *23* (0), 29-32, http://dx.doi.org/10.1016/j.phpro.2012.01.008
- Bedi, A.; Senanayak, S. P.; Das, S.; Narayan, K. S.; Zade, S. S., Cyclopenta[c]thiophene oligomers based solution processable D-A copolymers and their application as FET materials. *Polymer Chemistry* 2012 (Apr), *3* (6), 1453-1460, http://dx.doi.org/10.1039/C2PY20032E
- Radha, B.; Jayaraj, D.; Kulkarni, G. U.; Heun, S.; Ercolani, D.; Sorba, L., Large-Area Ohmic Top Contact to Vertically Grown Nanowires Using a Free-Standing Au Microplate Electrode. *ACS Applied Materials & Interfaces* 2012 (Apr), *4* (4), 1860-1864, http://dx.doi.org/10.1021/Am300063j
- 6. Reddy, S. M.; Datta, K. K. R.; Sreelakshmi, C.; Eswaramoorthy, M.; Reddy, B. V. S., Honey Mediated Green Synthesis of Pd Nanoparticles for Suzuki Coupling and Hydrogenation of Conjugated Olefins.

*Nanoscience and Nanotechnology Letters* **2012 (Apr)**, *4* (4), 420-425, http://dx.doi.org/10.1166/nnl.2012.1331

- Mukhopadhyay, S.; Narayan, K. S., Rationalization of donor-acceptor ratio in bulk heterojunction solar cells using lateral photocurrent studies. *Applied Physics Letters* 2012 (Apr 16), 100 (16), 163302 http://dx.doi.org/10.1063/1.4704654
- 8. Kolhe, N. B.; Devi, R. N.; Senanayak, S. P.; Jancy, B.; Narayan, K. S.; Asha, S. K., Structure engineering of naphthalene diimides for improved charge carrier mobility: self-assembly by hydrogen bonding, good or bad? *Journal of Materials Chemistry* **2012** (May), *22* (30), 15235-15246, http://dx.doi.org/10.1039/C2JM32554C
- 9. Krishna, K. S.; Kumar, B. V. V. S. P.; Eswaramoorthy, M., Shaping up: spontaneous formation of ordered mesoscopic salt bowls. *RSC Advances* **2012** (May), *2* (14), 5947-5949, http://dx.doi.org/10.1039/C2RA20596C
- 10. Ludwig, R.; Maginn, E.; Balasubramanian, S., Editorial: Ionic Liquids: The Fundamentals and Forces Driving Their Rise. *ChemPhysChem* **2012 (May)**, *13* (7), 1603-1603, http://dx.doi.org/10.1002/cphc.201200245
- 11. Kumari, G.; Narayana, C., New Nano Architecture for SERS Applications. *Journal of Physical Chemistry Letters* **2012 (May 3)**, *3* (9), 1130-1135, http://dx.doi.org/10.1021/Jz3001344
- 12. Singh Payal, R.; Balasubramanian, S., Orientational Ordering of Ionic Liquids near a Charged Mica Surface. *ChemPhysChem* 2012 (May 14), *13* (7), 1764-1771, http://dx.doi.org/10.1002/cphc.201100871
- 13. Gupta, R.; Sagade, A. A.; Kulkarni, G. U., A low cost optical hydrogen sensing device using nanocrystalline Pd grating. *International Journal of Hydrogen Energy* **2012 (Jun)**, *37* (11), 9443-9449, http://dx.doi.org/10.1016/j.ijhydene.2012.03.010
- 14. Payal, R. S.; Balasubramanian, S.; Rudra, I.; Tandon, K.; Mahlke, I.; Doyle, D.; Cracknell, R., Shear viscosity of linear alkanes through molecular simulations: quantitative tests for n-decane and n-hexadecane. *Molecular Simulation* **2012** (Jun), *38* (14-15), 1234-1241, http://dx.doi.org/10.1080/08927022.2012.702423
- Narayanamoorthy, B.; Datta, K. K. R.; Eswaramoorthy, M.; Balaji, S., Improved Oxygen Reduction Reaction Catalyzed by Pt/Clay/Nafion Nanocomposite for PEM Fuel Cells. *ACS Applied Materials & Interfaces* 2012 (Jul), 4 (7), 3620-3626, http://dx.doi.org/10.1021/am300697q
- 16. Kundu, P. P.; Narayana, C., Raman based imaging in biological application- a perspective. *Journal of Medical and Allied Sciences* **2012** (Jul), *2*, 41-48,
- 17. Gupta, R.; Thomas, R.; Kulkarni, G. U., Tunable solid state fluorescence behavior of a methoxy substituted oligo(phenyleneethynylene): influence of cooling rate and surface crystallization. *Journal of Materials Chemistry* **2012** (Jul), *22* (36), 19139-19145, http://dx.doi.org/10.1039/C2JM31903A
- Kumar, P.; Kumar, M.; Shivaprasad, S. M., Ga induced 2D superstructural phase diagram on trenched Si(5512) surface. *Surface Science* 2012 (Jul), 606 (13-14), 1045-1049, http://dx.doi.org/10.1016/j.susc.2012.02.024
- Kulriya, P. K.; Mehta, B. R.; Agarwal, D. C.; Kumar, P.; Shivaprasad, S. M.; Pivin, J. C.; Avasthi, D. K., Giant enhancement in ferromagnetic properties of Pd nanoparticle induced by intentionally created defects. *Journal of Applied Physics* 2012 (Jul 1), *112* (1), http://dx.doi.org/10.1063/1.4733950
- 20. Radha, B.; Kulkarni, G. U., An Electrical Rectifier Based on Au Nanoparticle Array Fabricated Using Direct-Write Electron Beam Lithography. *Advanced Functional Materials* **2012** (Jul 10), *22* (13), 2837-2845, http://dx.doi.org/ 10.1002/adfm.201103170

- 21. Bag, M.; Vidhyadhiraja, N. S.; Narayan, K. S., Fluctuations in photocurrent of bulk heterojunction polymer solar cells-A valuable tool to understand microscopic and degradation processes. *Applied Physics Letters* **2012** (Jul 23), *101* (4), http://dx.doi.org/10.1063/1.4738985
- Rajeswaran, B.; Mandal, P.; Saha, R.; Suard, E.; Sundaresan, A.; Rao, C. N. R., Ferroelectricity Induced by Cations of Nonequivalent Spins Disordered in the Weakly Ferromagnetic Perovskites, YCr1–xMxO3 (M = Fe or Mn). *Chemistry of Materials* 2012 (Aug), *24* (18), 3591-3595, http://dx.doi.org/10.1021/cm301944s
- 23. Selvi, R. B.; Chatterjee, S.; Jagadeesan, D.; Chaturbedy, P.; Suma, B. S.; Eswaramoorthy, M.; Kundu, T. K., ATP driven clathrin dependent entry of carbon nanospheres prefer cells with glucose receptors. *Journal of Nanobiotechnology* **2012** (Aug 2), *10*, 35, http://dx.doi.org/10.1186/1477-3155-10-35
- 24. Jayaramulu, K.; Datta, K. K. R.; Suresh, M. V.; Kumari, G.; Datta, R.; Narayana, C.; Eswaramoorthy, M.; Maji, T. K., Honeycomb Porous Framework of Zinc(II): Effective Host for Palladium Nanoparticles for Efficient Three-Component (A3) Coupling and Selective Gas Storage. *ChemPlusChem* 2012 (Sep), 77 (9), 743-747, http://dx.doi.org/10.1002/cplu.201200093
- Rajaram, S.; Shivanna, R.; Kandappa, S. K.; Narayan, K. S., Nonplanar Perylene Diimides as Potential Alternatives to Fullerenes in Organic Solar Cells. *Journal of Physical Chemistry Letters* 2012 (Sep 6), *3* (17), 2405-2408, http://dx.doi.org/10.1021/ Jz301047d
- 26. Payal, R. S.; Balasubramanian, S., Dynamic Atomic Force Microscopy for Ionic Liquids: Massless Model Shows the Way. *Chemphyschem* 2012 (Sep 17), *13* (13), 3085-3086, http://dx.doi.org/10.1002/cphc.201200380
- Kumar, P.; Tuteja, M.; Kesaria, M.; Waghmare, U. V.; Shivaprasad, S. M., Superstructure of self-aligned hexagonal GaN nanorods formed on nitrided Si(111) surface. *Applied Physics Letters* 2012 (Sep 24), *101* (13), 131605 http://dx.doi.org/10.1063 /1.4751986
- 28. Bhasker, H. P.; Dhar, S.; Sain, A.; Kesaria, M.; Shivaprasad, S. M., High electron mobility through the edge states in random networks of c-axis oriented wedge-shaped GaN nanowalls grown by molecular beam epitaxy. *Applied Physics Letters* **2012 (Sep 24)**, *101* (13), http://dx.doi.org/10.1063/1.4755775
- 29. Gupta, R.; Kulkarni, G. U., Pd grating obtained by direct micromolding for use in high resolution optical diffraction based sensing. *Bulletin of Materials Science* **2012 (Oct)**, *35* (5), 773-779, http://dx.doi.org/10.1007/s12034-012-0365-8
- Tangi, M.; Kuyyalil, J.; Shivaprasad, S. M., Role of native defects in nitrogen flux dependent carrier concentration of InN films grown by molecular beam epitaxy. *Journal of Applied Physics* 2012 (Oct 1), *112* (7), 073510 http://dx.doi.org/10.1063 /1.4757031
- 31. Kuyyalil, J.; Tangi, M.; Shivaprasad, S. M., Effect of interfacial lattice mismatch on bulk carrier concentration and band gap of InN. *Journal of Applied Physics* **2012 (Oct 15)**, *112* (8), 083521 http://dx.doi.org/10.1063/1.4759449
- 32. Kurra, N.; Bhadram, V. S.; Narayana, C.; Kulkarni, G. U., Field effect transistors and photodetectors based on nanocrystalline graphene derived from electron beam induced carbonaceous patterns. *Nanotechnology* 2012 (Oct 26), *23* (42), 425301, http://dx.doi.org/10.1088/0957-4484/23/42/425301
- 33. Chaturbedy, P.; Chatterjee, S.; Selvi, R. B.; Bhat, A.; Kavitha, M. K.; Tiwari, V.; Patel, A. B.; Kundu, T. K.; Maji, T. K.; Eswaramoothy, M., Multifunctional carbon nanospheres with magnetic and luminescent probes: probable brain theranostic agents. *Journal of Materials Chemistry B* 2012 (Nov), *1* (7), 939-945, http://dx.doi.org/10.1039/ C2TB00134A
- 34. Siddhanta, S.; Thakur, V.; Narayana, C.; Shivaprasad, S. M., Universal Metal-Semiconductor Hybrid Nanostructured SERS Substrate for Biosensing. *ACS Applied Materials & Interfaces* 2012 (Nov), 4

(11), 5807-5812, http://dx.doi.org/10.1021/am302102p

- Saha, R.; Shireen, A.; Shirodkar, S. N.; Waghmare, U. V.; Sundaresan, A.; Rao, C. N. R., Multiferroic and magnetoelectric nature of GaFeO3, AlFeO3 and related oxides. *Solid State Communications* 2012 (Nov), *152* (21), 1964-1968, http://dx.doi.org/10.1016/j.ssc.2012.07.018
- 36. Rajeswaran, B.; Khomskii, D. I.; Zvezdin, A. K.; Rao, C. N. R.; Sundaresan, A., Field-induced polar order at the Neel temperature of chromium in rare-earth orthochromites: Interplay of rare-earth and Cr magnetism. *Physical Review B* 2012 (Dec 10), *86* (21), 214409 http://dx.doi.org/10.1103/Physrevb.86.214409
- 37. Reddy, S. K.; Balasubramanian, S., Liquid Dimethyl Carbonate: A Quantum Chemical and Molecular Dynamics Study. *Journal of Physical Chemistry B* 2012 (Dec 27), *116* (51), 14892-14902, http://dx.doi.org/10.1021/jp309374m
- 38. Bhadram, V. S.; Rajeswaran, B.; Sundaresan, A.; Narayana, C., Spin-phonon coupling in multiferroic RCrO<sub>3</sub>(R-Y, Lu, Gd, Eu, Sm): A Raman study. *EPL (Europhysics Letters)* 2013 (Jan), *101* (1), 17008 http://dx.doi.org/10.1209/0295-5075/101/17008
- 39. Kurra, N.; Bhadram, V. S.; Narayana, C.; Kulkarni, G. U., Few layer graphene to graphitic films: infrared photoconductive versus bolometric response. *Nanoscale* **2013** (Jan), *5* (1), 381-389, http://dx.doi.org/10.1039/c2nr32861e
- 40. Mandal, P.; Serrao, C. R.; Suard, E.; Caignaert, V.; Raveau, B.; Sundaresan, A.; Rao, C. N. R., Spin reorientation and magnetization reversal in the perovskite oxides, YFe1-xMnxO3 (0 <= x <= 0.45): A neutron diffraction study. *Journal of Solid State Chemistry* **2013 (Jan)**, *197*, 408-413, http://dx.doi.org/10.1016/j.jssc.2012.09.005
- 41. Siddhanta, S.; Karthigeyan, D.; Kundu, P. P.; Kundu, T. K.; Narayana, C., Surface enhanced Raman spectroscopy of Aurora kinases: direct, ultrasensitive detection of autophosphorylation. *RSC Advances* **2013** (Jan), *3* (13), 4221-4230, http://dx.doi.org/10.1039/C3ra22676j
- 42. Narayan, B.; Senanayak, S. P.; Jain, A.; Narayan, K. S.; George, S. J., Self-Assembly of π-Conjugated Amphiphiles: Free Standing, Ordered Sheets with Enhanced Mobility. *Advanced Functional Materials* 2013 (Jan), *23*, 3053–3060, http://dx.doi.org/10.1002/adfm.201202298
- 43. Mukhopadhyay, S.; Das, A. J.; Narayan, K. S., High-Resolution Photocurrent Imaging of Bulk Heterojunction Solar Cells. *Journal of Physical Chemistry Letters* **2013 (Jan 3)**, *4* (1), 161-169, http://dx.doi.org/10.1021/Jz3018336
- Sagade, A. A.; Rao, K. V.; Mogera, U.; George, S. J.; Datta, A.; Kulkarni, G. U., High-Mobility Field Effect Transistors Based on Supramolecular Charge Transfer Nanofibres. *Advanced Materials* 2013 (Jan 25), 25 (4), 559-564, http://dx.doi.org/10.1002/ adma.201203926
- 45. Narayan, K. S.; Madhushankar, B. N.; Gautam, V.; Senanayak, S. P.; Shivanna, R., Water-Gated Phospholipid-Monolayer Organic Field Effect Transistor Through Modified Mueller-Montal Method. *IEEE Electron Device Letters* **2013 (Feb)**, *34* (2), 310-312, http://dx.doi.org/10.1109/Led.2012.2233192
- 46. Kuyyalil, J.; Tangi, M.; Shivaprasad, S. M., In induced reconstructions of Si(111) as superlattice matched epitaxial templates for InN growth. *Materials Research Bulletin* **2013 (Feb)**, *48* (2), 256-259, http://dx.doi.org/10.1016/j.materresbull.2012.10.011
- Kiran, S. R.; Babu, G. S.; Narayana, C.; Murthy, V. R. K.; Subramanian, V., Long range B-site cation ordering and Briet–Wigner–Fano line shape of A1g-like Raman mode in Nd1–xSmx(Mg0.5Ti0.5)03 microwave dielectric ceramics. *Materials Research Bulletin* 2013 (Feb), *48* (2), 194-199, http://dx.doi.org/10.1016/j.materresbull. 2012.09.056

- 48. Basori, R.; Das, K.; Kumar, P.; Narayan, K. S.; Raychaudhuri, A. K., Large photoresponse of Cu:7,7,8,8tetracyanoquinodimethane nanowire arrays formed as aligned nanobridges. *Applied Physics Letters* **2013 (Feb 11)**, *102* (6), 061111 http://dx.doi.org/10.1063/1.4792470
- 49. Gupta, R.; Kulkarni, G. U., Holistic Method for Evaluating Large Area Transparent Conducting Electrodes. *ACS Applied Materials & Interfaces* **2013 (Feb 13)**, *5* (3), 730-736, http://dx.doi.org/10.1021/am302264a
- 50. Radha, B.; Lim, S. H.; Saifullah, M. S. M.; Kulkarni, G. U., Metal hierarchical patterning by direct nanoimprint lithography. *Scientific Reports* **2013 (Feb 28)**, *3*, 1078, http://dx.doi.org/10.1038/srep01078
- 51. Rajeswaran, B.; Sanyal, D.; Chakrabarti, M.; Sundarayya, Y.; Sundaresan, A.; Rao, C. N. R., Interplay of 4f-3d magnetism and ferroelectricity in DyFeO3. *EPL (Europhysics Letters)* 2013 (Jan), *101* (1), 17001 http://dx.doi.org/10.1209/0295-5075/ 101/17001
- 52. Rao, K. D. M.; Radha, B.; Smith, K. C.; Fisher, T. S.; Kulkarni, G. U., Solution-processed soldering of carbon nanotubes for flexible electronics. *Nanotechnology* **2013** (Feb 22), *24* (7), 075301, http://dx.doi.org/10.1088/0957-4484/24/7/075301
- 53. Angmo, D.; Gevorgyan, S. A.; Larsen-Olsen, T. T.; Sondergaard, R. R.; Hosel, M.; Jorgensen, M.; Gupta, R.; Kulkarni, G. U.; Krebs, F. C., Scalability and stability of very thin, roll-to-roll processed, large area, indium-tin-oxide free polymer solar cell modules. *Organic Electronics* **2013 (Mar)**, *14* (3), 984-994, http://dx.doi.org/ 10.1016/j.orgel. 2012.12.033
- 54. Kulkarni, C.; Balasubramanian, S.; George, S. J., What Molecular Features Govern the Mechanism of Supramolecular Polymerization? *Chemphyschem* **2013** (Mar), *14* (4), 661-673, http://dx.doi.org/10.1002/cphc.201200801
- 55. Rao, K. V.; Datta, K. K. R.; Eswaramoorthy, M.; George, S. J., Highly Pure Solid-State White-Light Emission from Solution-Processable Soft-Hybrids. *Advanced Materials* **2013** (Mar 25), *25* (12), 1713-1718, http://dx.doi.org/10.1002/adma.201204407
- 56. Radha, B.; Liu, G.; Eichelsdoerfer, D. J.; Kulkarni, G. U.; Mirkin, C. A., Layer-by-layer assembly of a metallomesogen by dip-pen nanolithography. *ACS Nano* **2013** (Mar 26), *7* (3), 2602-9, http://dx.doi.org/10.1021/nn306013e

### **Book, Book Chapters and Conference Papers**

- 1. Graphene: Synthesis, Properties, and Phenomena. Wiley-VCH Verlag GmbH & Co. KGaA: Rao, C. N. R.; Sood, A. K., 2012, ISBN. 9783527651122.
- Goroshko, D. L.; Galkin, K. N.; Chusovitin, E. A.; Galkin, N. G.; Kumar, M.; Shivaprasad, S. M., An influence of Mg adsorption on the Si(5512) substrate conductivity and surface morphology. <u>In</u> *Asian School-Conference on Physics and Technology of Nanostructured Materials*, Galkin, N. G., Ed. Elsevier Science Bv: Amsterdam, **2012**; Vol. 23, pp 33-36.
- 3. Radha, B.; Kulkarni, G. U., Micromolding A Soft Lithography Technique. <u>In</u> *Micromanufacturing Processes*, Jain, V. K., Ed. CRC Press, Taylor and Francis Group: Boca Raton, USA, 2013; p 329.
- 4. Kulkarni, G. U., Nanolithography. <u>In</u> *A Textbook of Nanoscience and Nanotechnology*, Pradeep, T., Ed. MC Graw Hill: 2012; p 572, ISBN. 9781259007323.
- Arif, M.; Karthigeyan, D.; Siddhanta, S.; Kumar, G. V. P.; Narayana, C.; Kundu, T. K., Analysis of protein acetyltransferase structure-function relation by Surface-Enhanced Raman Scattering (SERS): A tool to screen and characterize small molecule modulators. <u>In</u> *Protein Acetylation: methods and protocols*, 2013 ed.; Hake, S. B.; Janzen, C. J., Eds. Humana Press: 2013; Vol. 981, pp 239-261, ISBN.

9781627033046, http://dx.doi.org/10.1007/978-1-62703-305-3\_19

- Galkin, K. N.; Chusovitin, E. A.; Kumar, M.; Shivaprasad, S. M.; Galkin, N. G.; Goroshko, D. L., The study of Si(5512) cleaning in the ultra-high vacuum conditions. <u>In</u> *Asian School-Conference on Physics and Technology of Nanostructured Materials*, Galkin, N. G., Ed. Elsevier Science Bv: Amsterdam, 2012; Vol. 23, pp 29-32.
- 7. Rao, C. N. R.; Maitra, U.; Matte, H. S. S. R., Synthesis, Characterization, and Selected Properties of Graphene. In Graphene: Synthesis, Properties, and Phenomena, Rao, C. N. R.; Sood, A. K., Eds. Wiley-VCH Verlag GmbH & Co. KGaA: 2012; pp 1-47, ISBN. 9783527651122.

## **Engineering Mechanics Unit**

- 1. Alam, M., Non-Modal Stability and Optimal Perturbations in Unbounded Granular Shear Flow: Three-Dimensionality and Particle Spin. *Progress of Theoretical Physics Supplement* **2012** *195*, 78-100, http://dx.doi.org/10.1143/PTPS.195.78
- 2. Mukund, R.; Narasimha, R.; Viswanath, P. R.; Crouch, J. D., Multiple laminar-turbulent transition cycles around a swept leading edge. *Experiments in Fluids* **2012 (Dec)**, *53* (6), 1915-1927, http://dx.doi.org/10.1007/s00348-012-1405-2
- 3. Narasimha, R., Cumulus clouds and convective boundary layers: a tropical perspective on two turbulent shear flows. *Journal of Turbulence* **2012** *13* (47), 1-25, N47 http://dx.doi.org/10.1080/14685248.2012.718782
- Ponnulakshmi, V. K.; Mukund, V.; Singh, D. K.; Sreenivas, K. R.; Subramanian, G., Hypercooling in the Nocturnal Boundary Layer: Broadband Emissivity Schemes. *Journal of the Atmospheric Sciences* 2012 (Sep), 69 (9), 2892-2905, http://dx.doi.org/10.1175/jas-d-11-0269.1
- Subudhi, S.; Sreenivas, K. R.; Arakeri, J. H., Study of Submerged Jet for Suction of Fluid. *Journal of Fluids Engineering-Transactions of the Asme* 2012 (Sep), *134* (9), 6, 094502 http://dx.doi.org/10.1115/1.4007266
- 6. Alam, M.; Shukla, P., Nonlinear stability, bifurcation and vortical patterns in three-dimensional granular plane Couette flow. *Journal of Fluid Mechanics* **2013 (Feb)**, *716*, 349-413, http://dx.doi.org/10.1017/jfm.2012.549
- Mukund, V.; Singh, D. K.; Ponnulakshmi, V. K.; Subramanian, G.; Sreenivas, K. R., Field and laboratory experiments on aerosol-induced cooling in the nocturnal boundary layer. *Quarterly Journal of the Royal Meteorological Society* 2013, Mar 18, http://dx.doi.org/10.1002/qj.2113
- 8. Ponnulakshmi, V. K.; Singh, D. K.; Mukund, V.; Sreenivas, K. R.; Subramanian, G., Hypercooling in the Atmospheric Boundary Layer: Beyond Broadband Emissivity Schemes. *Journal of the Atmospheric Sciences* **2013** (Jan), *70* (1), 278-283, http://dx.doi.org/10.1175/jas-d-12-095.1
- 9. Ramadugu, R.; Thampi, S. P.; Adhikari, R.; Succi, S.; Ansumali, S., Lattice differential operators for computational physics. *Europhysics Letters* **2013 (Mar)**, *101* (5), 6, 50006 http://dx.doi.org/10.1209/0295-5075/101/50006
- Shukla, P.; Alam, M., Nonlinear vorticity-banding instability in granular plane Couette flow: higherorder Landau coefficients, bistability and the bifurcation scenario. *Journal of Fluid Mechanics* 2013 (Mar), *718*, 131-180, http://dx.doi.org/10.1017/ jfm.2012.601
- Singh, D. K.; Ponnulakshami, V. K.; Mukund, V.; Subramanian, G.; Sreenivas, K. R., Radiation forcing by the atmospheric aerosols in the nocturnal boundary layer. *AIP Conference Proceedings* 2013 (May 10), *1531* (1), 596-599, http://dx.doi.org/10.1063/1.4804840
- 12. Singh, S.; Krithivasan, S.; Karlin, I. V.; Succi, S.; Ansumali, S., Energy Conserving Lattice Boltzmann

Models for Incompressible Flow Simulations *Communications in Computational Physics* **2013** *13* (3), 603-613, http://dx.doi.org/10.4208/ cicp.311011.170412s

- Subudhi, S.; Sreenivas, K. R.; Arakeri, J. H., Study of buoyant jets in natural ventilation of a model room. *International Journal of Heat and Mass Transfer* 2013 64 (0), 91-97, http://dx.doi.org/http://dx.doi.org/10.1016/j.ijheatmasstransfer.2013.04.027
- 14. Subudhi, S.; Sreenivas, K. R.; Arakeri, J. H., Removal of unwanted fluid. *Heat and Mass Transfer* **2013** (Jan), *49* (1), 95-106, http://dx.doi.org/10.1007/s00231-012-1068-9
- 15. Narasimha, R.; Roshko, A.; Gharib, M., Hans W. Liepmann, 1914-2009. *Annual Review of Fluid Mechanics* **2013** *45*, 1-17, http://dx.doi.org/10.1146/annurev-fluid-120710-101108
- 16. Suryanarayanan, S.; Narasimha, R.; Dass, N. D. H., The Turbulent 'Mixing' Layer as a Problem in the Non-equilibrium Statistical Mechanics of a Vortex Gas. **2013 (2013)**, arXiv:1212.6586, http://dx.doi.org/http://arxiv.org/abs/1212.6586
- 17. Suryanarayanan, S.; Singh, S.; Ansumali, S., Extended BGK Boltzmann for Dense Gases *Communications in Computational Physics* **2013** *13* (3), 629-648,
- Thampi, S. P.; Ansumali, S.; Adhikari, R.; Succi, S., Isotropic discrete Laplacian operators from lattice hydrodynamics. *Journal of Computational Physics* 2013 (Feb), *234*, 1-7, http://dx.doi.org/10.1016/j.jcp.2012.07.037

### **Book Chapters and Conference Papers**

- 1. Narasimha, R., Rockets in Mysore and Britain (AD 1750-1850). In *History of Technology in India*, Mukhia, H., Ed. Indian National Science Academy: New Delhi, 2012; Vol. II, pp 804-822,
- Narasimha, R.; Roshko, A.; Gharib, M., Hans W. Liepmann, 1914-2009. In *Annual Review of Fluid Mechanics, Vol 45*, Davis, S. H.; Moin, P., Eds. Annual Reviews: Palo Alto, 2013; Vol. 45, pp 1-17, ISBN. 0066-4189; 978-0-8243-0745-5, http://dx.doi.org/10.1146/ annurev-fluid-120710-101108
- 3. Alam, M.; Shukla, P. Vorticity Banding and Stress Localization in a Granular Fluid, *Proceedings of 23rd International Congress of Theoretical and Applied Mechanics (ICTAM2012)*, Beijing, China, **2012 (Aug 19-24)**
- 4. Alam, M.; Shukla, P. Gradient and vorticity banding phenomena in a sheared granular fluid, *65th Annual Meeting of the APS Divison of Fluid Dynamics*, San Diego, California, USA, Session L32: Granular Flows III **2012 (Nov 19)**
- 5. Ansari, I.; Alam, M. Patterns, Segregation and Hysteresis in vertically vibrated granular mixtures, 65th Annual Meeting of the APS Division of Fluid Dynamics, San Diego, California, USA, Session L32: Granular Flows III **2012 (Nov 19)**
- 6. Singh, D. K.; Ponnulakshmi, V. K.; Subramanian, G.; Sreenivas, K. R. Delay in convection in nocturnal boundary layer due to aerosol-induced cooling, *Bulletin of the American Physical Society, 65th Annual Meeting of the APS Division of Fluid Dynamics* Session L1: Geophysical: Atmospheric III 2012 (Nov 19)
- Paul, U.; Narasimha, R. From a Desingularized Vortex Sheet Model to a Turbulent Mixing Layer, *APS March Meeting 2013, Bulletin of the American Physical Society*, Baltimore, Maryland, Session T16: Climate Physics / Instabilities and Turbulence **2013 (Mar 18-22)** http://meetings.aps.org/Meeting/MAR13/Session/T16.12.

## **Evolutionary and Organismal Biology Unit**

1. De, J.; Varma, V.; Sharma, V. K., Adult Emergence Rhythm of Fruit Flies Drosophila melanogaster under Seminatural Conditions. *Journal of Biological Rhythms* **2012** (August 1, ), *27* (4), 280-286,

http://dx.doi.org/10.1177/0748730412448360

- Kannan, N. N.; Mukherjee, N.; Sharma, V. K., Robustness of Circadian Timing Systems Evolves in the Fruit Fly Drosophila melanogaster as a Correlated Response to Selection for Adult Emergence in a Narrow Window of Time. *Chronobiology International* 2012 *29* (10), 1312-1328, http://dx.doi.org/10.3109/07420528.2012.728550
- Kannan, N. N.; Varma, V.; De, J.; Sharma, V. K., Stability of Adult Emergence and Activity/Rest Rhythms in Fruit Flies Drosophila melanogaster under Semi-Natural Condition. *PLoS One* 2012 (Nov 28), 7 (11), e50379, http://dx.doi.org/10.1371/ journal.pone.0050379
- Kannan, N. N.; Vaze, K. M.; Sharma, V. K., Clock accuracy and precision evolve as a consequence of selection for adult emergence in a narrow window of time in fruit flies Drosophila melanogaster. *Journal of Experimental Biology* 2012 (Oct), *215* (20), 3527-3534, http://dx.doi.org/10.1242/Jeb.074534
- 5. M Ghosh, S.; Joshi, A., Evolution of reproductive isolation as a by-product of divergent life-history evolution in laboratory populations of Drosophila melanogaster. *Ecology and Evolution* 2012 (Dec), *2* (12), 3214-26, http://dx.doi.org/10.1002/ece3.413
- Mukherjee, N.; Kannan, N. N.; Yadav, P.; Sharma, V. K., A model based on oscillatory threshold and build-up of a developmental substance explains gating of adult emergence in Drosophila melanogaster. *The Journal of Experimental Biology* 2012 (September 1, ), *215* (17), 2960-2968, http://dx.doi.org/10.1242/jeb.071290
- 7. Potdar, S.; Sheeba, V., Large Ventral Lateral Neurons Determine the Phase of Evening Activity Peak across Photoperiods in Drosophila melanogaster. *Journal of Biological Rhythms* **2012 (Aug)**, *27* (4), 267-279, http://dx.doi.org/10.1177/0748730412449820
- 8. Prabhakaran, P. M.; Sheeba, V., Sympatric Drosophilid Species melanogaster and ananassae Differ in Temporal Patterns of Activity. *Journal of Biological Rhythms* **2012 (Oct)**, *27* (5), 365-376, http://dx.doi.org/10.1177/0748730412458661
- 9. Vaze, K. M.; Kannan, N. N.; Abhilash, L.; Sharma, V. K., Chronotype differences in Drosophila are enhanced by semi-natural conditions. *Naturwissenschaften* **2012** (Nov), *99* (11), 967-971, http://dx.doi.org/10.1007/s00114-012-0978-1
- Vaze, K. M.; Nikhil, K. L.; Abhilash, L.; Sharma, V. K., Early- and Late-Emerging Drosophila melanogaster Fruit Flies Differ in Their Sensitivity to Light During Morning and Evening. *Chronobiology International* 2012 (Dec), 29 (6), 674-682, http://dx.doi.org/10.3109/07420528.2012.680557
- 11. Dey, S.; Joshi, A., Effects of constant immigration on the dynamics and persistence of stable and unstable Drosophila populations. *Scientific Reports* **2013** (Mar 8), *3*, 1405, http://dx.doi.org/10.1038/srep01405

### **Book chapter**

 Johnsson, A.; Sharma, V. K.; Engelmann, W., The Telegraph Plant: Codariocalyx motorius (Formerly Also Desmodium gyrans). In Plant Electrophysiology, Volkov, A. G., Ed. Springer: 2012; pp 85-123, ISBN. 978-3-642-30676-1.

## **Molecular Biology and Genetics Unit**

1. Arivazhagan, A.; Kumar, D. M.; Sagar, V.; Patric, I. R. P.; Sridevi, S.; Thota, B.; Srividya, M. R.; Prasanna, K.; Thennarasu, K.; Mondal, N.; Hegde, A. S.; Chandramouli, B. A.; Santosh, V.; Rao, M. R. S.; Kondaiah, P.; Somasundaram, K., Higher topoisomerase 2 alpha gene transcript levels predict better prognosis in GBM patients receiving temozolomide chemotherapy: identification of temozolomide as a TOP2A inhibitor. *Journal of Neuro-Oncology* **2012** (Apr), *107* (2), 289-297, http://dx.doi.org/10.1007/s11060-011-0758-3

- Jain, M.; Bhat, G. P.; VijayRaghavan, K.; Inamdar, M. S., Rudhira/BCAS3 is a cytoskeletal protein that controls Cdc42 activation and directional cell migration during angiogenesis. *Experimental Cell Research* 2012 (Apr), *318* (6), 753-767, http://dx.doi.org/10.1016/j.yexcr.2012.01.016
- Maity, K.; Bajaj, P.; Surolia, N.; Surolia, A.; Suguna, K., Insights into the Substrate Specificity of a Thioesterase Rv0098 of Mycobacterium Tuberculosis through X-ray Crystallographic and Molecular Dynamics Studies. *Journal of Biomolecular Structure & Dynamics* 2012 (Apr), 29 (5), 973-983,
- Mehrotra, S.; Ningappa, M. B.; Raman, J.; Anand, R. P.; Balaram, H., Mutational analysis of cysteine 328 and cysteine 368 at the interface of Plasmodium falciparum adenylosuccinate synthetase. *Biochimica Et Biophysica Acta-Proteins and Proteomics* 2012 (Apr), *1824* (4), 589-597, http://dx.doi.org/10.1016/ j.bbapap.2012.01.007
- Thakur, J.; Sanyal, K., A Coordinated Interdependent Protein Circuitry Stabilizes the Kinetochore Ensemble to Protect CENP-A in the Human Pathogenic Yeast Candida albicans. *PLoS Genetics* 2012 (Apr), *8* (4), 466-481, e1002661 http://dx.doi.org/ 10.1371/journal.pgen.1002661
- Modak, R.; Mitra, S. D.; Krishnamoorthy, P.; Bhat, A.; Banerjee, A.; Gowsica, B. R.; Bhuvana, M.; Dhanikachalam, V.; Natesan, K.; Shome, R.; Shome, B. R.; Kundu, T. K., Histone H3K14 and H4K8 hyperacetylation is associated with Escherichia coli induced mastitis in mice. *Epigenetics* 2012 (May), 7 (5), 492-501, http://dx.doi.org/10.4161/ epi.19742
- Ramana, L. N.; Sharma, S.; Sethuraman, S.; Ranga, U.; Krishnan, U. M., Investigation on the stability of saquinavir loaded liposomes: Implication on stealth, release characteristics and cytotoxicity. *International Journal of Pharmaceutics* 2012 (Jul), *431* (1-2), 120-129, http://dx.doi.org/10.1016/j.ijpharm.2012.04.054
- 8. Selvi, R. B.; Chatterjee, S.; Jagadeesan, D.; Chaturbedy, P.; Suma, B. S.; Eswaramoorthy, M.; Kundu, T. K., ATP driven clathrin dependent entry of carbon nanospheres prefer cells with glucose receptors.
  *Journal of Nanobiotechnology* 2012 (Aug 2), *10*, 35, http://dx.doi.org/10.1186/1477-3155-10-35
- Arun, G.; Akhade, V. S.; Donakonda, S.; Rao, M. R. S., mrhl RNA, a Long Noncoding RNA, Negatively Regulates Wnt Signaling through Its Protein Partner Ddx5/p68 in Mouse Spermatogonial Cells. *Molecular and Cellular Biology* 2012 (Aug), 32 (15), 3140-3152, http://dx.doi.org/10.1128/mcb.00006-12
- Bodhini, D.; Sandhiya, M.; Ghosh, S.; Majumder, P. P.; Rao, M. R. S.; Mohan, V.; Radha, V., Association of His1085His INSR Gene Polymorphism with Type 2 Diabetes in South Indians. *Diabetes Technology & Therapeutics* 2012 (Aug), 14 (8), 696-700, http://dx.doi.org/10.1089/dia.2012.0009
- Neogi, U.; Gupta, S.; Sahoo, P. N.; Shet, A.; Rao, S. D.; Ranga, U.; Prasad, V. R., Genetic Characterization of HIV Type 1 Tat Exon 1 from a Southern Indian Clinical Cohort: Identification of Unique Epidemiological Signature Residues. *AIDS Research and Human Retroviruses* 2012 (Sep), 28 (9), 952-956, http://dx.doi.org/10.1089/aid.2011.0380
- 12. Inamdar, M. S.; Healy, L.; Sinha, A.; Stacey, G., Global Solutions to the Challenges of Setting up and Managing a Stem Cell Laboratory. *Stem Cell Reviews and Reports* **2012 (Sep)**, *8* (3), 830-843, http://dx.doi.org/10.1007/s12015-011-9326-7
- 13. Ali, R.; Kumar, S.; Balaram, H.; Sarma, S. P., H-1, C-13, N-15 assignment and secondary structure determination of glutamine amido transferase subunit of gaunosine monophosphate synthetase from Methanocaldococcus jannaschii. *Biomolecular NMR Assignments* **2012 (Oct)**, *6* (2), 193-196, http://dx.doi.org/10.1007/s12104-011-9354-x
- 14. Bachu, M.; Mukthey, A. B.; Murali, R. V.; Cheedarla, N.; Mahadevan, A.; Shankar, S. K.; Satish, K. S.; Kundu, T. K.; Ranga, U., Sequence Insertions in the HIV Type 1 Subtype C Viral Promoter

Predominantly Generate an Additional NF-kappa B Binding Site. *AIDS Research and Human Retroviruses* **2012 (Oct)**, *28* (10), 1362-1368, http://dx.doi.org/10.1089/aid.2011.0388

- 15. Banerjee, S.; Arif, M.; Rakshit, T.; Roy, N. S.; Kundu, T. K.; Roy, S.; Mukhopadhyay, R., Structural features of human histone acetyltransferase p300 and its complex with p53. *FEBS Letters* **2012 (Nov)**, *586* (21), 3793-3798, http://dx.doi.org/10.1016/ j.febslet. 2012.09.012
- Vasudevarao, M. D.; Dhanasekaran, K.; Selvi, R. B.; Kundu, T. K., Inhibition of acetyltransferase alters different histone modifications: probed by small molecule inhibitor plumbagin. *Journal of Biochemistry* 2012 (Nov), *152* (5), 453-462, http://dx.doi.org/10.1093/jb/mvs093
- Banerjee, T.; Jaijyan, D. K.; Surolia, N.; Singh, A. P.; Surolia, A., Apicoplast triose phosphate transporter (TPT) gene knockout is lethal for Plasmodium. *Molecular and Biochemical Parasitology* 2012 (Nov), *186* (1), 44-50, http://dx.doi.org/10.1016/ j.molbiopara.2012.09.008
- 18. Bachu, M.; Yalla, S.; Asokan, M.; Verma, A.; Neogi, U.; Sharma, S.; Murali, R. V.; Mukthey, A. B.; Bhatt, R.; Chatterjee, S.; Rajan, R. E.; Cheedarla, N.; Yadavalli, V. S.; Mahadevan, A.; Shankar, S. K.; Rajagopalan, N.; Shet, A.; Saravanan, S.; Balakrishnan, P.; Solomon, S.; Vajpayee, M.; Satish, K. S.; Kundu, T. K.; Jeang, K. T.; Ranga, U., Multiple NF-kappa B Sites in HIV-1 Subtype C Long Terminal Repeat Confer Superior Magnitude of Transcription and Thereby the Enhanced Viral Predominance. *Journal of Biological Chemistry* 2012 (Dec), *287* (53), 44714-44735, http://dx.doi.org/10.1074/jbc.M112.397158
- 19. Chaturbedy, P.; Chatterjee, S.; Selvi, R. B.; Bhat, A.; Kavitha, M. K.; Tiwari, V.; Patel, A. B.; Kundu, T. K.; Maji, T. K.; Eswaramoothy, M., Multifunctional carbon nanospheres with magnetic and luminescent probes: probable brain theranostic agents. *Journal of Materials Chemistry B* 2013 *1* (7), 939-945, http://dx.doi.org/10.1039/c2tb00134a
- 20. Siddhanta, S.; Karthigeyan, D.; Kundu, P. P.; Kundu, T. K.; Narayana, C., Surface enhanced Raman spectroscopy of Aurora kinases: direct, ultrasensitive detection of autophosphorylation. *RSC Advances* **2013** *3* (13), 4221-4230, http://dx.doi.org/10.1039/c3ra22676j
- 21. Collins, H. M.; Abdelghany, M. K.; Messmer, M.; Yue, B. G.; Deeves, S. E.; Kindle, K. B.; Mantelingu, K.; Aslam, A.; Winkler, G. S.; Kundu, T. K.; Heery, D. M., Differential effects of garcinol and curcumin on histone and p53 modifications in tumour cells. *BMC Cancer* 2013 (Jan), *13*, 11, 37 http://dx.doi.org/10.1186/1471-2407-13-37
- 22. Maity, D.; Karthigeyan, D.; Kundu, T. K.; Govindaraju, T., FRET-based rational strategy for ratiometric detection of Cu2+ and live cell imaging. *Sensors and Actuators B-Chemical* 2013 (Jan), *176*, 831-837, http://dx.doi.org/10.1016/j.snb.2012.09.071
- 23. Roy, B.; Varshney, N.; Yadav, V.; Sanyal, K., The process of kinetochore assembly in yeasts. *FEMS Microbiology Letters* **2013 (Jan)**, *338* (2), 107-117, http://dx.doi.org/10.1111/1574-6968.12019
- Majumder, P.; Banerjee, A.; Shandilya, J.; Senapati, P.; Chatterjee, S.; Kundu, T. K.; Dasgupta, D., Minor Groove Binder Distamycin Remodels Chromatin but Inhibits Transcription. *PLoS One* 2013 (Feb), 8 (2), 9, e57693 http://dx.doi.org/10.1371/ journal.pone.0057693
- 25. Das, S.; Cong, R.; Shandilya, J.; Senapati, P.; Moindrot, B.; Monier, K.; Delage, H.; Mongelard, F.; Kumar, S.; Kundu, T. K.; Bouvet, P., Characterization of nucleolin K88 acetylation defines a new pool of nucleolin colocalizing with pre-mRNA splicing factors. *FEBS Letters* **2013 (Mar)**, *587* (5), 417-424, http://dx.doi.org/10.1016/ j.febslet.2013.01.035

### **Book Edited and Book Chapters**

- 1. Kundu, T. K., *Epigenetics: Development and Disease*. Springer: 2013; Vol. Vol. 61, p XXVI, 689 p., ISBN. 978-94-007-4524-7.
- 2. Chatterjee, S.; Senapati, P.; Kundu, T. K., Post-translational modifications of lysine in DNA-damage

repair. In *Lysine-Based Post-Translational Modification of Proteins*, Essays in Biochemistry, Scott, I., Ed. Portland Press Ltd: London, 2012; Vol. 52, pp 93-111, ISBN. 978-1-85578-185-6.

- 3. Arif, M.; Karthigeyan, D.; Siddhanta, S.; Kumar, G. V. P.; Narayana, C.; Kundu, T., Analysis of Protein Acetyltransferase Structure–Function Relation by Surface-Enhanced Raman Scattering (SERS): A Tool to Screen and Characterize Small Molecule Modulators. In *Protein Acetylation*, Methods in Molecular Biology, Hake, S. B.; Janzen, C. J., Eds. Humana Press: 2013; Vol. 981, pp 239-261, ISBN. 978-1-62703-304-6.
- Kumari, S.; Swaminathan, A.; Chatterjee, S.; Senapati, P.; Boopathi, R.; Kundu, T., Chromatin Organization, Epigenetics and Differentiation: An Evolutionary Perspective. In *Epigenetics: Development and Disease*, Subcellular Biochemistry, Kundu, T. K., Ed. Springer Netherlands: 2013; Vol. 61, pp 3-35, ISBN. 978-94-007-4524-7.
- 5. Selvi, B. R.; Chatterjee, S.; Modak, R.; Eswaramoorthy, M.; Kundu, T., Histone Acetylation as a Therapeutic Target. In *Epigenetics: Development and Disease*, Subcellular Biochemistry, Kundu, T. K., Ed. Springer Netherlands: 2013; Vol. 61, pp 567-596, ISBN. 978-94-007-4524-7.

## **New Chemistry Unit**

- 1. Ren, Z.; Kim, E.; Pattinson, S. W.; Subrahmanyam, K. S.; Rao, C. N. R.; Cheetham, A. K.; Eder, D., Hybridizing photoactive zeolites with graphene: a powerful strategy towards superior photocatalytic properties. *Chemical Science* **2012** *3* (1), 209-216 http://dx.doi.org/10.1039/C1sc00511a
- Rao, C. N. R.; Matte, H. S. S. R.; Subrahmanyam, K. S.; Maitra, U., Unusual magnetic properties of graphene and related materials. *Chemical Science* 2012 3 (1), 45-52 http://dx.doi.org/10.1039/C1sc00726b
- Samanta, P. K.; Periyasamy, G.; Manna, A. K.; Pati, S. K., Computational studies on structural and optical properties of single-stranded DNA encapsulated silver/gold clusters. *Journal of Materials Chemistry* 2012 22 (14), 6774-6781 http://dx.doi.org/ 10.1039/C2jm16068d
- 4. Matte, H. S. S. R.; Jain, A.; George, S. J., A covalently linked graphene-oligo(phenylenevinylene) adduct: self-organization and photo-physical properties. *RSC Advances* **2012** *2* (15), 6290-6294 http://dx.doi.org/10.1039/C2ra20455j
- 5. Manchineella, S.; Govindaraju, T., Hydrogen bond directed self-assembly of cyclic dipeptide derivatives: gelation and ordered hierarchical architectures. *RSC Advances* 2012 *2* (13), 5539-5542 http://dx.doi.org/10.1039/C2ra20342a
- 6. Maitra, U.; Matte, H. S.; Kumar, P.; Rao, C. N., Strategies for the synthesis of graphene, graphene nanoribbons, nanoscrolls and related materials. *Chimia (Aarau)* **2012** *66* (12), 941-8 http://dx.doi.org/10.2533/chimia.2012.941
- Haldar, R.; Maji, T. K., Selective carbon dioxide uptake and crystal-to-crystal transformation: porous 3D framework to 1D chain triggered by conformational change of the spacer. *Crystengcomm* 2012 14 (2), 684-690 http://dx.doi.org/10.1039/ C1ce05847a
- 8. Gopalakrishnan, K.; Subrahmanyam, K. S.; Kumar, P.; Govindaraj, A.; Rao, C. N. R., Reversible chemical storage of halogens in few-layer graphene. *RSC Advances* **2012** *2* (4), 1605-1608 http://dx.doi.org/10.1039/C1ra00403d
- 9. Ghosh, S.; Yamijala, S. R. K. C. S.; Pati, S. K.; Rao, C. N. R., The interaction of halogen molecules with SWNTs and graphene. *RSC Advances* **2012** *2* (3), 1181-1188 http://dx.doi.org/10.1039/C1ra00295c
- Kumar, P.; Bera, A.; Muthu, D. V. S.; Shirodkar, S. N.; Saha, R.; Shireen, A.; Sundaresan, A.; Waghmare, U. V.; Sood, A. K.; Rao, C. N. R., Coupled phonons, magnetic excitations, and ferroelectricity in AlFeO<sub>3</sub>: Raman and first-principles studies. *Physical Review B* 2012 (Apr), *85* (13), 134449

http://dx.doi.org/10.1103/PhysRevB.85.134449

- 11. Iyer, A. K.; Peter, S. C., EuLiGe2 and YbLiGe<sub>2</sub>-A Divalent and an Intermediate-Valent Compound with CaLiSi<sub>2</sub>-Type Structures. *European Journal of Inorganic Chemistry* **2012 (Apr)**, (11), 1790-1794 http://dx.doi.org/10.1002/ejic.201101370
- 12. Shiva, K.; Rajendra, H. B.; Subrahmanyam, K. S.; Bhattacharyya, A. J.; Rao, C. N. R., Improved Lithium Cyclability and Storage in Mesoporous SnO<sub>2</sub> Electronically Wired with Very Low Concentrations (=1?%) of Reduced Graphene Oxide. *Chemistry-a European Journal* **2012 (Apr)**, *18* (15), 4489-4494 http://dx.doi.org/10.1002/ chem.201200352
- 13. Maitra, U.; Pandeeswar, M.; Govindaraju, T., Covalent crosslinking of carbon nanostructures. *Journal of Chemical Sciences* **2012** (May), *124* (3), 551-556
- 14. Haldar, R.; Rao, K. V.; George, S. J.; Maji, T. K., Exciplex formation and energy transfer in a selfassembled metal-organic hybrid system. *Chemistry-a European Journal* **2012 (May 7)**, *18* (19), 5848-52 http://dx.doi.org/10.1002/chem.201103827
- 15. Rao, C. N. R.; Matte, H.; Voggu, R.; Govindaraj, A., Recent progress in the synthesis of inorganic nanoparticles. *Dalton Transactions* **2012** (May 7), *41* (17), 5089-5120 http://dx.doi.org/10.1039/c2dt12266a
- 16. Chakraborty, A.; Gurunatha, K. L.; Muthulakshmi, A.; Dutta, S.; Pati, S. K.; Maji, T. K., Assembly of trinuclear and tetranuclear building units of Cu<sub>2+</sub> towards two 1D magnetic systems: synthesis and magneto-structural correlations. *Dalton Transactions* 2012 (May 21), *41* (19), 5879-88 http://dx.doi.org/10.1039/c2dt12511k.
- 17. Subbarao, U.; Peter, S. C., Crystal Structure of YbCu6In6 and Mixed Valence Behavior of Yb in YbCu<sub>6-x</sub>In<sub>6+x</sub> (x=0, 1, and 2) Solid Solution. *Inorganic Chemistry* 2012 (Jun 4), *51* (11), 6326-6332 http://dx.doi.org/10.1021/ic300552w
- Kumar, P.; Das, B.; Chitara, B.; Subrahmanyam, K. S.; Gopalakrishnan, K.; Krupanidhi, S. B.; Rao, C. N. R., Novel Radiation-Induced Properties of Graphene and Related Materials. *Macromolecular Chemistry and Physics* 2012 (Jun 14), *213* (10-11), 1146-1163 http://dx.doi.org/10.1002/macp.201100451
- 19. Late, D. J.; Liu, B.; Matte, H. S.; Dravid, V. P.; Rao, C. N., Hysteresis in single-layer MoS<sub>2</sub> field effect transistors. *ACS Nano* 2012 (Jun 26), 6 (6), 5635-41 http://dx.doi.org/10.1021/nn301572c
- 20. Late, D. J.; Liu, B.; Luo, J. J.; Yan, A. M.; Matte, H.; Grayson, M.; Rao, C. N. R.; Dravid, V. P., GaS and GaSe Ultrathin Layer Transistors. *Advanced Materials* **2012** (Jul), *24* (26), 3549-3554 http://dx.doi.org/10.1002/adma.201201361
- 21. Nagaraja, C. M.; Maji, T. K.; Rao, C. N. R., Synthesis, structure and magnetic properties of two organically-templated coordination polymers, {[EDAH<sub>2</sub>][M<sub>1</sub>M<sub>2</sub>F<sub>2</sub>(SO<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]}<sub>n</sub> (M<sub>1</sub> = M<sub>2</sub> = Ni<sup>II</sup> and M<sub>1</sub> = Co<sup>II</sup>, M<sub>2</sub> = Ni<sup>II</sup>). *Inorganica Chimica Acta* 2012 (Jul 1), *389*, 85-89 http://dx.doi.org/10.1016/j.ica.2012.01.060
- 22. Samanta, P. K.; Manna, A. K.; Pati, S. K., Thieno Analogues of RNA Nucleosides: A Detailed Theoretical Study. *Journal of Physical Chemistry B* 2012 (Jul 5), *116* (26), 7618-7626 http://dx.doi.org/10.1021/jp301752k
- 23. Avinash, M. B.; Govindaraju, T., Amino acid derivatized arylenediimides: a versatile modular approach for functional molecular materials. *Advanced Materials* **2012** (Aug 2), *24* (29), 3905-22 http://dx.doi.org/10.1002/adma.201201544
- 24. Brovelli, S.; Galland, C.; Viswanatha, R.; Klimov, V. I., Tuning radiative recombination in Cu-doped nanocrystals via electrochemical control of surface trapping. *Nano letters* **2012** (Aug 8), *12* (8),

4372-9 http://dx.doi.org/10.1021/nl302182u

- 25. Viswanatha, R.; Naveh, D.; Chelikowsky, J. R.; Kronik, L.; Sarma, D. D., Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. *Journal of Physical Chemistry Letters* **2012** (Aug 2), *3* (15), 2009-2014 http://dx.doi.org/10.1021/Jz300741z
- 26. Rao, C. N. R.; Sundaresan, A.; Saha, R., Multiferroic and Magnetoelectric Oxides: The Emerging Scenario. *Journal of Physical Chemistry Letters* **2012** (Aug 16), *3* (16), 2237-2246 http://dx.doi.org/10.1021/Jz300688b
- 27. Hoque, J.; Kumar, P.; Aswal, V. K.; Haldar, J., Aggregation properties of amide bearing cleavable gemini surfactants by small angle neutron scattering and conductivity studies. *The journal of Physical Chemistry. B* 2012 (Aug 16), *116* (32), 9718-26 http://dx.doi.org/10.1021/ jp305590f
- 28. Manna, A. K.; Pati, S. K., Designing Tunable Electronic and Magnetic Properties of Graphene: A Theoretical Perspective. *International Journal of Modern Physics B* 2012 (Aug 20), *26* (21), 1242003 http://dx.doi.org/10.1142/S0217979212420039
- Hoque, J.; Akkapeddi, P.; Yarlagadda, V.; Uppu, D. S.; Kumar, P.; Haldar, J., Cleavable cationic antibacterial amphiphiles: synthesis, mechanism of action, and cytotoxicities. *Langmuir* 2012 (Aug 21), *28* (33), 12225-34 http://dx.doi.org/10.1021/la302303d
- 30. Ghosh, D.; Parida, P.; Pati, S. K., Electronic, Magnetic, and Transport Properties of  $Fe_n$ -bis(*n*-acene) and  $Fe_n$ -bis(*n*-BNacene) [n = 1,2,
- 31. Das, B.; Kumar, P.; Rao, C. N. R., Factors Affecting Laser-Excited Photoluminescence from ZnO Nanostructures. *Journal of Cluster Science* 2012 (Sep), *23* (3), 649-659 http://dx.doi.org/10.1007/s10876-012-0453-3
- 32. Rao, B. G.; Matte, H. S. S. R.; Rao, C. N. R., Decoration of Few-Layer Graphene-Like MoS<sub>2</sub> and MoSe<sub>2</sub> by Noble Metal Nanoparticles. *Journal of Cluster Science* **2012 (Sep)**, *23* (3), 929-937 http://dx.doi.org/10.1007/s10876-012-0504-9
- 33. Kanoo, P.; Reddy, S. K.; Kumari, G.; Haldar, R.; Narayana, C.; Balasubramanian, S.; Maji, T. K., Unusual room temperature CO<sub>2</sub> uptake in a fluoro-functionalized MOF: insight from Raman spectroscopy and theoretical studies. *Chemical communications* **2012** (Sep 4), *48* (68), 8487-9 http://dx.doi.org/10.1039/c2cc34276f
- 34. Gopalakrishnan, K.; Moses, K.; Dubey, P.; Rao, C. N. R., A Raman study of the interaction of electrondonor and -acceptor molecules with chemically doped graphene. *Journal of Molecular Structure* 2012 (Sep 12), 1023, 2-6 http://dx.doi.org/10.1016/ j.molstruc.2011.12.031
- Rajeswaran, B.; Mandal, P.; Saha, R.; Suard, E.; Sundaresan, A.; Rao, C. N. R., Ferroelectricity Induced by Cations of Nonequivalent Spins Disordered in the Weakly Ferromagnetic Perovskites, YCr1-xMxO3 (M = Fe or Mn). *Chemistry of Materials* 2012 (Sep 25), *24* (18), 3591-3595 http://dx.doi.org/10.1021/cm301944s
- 36. Haldar, R.; Narayan, R. P.; Maji, T. K., Selective CO<sub>2</sub> uptake in a bi-pillared layer 3D metal-organic framework of Zn(II). *Indian Journal of Chemistry Section a-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry* **2012 (Sep-Oct)**, *51* (9-10), 1231-1237
- 37. George, S. J.; de Bruijn, R.; Tomovic, Z.; Van Averbeke, B.; Beljonne, D.; Lazzaroni, R.; Schenning, A.; Meijer, E. W., Asymmetric Noncovalent Synthesis of Self-Assembled One-Dimensional Stacks by a Chiral Supramolecular Auxiliary Approach. *Journal of the American Chemical Society* 2012 (Oct), *134* (42), 17789-17796 http://dx.doi.org/ 10.1021/ja3086005
- 38. Jayaramulu, K.; Narayanan, R. P.; George, S. J.; Maji, T. K., Luminescent Microporous Metal-Organic Framework with Functional Lewis Basic Sites on the Pore Surface: Specific Sensing and Removal of

Metal Ions. *Inorganic Chemistry* **2012 (Oct)**, *51* (19), 10089-10091 http://dx.doi.org/10.1021/ic3017547

- 39. Avinash, M. B.; Verheggen, E.; Schmuck, C.; Govindaraju, T., Self-cleaning functional molecular materials. *Angewandte Chemie Int Ed Engl* 2012 (Oct 8), *51* (41), 10324-8 http://dx.doi.org/10.1002/anie.201204608
- Peter, S. C.; Sarkar, S.; Kanatzidis, M. G., Metallic Yb<sub>2</sub>AuGe<sub>3</sub>: An Ordered Superstructure in the AlB<sub>2</sub>. Type Family with Mixed-Valent Yb and a High-Temperature Phase Transition. *Inorganic Chemistry* 2012 (Oct 15), *51* (20), 10793-10799 http://dx.doi.org/10.1021/ic301197w
- 41. Govindaraju, T.; Avinash, M. B., Two-dimensional nanoarchitectonics: organic and hybrid materials. *Nanoscale* **2012** (Oct **21**), *4* (20), 6102-17 http://dx.doi.org/10.1039/c2nr31167d
- Saha, R.; Shireen, A.; Shirodkar, S. N.; Waghmare, U. V.; Sundaresan, A.; Rao, C. N. R., Multiferroic and magnetoelectric nature of GaFeO<sub>3</sub>, AlFeO<sub>3</sub> and related oxides. *Solid State Communications* 2012 (Nov), *152* (21), 1964-1968 http://dx.doi.org/10.1016/j.ssc.2012.07.018
- 43. Samanta, P. K.; Manna, A. K.; Pati, S. K., Structural, Electronic, and Optical Properties of Metallo Base Pairs in Duplex DNA: A Theoretical Insight. *Chemistry-an Asian Journal* **2012** (Nov), 7 (11), 2718-2728 http://dx.doi.org/10.1002/asia.201200630
- 44. Sarkar, S.; Peter, S. C., Single crystal growth of europium and ytterbium based intermetallic compounds using metal flux technique. *Journal of Chemical Sciences* **2012** (Nov), *124* (6), 1385-1390 http://dx.doi.org/10.1007/s12039-012-0335-0
- 45. Rao, K. V.; George, S. J., Supramolecular Alternate Co-Assembly through a Non-Covalent Amphiphilic Design: Conducting Nanotubes with a Mixed D-A Structure. *Chemistry-a European Journal* 2012 (Nov), *18* (45), 14286-14291 http://dx.doi.org/10.1002/ chem.201202168
- 46. Grandhi, G. K.; Tomar, R.; Viswanatha, R., Study of Surface and Bulk Electronic Structure of II-VI Semiconductor Nanocrystals Using Cu as a Nanosensor. *ACS Nano* 2012 (Nov), *6* (11), 9751-9763 http://dx.doi.org/10.1021/Nn304149s
- 47. Kumar, M.; Jonnalagadda, N.; George, S. J., Molecular recognition driven self-assembly and chiral induction in naphthalene diimide amphiphiles. *Chem Commun (Camb)* **2012 (Nov 18)**, *48* (89), 10948-50 http://dx.doi.org/10.1039/c2cc35438a
- 48. Matte, H. S. S. R.; Maitra, U.; Kumar, P.; Rao, B. G.; Pramoda, K.; Rao, C. N. R., Synthesis, Characterization, and Properties of Few-layer Metal Dichalcogenides and their Nanocomposites with Noble Metal Particles, Polyaniline, and Reduced Graphene Oxide. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* 2012 (Dec), 638 (15), 2617-2624 http://dx.doi.org/10.1002/zaac.201200283
- 49. Pandey, A.; Brovelli, S.; Viswanatha, R.; Li, L.; Pietryga, J. M.; Klimov, V. I.; Crooker, S. A., Long-lived photoinduced magnetization in copper-doped ZnSe-CdSe core-shell nanocrystals. *Nature nanotechnology* **2012 (Dec)**, *7* (12), 792-7 http://dx.doi.org/10.1038/nnano.2012.210
- Kumar, S. V.; Saraiah, B.; Misra, N. C.; Ila, H., Synthesis of 2-Phenyl-4,5-Substituted Oxazoles by Copper-Catalyzed Intramolecular Cyclization of Functionalized Enamides. *Journal of Organic Chemistry* 2012 (Dec 7), 77 (23), 10752-10763 http://dx.doi.org/10.1021/Jo3021192
- 51. Rajeswaran, B.; Khomskii, D. I.; Zvezdin, A. K.; Rao, C. N. R.; Sundaresan, A., Field-induced polar order at the Neel temperature of chromium in rare-earth orthochromites: Interplay of rare-earth and Cr magnetism. *Physical Review B* 2012 (Dec 10), *86* (21), 214409 http://dx.doi.org/10.1103/Physrevb.86.214409
- 52. Lee, C. M.; Weight, A. K.; Haldar, J.; Wang, L.; Klibanov, A. M.; Chen, J. Z., Polymer-attached zanamivir inhibits synergistically both early and late stages of influenza virus infection. *Proceedings of the*

*National Academy of Sciences of the United States of America* **2012** (Dec **11**), *109* (50), 20385-20390 http://dx.doi.org/10.1073/pnas.1219155109

- 53. Lo, S. H.; He, J. Q.; Biswas, K.; Kanatzidis, M. G.; Dravid, V. P., Phonon Scattering and Thermal Conductivity in p-Type Nanostructured PbTe-BaTe Bulk Thermoelectric Materials. *Advanced Functional Materials* 2012 (Dec 19), 22 (24), 5175-5184 http://dx.doi.org/10.1002/adfm.201201221
- 54. Neihsial, S.; Periyasamy, G.; Samanta, P. K.; Pati, S. K., Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study. *Journal of Physical Chemistry B* 2012 (Dec 27), *116* (51), 14754-14759 http://dx.doi.org/ 10.1021/Jp305894c
- 55. Ila, H.; Junjappa, H., Molecular Diversity through Novel Organosulfur Synthons: Versatile Templates for Heterocycle Synthesis. *Chimia* **2013** *67* (1-2), 17-22 http://dx.doi.org/10.2533/chimia.2013.17
- 56. Kumar, R.; Jayaramulu, K.; Maji, T. K.; Rao, C. N. R., Hybrid nanocomposites of ZIF-8 with graphene oxide exhibiting tunable morphology, significant CO<sub>2</sub> uptake and other novel properties. *Chemical Communications* **2013** *49* (43), 4947-4949 http://dx.doi.org/10.1039/c3cc00136a
- 57. Subbarao, U.; Sebastian, A.; Rayaprol, S.; Yadav, C. S.; Svane, A.; Vaitheeswaran, G.; Peter, S. C., Metal Flux Crystal Growth Technique in the Determination of Ordered Superstructure in EuInGe. *Crystal Growth & Design* 2013 (Jan), *13* (1), 352-359 http://dx.doi.org/10.1021/Cg301532b
- 58. Swaroop, T. R.; Roopashree, R.; Ila, H.; Rangappa, K. S., Attempted Simmon-Smith reaction on betaalkylthio-alpha,beta-unsaturated ketones: a regiospecific synthesis of 2,4-disubstituted thiophenes. *Tetrahedron Letters* **2013 (Jan)**, *54* (2), 147-150 http://dx.doi.org/10.1016/j.tetlet.2012.10.110
- 59. Rao, C. N. R.; Matte, H.; Subrahmanyam, K. S., Synthesis and Selected Properties of Graphene and Graphene Mimics. *Accounts of Chemical Research* **2013** (Jan 15), *46* (1), 149-159 http://dx.doi.org/10.1021/ar300033m
- 60. Sanyal, S.; Manna, A. K.; Pati, S. K., Effect of Imide Functionalization on the Electronic, Optical, and Charge Transport Properties of Coronene: A Theoretical Study. *Journal of Physical Chemistry C* 2013 (Jan 17), *117* (2), 825-836 http://dx.doi.org/10.1021/ Jp310362c
- 61. Sagade, A. A.; Rao, K. V.; Mogera, U.; George, S. J.; Datta, A.; Kulkarni, G. U., High-Mobility Field Effect Transistors Based on Supramolecular Charge Transfer Nanofibres. *Advanced Materials* **2013 (Jan 25)**, *25* (4), 559-564 http://dx.doi.org/10.1002/ adma.201203926
- 62. Chakraborty, B.; Matte, H.; Sood, A. K.; Rao, C. N. R., Layer-dependent resonant Raman scattering of a few layer MoS<sub>2</sub>. *Journal of Raman Spectroscopy* **2013** (Jan), *44* (1), 92-96 http://dx.doi.org/10.1002/jrs.4147
- 63. Dey, S.; Das, B.; Voggu, R.; Nag, A.; Sarma, D. D.; Rao, C. N. R., Interaction of CdSe and ZnO nanocrystals with electron-donor and -acceptor molecules. *Chemical Physics Letters* **2013 (Jan 29)**, 556, 200-206 http://dx.doi.org/10.1016/j.cplett.2012.11.046
- 64. Gopalakrishnan, K.; Moses, K.; Govindaraj, A.; Rao, C. N. R., Supercapacitors based on nitrogen-doped reduced graphene oxide and borocarbonitrides. *Solid State Communications* **2013 (Feb)**, http://dx.doi.org/10.1016/j.ssc.2013.02.005
- 65. Grandhi, G. K.; Viswanatha, R., Tunable Infrared Phosphors Using Cu Doping in Semiconductor Nanocrystals: Surface Electronic Structure Evaluation. *Journal of Physical Chemistry Letters* **2013** (Feb 7), 4 (3), 409-415 http://dx.doi.org/10.1021/ Jz3021588
- Avinash, M. B.; Govindaraju, T., Extremely Slow Dynamics of an Abiotic Helical Assembly: Unusual Relevance to the Secondary Structure of Proteins. *Journal of Physical Chemistry Letters* 2013 (Feb 21), 4 (4), 583-588 http://dx.doi.org/ 10.1021/Jz4001642

- 67. Jayaramulu, K.; Haldar, R.; Maji, T. K., Self-assembly of tetrabromoterephthalic acid with different metal system: Diversity in dimensionalities, structures and gas adsorption. *Polyhedron* **2013 (Mar)**, *52*, 553-559 http://dx.doi.org/10.1016/j.poly.2012.08.029
- 68. Kulkarni, C.; Balasubramanian, S.; George, S. J., What Molecular Features Govern the Mechanism of Supramolecular Polymerization? *Chemphyschem* **2013 (Mar 18)**, *14* (4), 661-673 http://dx.doi.org/10.1002/cphc.201200801
- Mandal, P.; Serrao, C. R.; Suard, E.; Caignaert, V.; Raveau, B.; Sundaresan, A.; Rao, C. N. R., Spin reorientation and magnetization reversal in the perovskite oxides, YFe<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> (0≤x≤0.45): A neutron diffraction study. *Journal of Solid State Chemistry* 2013 (Jan), *197*, 408-413 http://dx.doi.org/10.1016/j.jssc.2012.09.005
- 70. Manna, A. K.; Pati, S. K., Theoretical understanding of single-stranded DNA assisted dispersion of graphene. *Journal of Materials Chemistry B* 2013 1 (1), 91-100 http://dx.doi.org/10.1039/C2tb00184e
- Narayan, B.; Kulkarni, C.; George, S. J., Synthesis and self-assembly of a C-3-symmetric benzene-1,3,5-tricarboxamide (BTA) anchored naphthalene diimide disc. *Journal of Materials Chemistry C* 2013 1 (4), 626-629 http://dx.doi.org/10.1039/c2tc00742h
- 72. Rajeswaran, B.; Sanyal, D.; Chakrabarti, M.; Sundarayya, Y.; Sundaresan, A.; Rao, C. N. R., Interplay of 4f-3d magnetism and ferroelectricity in DyFeO3. *EPL-Europhysics Letters* **2013** (Jan), *101* (1), 17001 http://dx.doi.org/10.1209/0295-5075/101/17001
- 73. Rao, K. V.; Datta, K. K. R.; Eswaramoorthy, M.; George, S. J., Highly Pure Solid-State White-Light Emission from Solution-Processable Soft-Hybrids. *Advanced Materials* **2013 (Mar 25)**, *25* (12), 1713-1718 http://dx.doi.org/10.1002/adma.201204407
- 74. Subbarao, U.; Gutmann, M. J.; Peter, S. C., New Structure Type in the Mixed-Valent Compound YbCu4Ga8. *Inorganic Chemistry* 2013 (Feb 18), *52* (4), 2219-2227 http://dx.doi.org/10.1021/ic302688n
- Subbarao, U.; Peter, S. C., Crystal Growth and Properties of YbCuGa<sub>3</sub>: First Monoclinic System in the RETX<sub>3</sub> Family. *Crystal Growth & Design* 2013 (Feb), *13* (2), 953-959 http://dx.doi.org/10.1021/Cg301765f
- 76. Yamijala, S.; Pati, S. K., Electronic and Magnetic Properties of Zigzag Boron-Nitride Nanoribbons with Even and Odd-Line Stone-Wales (5-7 Pair) Defects. *Journal of Physical Chemistry C* 2013 (Feb 21), *117* (7), 3580-3594 http://dx.doi.org/10.1021/ Jp310614u

## **Book Chapters and Conference Papers**

- Muthu, D. V. S.; Midgley, A. E.; Scott, P. R.; Kruger, M. B.; Sahu, J. R.; Sood, A. K.; Rao, C. N. R., Highpressure synchrotron x-ray diffraction study of RMnO3 (R=Eu, Gd, Tb and Dy) upto 50 GPa. In *23rd International Conference on High Pressure Science and Technology*, 2012; Vol. 377, ISBN. 1742-6588,
- 2. Viswanatha, R.; Pandey, A., Optical studies of quantum dots. In *Spectroscopic Properties of Inorganic and Organometallic Compounds: Techniques, Materials and Applications Volume 44*, The Royal Society of Chemistry: 2013; Vol. 44, pp 123-155,

## **Theoretical Sciences Unit**

 Chakraborty, B.; Bera, A.; Muthu, D. V. S.; Bhowmick, S.; Waghmare, U. V.; Sood, A. K., Symmetrydependent phonon renormalization in monolayer MoS2 transistor. *Physical Review B* 2012 (Apr 6), *85* (16), 161403 http://dx.doi.org/10.1103/ Physrevb.85.161403

- Kumar, P.; Bera, A.; Muthu, D. V. S.; Shirodkar, S. N.; Saha, R.; Shireen, A.; Sundaresan, A.; Waghmare, U. V.; Sood, A. K.; Rao, C. N. R., Coupled phonons, magnetic excitations, and ferroelectricity in AlFeO3: Raman and first-principles studies. *Physical Review B* 2012 (Apr 27), *85* (13), 134449, 134449 http://dx.doi.org/10.1103/Physrevb.85.134449
- 3. Chakraborty, A.; Gurunatha, K. L.; Muthulakshmi, A.; Dutta, S.; Pati, S. K.; Maji, T. K., Assembly of trinuclear and tetranuclear building units of Cu2+ towards two 1D magnetic systems: synthesis and magneto-structural correlations. *Dalton Transactions* **2012 (May 21)**, *41* (19), 5879-5888, http://dx.doi.org/10.1039/ c2dt12511k
- 4. Jaiswal, P. K.; Puri, S.; Das, S. K., Surface-directed spinodal decomposition: A molecular dynamics study. *Physical Review E* 2012 (May 29), *85* (5), 051137 http://dx.doi.org/ 10.1103/PhysRevE.85.051137
- Adjokatse, S. K.; Mishra, A. K.; Waghmare, U. V., Dielectric and piezoelectric responses of nylon-7: A first-principles study. *Polymer* 2012 (Jun 7), *53* (13), 2751-2757, http://dx.doi.org/10.1016/j.polymer.2012.04.042
- 6. Samanta, P. K.; Manna, A. K.; Pati, S. K., Thieno Analogues of RNA Nucleosides: A Detailed Theoretical Study. *Journal of Physical Chemistry B* 2012 (Jul 5), *116* (26), 7618-7626, http://dx.doi.org/10.1021/jp301752k
- Bag, M.; Vidhyadhiraja, N. S.; Narayan, K. S., Fluctuations in photocurrent of bulk heterojunction polymer solar cells-A valuable tool to understand microscopic and degradation processes. *Applied Physics Letters* 2012 (Jul 23), *101* (4), 043903-5, 043903 http://dx.doi.org/10.1063/1.4738985
- K. Das, S.; Kim, Y. C.; Fisher, M. E., Near critical electrolytes: Are the charge-charge sum rules obeyed? *The Journal of Chemical Physics* 2012 (Aug), *137* (7), 074902 http://dx.doi.org/10.1063/1.4743957
- Ghosh, D.; Parida, P.; Pati, S. K., Electronic, Magnetic, and Transport Properties of Fe<sub>n</sub>-bis(n-acene) and Fe<sub>n</sub>-bis(n-BNacene) [n = 1,2,]: A Theoretical Study. *The Journal of Physical Chemistry C* 2012 (Aug 9), *116* (34), 18487-18494, http://dx.doi.org/10.1021/jp304592h
- 10. Manna, A. K.; Pati, S. K., Designing Tunable Electronic and Magnetic Properties of Graphene: a Theoretical Perspective. *International Journal of Modern Physics B* 2012 (Aug 20), *26* (21), 1242003, 1242003 http://dx.doi.org/10.1142/S0217979212420039
- 11. Sen, S.; Vidhyadhiraja, N. S., Protocols for characterising quantum transport through nano-structures. *Applied Physics Letters* **2012 (Sep)**, *101* (13), 133106 http://dx.doi.org/10.1063/1.4754620
- Kumar, P.; Tuteja, M.; Kesaria, M.; Waghmare, U. V.; Shivaprasad, S. M., Superstructure of self-aligned hexagonal GaN nanorods formed on nitrided Si(111) surface. *Applied Physics Letters* 2012 (Sep 24), *101* (13), 131605, 131605 http://dx.doi.org/10.1063/1.4751986
- 13. Shirodkar, S. N.; Waghmare, U. V., Electronic and vibrational signatures of Stone-Wales defects in graphene: First-principles analysis. *Physical Review B* 2012 (Oct 1), *86* (16), 165401, 165401 http://dx.doi.org/10.1103/Physrevb.86.165401
- 14. Saha, B.; Sands, T. D.; Waghmare, U. V., Thermoelectric properties of HfN/ScN metal/semiconductor superlattices: a first-principles study. *Journal of Physics-Condensed Matter* **2012 (Oct 17)**, *24* (41), 415303, http://dx.doi.org/10.1088/0953-8984/24/41/415303
- 15. Manna, A. K.; Pati, S. K., Theoretical understanding of single-stranded DNA assisted dispersion of graphene. *Journal of Materials Chemistry B* 2012 (Oct 18), *1* (1), 91-100, http://dx.doi.org/10.1039/c2tb00184e
- 16. Saha, R.; Shireen, A.; Shirodkar, S. N.; Waghmare, U. V.; Sundaresan, A.; Rao, C. N. R., Multiferroic and

magnetoelectric nature of GaFeO3, AlFeO3 and related oxides. *Solid State Communications* **2012** (Nov), *152* (21), 1964-1968, http://dx.doi.org/ 10.1016/j.ssc.2012.07.018

- Samanta, P. K.; Manna, A. K.; Pati, S. K., Structural, Electronic, and Optical Properties of Metallo Base Pairs in Duplex DNA: A Theoretical Insight. *Chemistry – An Asian Journal* 2012 (Nov), 7 (11), 2718-2728, http://dx.doi.org/10.1002/asia.201200630
- 18. Niranjan, M. K.; Waghmare, U. V., Relation between the work function and Young's modulus of RhSi and estimate of Schottky-barrier height at RhSi/Si interface: An ab-initio study. *Journal of Applied Physics* **2012** (Nov 1), *112* (9), 093702, 093702 http://dx.doi.org/10.1063/1.4761994
- Nishimatsu, T.; Aoyagi, K.; Kiguchi, T.; Konno, T. J.; Kawazoe, Y.; Funakubo, H.; Kumar, A.; Waghmare, U. V., Molecular Dynamics Simulation of 90 degrees Ferroelectric Domains in PbTiO3. *Journal of the Physical Society of Japan* 2012 (Dec), *81* (12), 124702 http://dx.doi.org/10.1143/Jpsj.81.124702
- 20. Ahmad, S.; Corberi, F.; Das, S. K.; Lippiello, E.; Puri, S.; Zannetti, M., Aging and crossovers in phaseseparating fluid mixtures. *Physical Review E* 2012 (Dec), *86* (6), 061129, 061129 http://dx.doi.org/10.1103/PhysRevE.86.061129
- 21. Mukri, B. D.; Dutta, G.; Waghmare, U. V.; Hegde, M. S., Activation of Lattice Oxygen of TiO2 by Pd2+ Ion: Correlation of Low-Temperature CO and Hydrocarbon Oxidation with Structure of Ti1-xPdxO2-x (x=0.01-0.03). *Chemistry of Materials* **2012 (Dec 11)**, *24* (23), 4491-4502, http://dx.doi.org/10.1021/cm301704u
- 22. Neihsial, S.; Periyasamy, G.; Samanta, P. K.; Pati, S. K., Understanding the Binding Mechanism of Various Chiral SWCNTs and ssDNA: A Computational Study. *Journal of Physical Chemistry B* 2012 (Dec 27), *116* (51), 14754-14759, http://dx.doi.org/ 10.1021/Jp305894c
- 23. Das, S. K., Unlocking of frozen dynamics in the complex Ginzburg-Landau equation. *Physical Review. E, Statistical, nonlinear, and soft matter physics* **2013** (Jan), *87* (1), 012135 http://dx.doi.org/10.1103/PhysRevE.87.012135
- 24. Sanyal, S.; Manna, A. K.; Pati, S. K., Effect of Imide Functionalization on the Electronic, Optical, and Charge Transport Properties of Coronene: A Theoretical Study. *Journal of Physical Chemistry C* 2013 (Jan 17), *117* (2), 825-836, http://dx.doi.org/10.1021/ Jp310362c
- 25. Kumar, A.; Rabe, K. M.; Waghmare, U. V., Domain formation and dielectric response in PbTiO3: A firstprinciples free-energy landscape analysis. *Physical Review B* 2013 (Jan 22), *87* (2), 024107, 024107 http://dx.doi.org/10.1103/Physrevb.87.024107
- Maliyekkal, S. M.; Sreeprasad, T. S.; Krishnan, D.; Kouser, S.; Mishra, A. K.; Waghmare, U. V.; Pradeep, T., Graphene: a reusable substrate for unprecedented adsorption of pesticides. *Small* 2013 (Jan 28), 9 (2), 273-83, http://dx.doi.org/10.1002/smll. 201201125
- 27. Yamijala, S. R.; Sharma, K. C.; Pati, S. K., Electronic and Magnetic Properties of Zigzag Boron-Nitride Nanoribbons with Even and Odd-Line Stone-Wales (5-7 Pair) Defects. *Journal of Physical Chemistry C* 2013 (Feb 21), *117* (7), 3580-3594, http://dx.doi.org/Doi 10.1021/Jp310614u
- Bothra, P.; Periyasamy, G.; Pati, S. K., Methane formation from the hydrogenation of carbon dioxide on Ni(110) surface a density functional theoretical study. *Physical Chemistry Chemical Physics* 2013 (Feb 22), *15* (15), 5701-5706, http://dx.doi.org/10.1039/c3cp44495c
- 29. Roy, S.; Das, S. K., Dynamics and growth of droplets close to the two-phase coexistence curve in fluids. *Soft Matter* **2013 (Mar 7)**, *9* (16), 4178-4187, http://dx.doi.org/ 10.1039/C3sm50196e
- 30. Bera, A.; Pal, K.; Muthu, D. V.; Sen, S.; Guptasarma, P.; Waghmare, U. V.; Sood, A. K., Sharp Raman anomalies and broken adiabaticity at a pressure induced transition from band to topological insulator in Sb2Se3. *Physical Review Letters* **2013 (Mar 8)**, *110* (10), 107401 http://

dx.doi.org/10.1103/PhysRevLett.110.107401

#### **Book Chapters and Conference papers**

- 1. Shirodkar, S. N.; Waghmare, U. V., Topological Defects in Graphene and Related 2-D Materials. In *Graphene: Synthesis, Properties, and Phenomena*, Rao, C. N. R.; Sood, A. K., Eds. Wiley-VCH: Weinheim, 2012; pp 235-266, ISBN. 978-3-527-33258-8.
- 2. Waghmare, U. V., Multiferroics with Magnetoelectric Coupling. In *Functional Metal Oxides: New Science and Novel Applications*, Ogale, S. B.; Venkatesan, T. V.; Blamire, M., Eds. Wiley-VCH: Weinheim, 2013; pp 267-282, ISBN. 978-3-527-33179-6.
- Sreepad, H. R.; Ravi, H. R.; Ahmed, K.; Waghmare, U. V. Radiation Induced Changes in Electronic and Dielectric Properties of Polyoxymethylene, In *AIP Conference Proceedings: Proceedings of the 56th DAE Solid State Physics Symposium 2011, 19-23 December 2011*,SRM University, Kattankulathur, Tamilnadu, India, 2012, 793-794.
- 4. Sreepad, H. R.; Ravi, H. R.; Hembram, K. P. S. S.; Waghmare, U. V. First-principles Study of Structure and Properties of the Cyclic Pentamer of Formaldehyde, In *AIP Conference Proceedings: Proceedings of the 56th DAE Solid State Physics Symposium 2011, 19-23 December 2011*,SRM University, Kattankulathur, Tamilnadu, India, **2012**, 795-796.

## **International Centre for Materials Science**

- 1. Bhasker, H. P.; Dhar, S.; Sain, A.; Kesaria, M.; Shivaprasad, S. M., High electron mobility through the edge states in random networks of c-axis oriented wedge-shaped GaN nanowalls grown by molecular beam epitaxy. *Applied Physics Letters* **2012 (Sep 28)**, *101* (13), 132109-5, 132109 http://dx.doi.org/10.1063/1.4755775
- 2. Brovelli, S.; Galland, C.; Viswanatha, R.; Klimov, V. I., Tuning radiative recombination in Cu-doped nanocrystals via electrochemical control of surface trapping. *Nano letters* **2012** (Aug 8), *12* (8), 4372-9, http://dx.doi.org/10.1021/nl302182u
- 3. Das, B.; Kumar, P.; Rao, C. N. R., Factors Affecting Laser-Excited Photoluminescence from ZnO Nanostructures. *Journal of Cluster Science* 2012 (Sep), *23* (3), 649-659, http://dx.doi.org/10.1007/s10876-012-0453-3
- Datta, R.; Loukya, B.; Li, N.; Gupta, A., Structural features of epitaxial NiFe2O4 thin films grown on different substrates by direct liquid injection chemical vapor deposition. *Journal of Crystal Growth* 2012 (Apr 15), 345 (1), 44-50, http://dx.doi.org/ 10.1016/j.jcrysgro.2012.02.007
- 5. Gokhale, S.; Nagamanasa, K. H.; Santhosh, V.; Sood, A. K.; Ganapathy, R., Directional grain growth from anisotropic kinetic roughening of grain boundaries in sheared colloidal crystals. *Proceedings of the National Academy of Sciences* 2012 (December 11, ), *109* (50), 20314-20319, http://dx.doi.org/10.1073/pnas.1210456109
- Gopalakrishnan, K.; Moses, K.; Dubey, P.; Rao, C. N. R., A Raman study of the interaction of electrondonor and -acceptor molecules with chemically doped graphene. *Journal of Molecular Structure* 2012 (Sep 12), *1023* (0), 2-6, http://dx.doi.org/10.1016/ j.molstruc.2011.12.031
- 7. Govinda Rao, B.; Matte, H. S. S. R.; Rao, C. N. R., Decoration of Few-Layer Graphene-Like MoS2 and MoSe2 by Noble Metal Nanoparticles. *Journal of Cluster Science* **2012** (Sep), *23* (3), 929-937,
- 8. Grandhi, G. K.; Tomar, R.; Viswanatha, R., Study of Surface and Bulk Electronic Structure of VI Semiconductor Nanocrystals Using Cu as a Nanosensor. *ACS Nano* 2012 (Oct 17), 6 (11), 9751-9763,
- 9. Jayaramulu, K.; Datta, K. K. R.; Suresh, M. V.; Kumari, G.; Datta, R.; Narayana, C.; Eswaramoorthy, M.;

Maji, T. K., Honeycomb Porous Framework of Zinc(II): Effective Host for Palladium Nanoparticles for Efficient Three-Component (A3) Coupling and Selective Gas Storage. *ChemPlusChem* **2012 (Sep)**, 77 (9), 743-747, http://dx.doi.org/10.1002/cplu.201200093

- Kulriya, P. K.; Mehta, B. R.; Agarwal, D. C.; Kumar, P.; Shivaprasad, S. M.; Pivin, J. C.; Avasthi, D. K., Giant enhancement in ferromagnetic properties of Pd nanoparticle induced by intentionally created defects. *Journal of Applied Physics* 2012 (July), *112* (1), 014318-7, 014318 http://dx.doi.org/10.1063/1.4733950
- 11. Kumar, P.; Bera, A.; Muthu, D. V. S.; Shirodkar, S. N.; Saha, R.; Shireen, A.; Sundaresan, A.; Waghmare, U. V.; Sood, A. K.; Rao, C. N. R., Coupled phonons, magnetic excitations, and ferroelectricity in AlFeO\_{3}: Raman and first-principles studies. *Physical Review B* 2012 (Apr 27), *85* (13), 134449, http://dx.doi.org/10.1103/PhysRevB.85.134449
- 12. Kumar, P.; Das, B.; Chitara, B.; Subrahmanyam, K. S.; Gopalakrishnan, K.; Krupanidhi, S. B.; Rao, C. N. R., Novel Radiation-Induced Properties of Graphene and Related Materials. *Macromolecular Chemistry and Physics* 2012 (Jun 14), *213* (10-11), 1146-1163, http://dx.doi.org/10.1002/macp.201100451
- 13. Kumar, P.; Kumar, M.; Shivaprasad, S. M., Ga induced 2D superstructural phase diagram on trenched Si(5 5 12) surface. *Surface Science* **2012 (July)**, *606* (13–14), 1045-1049, http://dx.doi.org/10.1016/j.susc.2012.02.024
- 14. Kumar, P.; Tuteja, M.; Kesaria, M.; Waghmare, U. V.; Shivaprasad, S. M., Superstructure of self-aligned hexagonal GaN nanorods formed on nitrided Si(111) surface. *Applied Physics Letters* **2012 (Sep 28)**, *101* (13), 131605-4, 131605 http://dx.doi.org/10.1063/1.4751986
- 15. Kuyyalil, J.; Tangi, M.; Shivaprasad, S. M., Effect of interfacial lattice mismatch on bulk carrier concentration and band gap of InN. *Journal of Applied Physics* **2012 (Oct 15)**, *112* (8), 083521 http://dx.doi.org/10.1063/1.4759449
- 16. Late, D. J.; Liu, B.; Luo, J.; Yan, A.; Matte, H. S. S. R.; Grayson, M.; Rao, C. N. R.; Dravid, V. P., GaS and GaSe Ultrathin Layer Transistors. *Advanced Materials* **2012** (July 10), *24* (26), 3549-3554, http://dx.doi.org/10.1002/adma.201201361
- 17. Late, D. J.; Liu, B.; Matte, H. S. S. R.; Dravid, V. P.; Rao, C. N. R., Hysteresis in Single-Layer MoS2 Field Effect Transistors. *ACS Nano* 2012 (May 12), 6 (6), 5635-5641, http://dx.doi.org/10.1021/nn301572c
- 18. Li, N.; Schafer, S.; Datta, R.; Mewes, T.; Klein, T. M.; Gupta, A., Microstructural and ferromagnetic resonance properties of epitaxial nickel ferrite films grown by chemical vapor deposition. *Applied Physics Letters* **2012 (Sep 25)**, *101* (13), 132409 http://dx.doi.org/10.1063/1.4754847
- 19. Loukya, B.; Zhang, X.; Gupta, A.; Datta, R., Electron magnetic chiral dichroism in CrO2 thin films using monochromatic probe illumination in a transmission electron microscope. *Journal of Magnetism and Magnetic Materials* **2012 (Nov)**, *324* (22), 3754-3761, http://dx.doi.org/10.1016/j.jmmm.2012.06.012
- Maitra, U.; Matte, H. S. S. R.; Kumar, P.; Rao, C. N. R., Strategies for the Synthesis of Graphene, Graphene Nanoribbons, Nanoscrolls and Related Materials. *CHIMIA International Journal for Chemistry* 2012 (Dec), 66 (12), 941-948, http://dx.doi.org/10.2533/chimia.2012.941
- 21. Matte, H. S. S. R.; Maitra, U.; Kumar, P.; Govinda Rao, B.; Pramoda, K.; Rao, C. N. R., Synthesis, Characterization, and Properties of Few-layer Metal Dichalcogenides and their Nanocomposites with Noble Metal Particles, Polyaniline, and Reduced Graphene Oxide. *Zeitschrift für anorganische und allgemeine Chemie* 2012 (Dec), *638* (15), 2617-2624, http://dx.doi.org/10.1002/zaac.201200283
- 22. Nagaraja, C. M.; Maji, T. K.; Rao, C. N. R., Synthesis, structure and magnetic properties of two organically-templated coordination polymers, {[EDAH(2)] [M1M2F2 (SO4)(2)(H2O)(2)]}(n) (M-1 =

M-2 = Ni-II and M-1 = Co-II, M-2 = Ni-II). *Inorganica Chimica Acta* **2012** (Jul 1), *389*, 85-89, http://dx.doi.org/10.1016/j.ica.2012.01.060

- PandeyA; BrovelliS; ViswanathaR; LiL; Pietryga, J. M.; Klimov, V. I.; Crooker, S. A., Long-lived photoinduced magnetization in copper-doped ZnSe-CdSe core-shell nanocrystals. *Nature Nanotechnology* 2012 (Dec 2), 7 (12), 792-797, http://dx.doi.org/10.1038/nnano.2012.210
- 24. Rajeswaran, B.; Khomskii, D. I.; Zvezdin, A. K.; Rao, C. N. R.; Sundaresan, A., Field-induced polar order at the Neel temperature of chromium in rare-earth orthochromites: Interplay of rare-earth and Cr magnetism. *Physical Review B* 2012 (Dec 10), *86* (21), 214409 http://dx.doi.org/10.1103/Physrevb.86.214409
- Rajeswaran, B.; Mandal, P.; Saha, R.; Suard, E.; Sundaresan, A.; Rao, C. N. R., Ferroelectricity Induced by Cations of Nonequivalent Spins Disordered in the Weakly Ferromagnetic Perovskites, YCr1–xMxO3 (M = Fe or Mn). *Chemistry of Materials* 2012 (Aug 27), *24* (18), 3591-3595, http://dx.doi.org/10.1021/cm301944s
- 26. Rao, C. N. R.; Sundaresan, A.; Saha, R., Multiferroic and Magnetoelectric Oxides: The Emerging Scenario. *Journal of Physical Chemistry Letters* **2012** (Aug 16), *3* (16), 2237-2246, http://dx.doi.org/10.1021/Jz300688b
- Saha, R.; Shireen, A.; Shirodkar, S. N.; Waghmare, U. V.; Sundaresan, A.; Rao, C. N. R., Multiferroic and magnetoelectric nature of GaFeO3, AlFeO3 and related oxides. *Solid State Communications* 2012 (Nov), *152* (21), 1964-1968, http://dx.doi.org/10.1016/j.ssc.2012.07.018
- 28. Sasidharan, A.; Panchakarla, L. S.; Sadanandan, A. R.; Ashokan, A.; Chandran, P.; Girish, C. M.; Menon, D.; Nair, S. V.; Rao, C. N. R.; Koyakutty, M., Hemocompatibility and Macrophage Response of Pristine and Functionalized Graphene. *Small* 2012 (Apr 23), 8 (8), 1251-1263, http://dx.doi.org/10.1002/smll.201102393
- 29. Shiva, K.; Rajendra, H. B.; Subrahmanyam, K. S.; Bhattacharyya, A. J.; Rao, C. N. R., Improved Lithium Cyclability and Storage in Mesoporous SnO2 Electronically Wired with Very Low Concentrations (≤1%) of Reduced Graphene Oxide. *Chemistry A European Journal* 2012 (Apr 10), *18* (15), 4489-4494, http://dx.doi.org/10.1002/ chem.201200352
- Siddhanta, S.; Thakur, V.; Narayana, C.; Shivaprasad, S. M., Universal Metal-Semiconductor Hybrid Nanostructured SERS Substrate for Biosensing. *ACS Applied Materials & Interfaces* 2012 (Oct 8), 4 (11), 5807-5812, http://dx.doi.org/10.1021/ am302102p
- Tangi, M.; Kuyyalil, J.; Shivaprasad, S. M., Role of native defects in nitrogen flux dependent carrier concentration of InN films grown by molecular beam epitaxy. *Journal of Applied Physics* 2012 (Oct), *112* (7), 073510 http://dx.doi.org/ 10.1063/1.4757031
- 32. Viswanatha, R.; Naveh, D.; Chelikowsky, J. R.; Kronik, L.; Sarma, D. D., Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. *Journal of Physical Chemistry Letters* **2012** (Aug 2), *3* (15), 2009-2014, http://dx.doi.org/10.1021/Jz300741z
- 33. Chakraborty, B.; Matte, H. S. S. R.; Sood, A. K.; Rao, C. N. R., Layer-dependent resonant Raman scattering of a few layer MoS2. *Journal of Raman Spectroscopy* **2013** (Jan), *44* (1), 92-96, http://dx.doi.org/10.1002/Jrs.4147
- 34. Dey, S.; Das, B.; Voggu, R.; Nag, A.; Sarma, D. D.; Rao, C. N. R., Interaction of CdSe and ZnO nanocrystals with electron-donor and -acceptor molecules. *Chemical Physics Letters* **2013 (Jan 29)**, *556*, 200-206, http://dx.doi.org/10.1016/j.cplett.2012.11.046
- 35. Grandhi, G. K.; Viswanatha, R., Tunable Infrared Phosphors Using Cu Doping in Semiconductor Nanocrystals: Surface Electronic Structure Evaluation. *Journal of Physical Chemistry Letters* **2013** (Feb 7), 4 (3), 409-415, http://dx.doi.org/10.1021/ Jz3021588

- Kumar, N.; Moses, K.; Pramoda, K.; Shirodkar, S. N.; Mishra, A. K.; Waghmare, U. V.; Sundaresan, A.; Rao,
  C. N. R., Borocarbonitrides, BxCyNz. *Journal of Materials Chemistry A* 2013 (Feb 1), *1* (19), 5806-5821, http://dx.doi.org/10.1039/C3ta01345f
- 37. Kuyyalil, J.; Tangi, M.; Shivaprasad, S. M., In induced reconstructions of Si(1 1 1) as superlattice matched epitaxial templates for InN growth. *Materials Research Bulletin* **2013 (Feb)**, *48* (2), 256-259, http://dx.doi.org/10.1016/j.materresbull.2012.10.011
- 38. Mandal, P.; Serrao, C. R.; Suard, E.; Caignaert, V.; Raveau, B.; Sundaresan, A.; Rao, C. N. R., Spin reorientation and magnetization reversal in the perovskite oxides, YFe1−xMnxO3 (0≤x≤0.45): A neutron diffraction study. *Journal of Solid State Chemistry* 2013 (Jan), 197, 408-413, http://dx.doi.org/10.1016/j.jssc.2012.09.005
- Rajeswaran, B.; Sanyal, D.; Chakrabarti, M.; Sundarayya, Y.; Sundaresan, A.; Rao, C. N. R., Interplay of 4f-3d magnetism and ferroelectricity in DyFeO 3. *EPL (Europhysics Letters): Condensed Matter: Electronic Structure, Electrical, Magnetic and Optical Properties* 2013 (Jan 11), *101* (1), 17001, http://dx.doi.org/10.1209/0295-5075/ 101/17001
- 40. Rao, C. N. R.; Matte, H. S. S. R.; Subrahmanyam, K. S., Synthesis and Selected Properties of Graphene and Graphene Mimics. *Accounts of Chemical Research* **2013** (Jan 15), *46* (1), 149-159, http://dx.doi.org/10.1021/ar300033m
- 41. Bera, S.; Dhara, S.; Milekhin, A.; Chu, M. W.; Shivaprasad, S. M., Spectroscopic and Structural Insight into the Size-Dependent Behavior of the Nanophase. *International Journal of Spectroscopy* **2012** (2012), 197064 http://dx.doi.org/10.1155/2012/197064
- 42. Mitra, J.; Abraham, G. J.; Kesaria, M.; Bhal, S.; Gupta, A.; Shivaprasad, S. M.; Viswanadham, C. S.; Kulkarni, U. D.; Dey, G. K., Role of substrate temperature in the pulsed laser deposition of zirconium oxide thin film. *Materials Science Forum* **2012** *710*, 757.

### **Book Chapters**

- Galkin, K. N.; Chusovitin, E. A.; Kumar, M.; Shivaprasad, S. M.; Galkin, N. G.; Goroshko, D. L., The study of Si(5512) cleaning in the ultra-high vacuum conditions. In *Asian School-Conference on Physics and Technology of Nanostructured Materials*, Physics Procedia, 2012; Vol. 23, pp 29-32, ISBN. 1875-3892.
- Goroshko, D. L.; Galkin, K. N.; Chusovitin, E. A.; Galkin, N. G.; Kumar, M.; Shivaprasad, S. M., An influence of Mg adsorption on the Si(5512) substrate conductivity and surface morphology. In *Asian School-Conference on Physics and Technology of Nanostructured Materials*, Physics Procedia, 2012; Vol. 23, pp 33-36, ISBN. 1875-3892.
- Muthu, D. V. S.; Midgley, A. E.; Scott, P. R.; Kruger, M. B.; Sahu, J. R.; Sood, A. K.; Rao, C. N. R., High-pressure synchrotron x-ray diffraction study of RMnO3 (R=Eu, Gd, Tb and Dy) upto 50 GPa. In 23rd International Conference on High Pressure Science and Technology, Journal of Physics Conference Series, IOP: 2012; Vol. 377, p 012025, ISBN. 1742-6588.

### **RESEARCH PUBLICATIONS OF HON. PROFESSORS /HON.FACULTY/ENDOWED PROFESSORS**

- 1. Resmi, V.; Ambika, G.; Amritkar, R. E.; Rangarajan, G., Amplitude death in complex networks induced by environment. *Physical Review E* 2012 (Apr 16), *85* (4), 046211 http://dx.doi.org/10.1103/PhysRevE.85.046211
- Thakare, V.; Xing, G.; Peng, H.; Rana, A.; Game, O.; Kumar, P. A.; Banpurkar, A.; Kolekar, Y.; Ghosh, K.; Wu, T.; Sarma, D. D.; Ogale, S. B., High sensitivity low field magnetically gated resistive switching in CoFe<sub>2</sub>O<sub>4</sub>/La<sub>0.66</sub>Sr<sub>0.34</sub>MnO<sub>3</sub> heterostructure. *Applied Physics Letters* 2012 (April 26), *100* (17), 172412-4, http://dx.doi.org/10.1063/1.4707373
- 3. A. Mitra; Gadagkar, R., Queen signal should be honest to be involved in maintenance of eusociality:

chemical correlates of fertility in Ropalidia marginata. *Insectes Sociaux* 2012 (May), 59 (2), 251-255, http://dx.doi.org/10.1007/s00040-011-0214-6

- Kumar, P. A.; Ray, S.; Chakraverty, S.; Sarma, D. D., Magnetoresistance and electroresistance effects in Fe304 nanoparticle system. *Journal of Experimental Nanoscience* 2012 (May 14), 1-7, http://dx.doi.org/10.1080/17458080.2012. 662657
- A. Mitra; Gadagkar, R., Road to Royalty Transition of Potential Queen to Queen in the Primitively Eusocial Wasp Ropalidia marginata. *Ethology* 2012 (June 11), *118*, 694-702, http://dx.doi.org/10.1111/j.1439-0310.2012.02059.x
- 6. Kumar, P. A.; Sarma, D. D., Effect of ``dipolar-biasing'' on the tunability of tunneling magnetoresistance in transition metal oxide systems. *Applied Physics Letters* **2012 (June 27)**, *100* (26), 262407-4,
- Kolakkandy, S.; Giri, K.; Sathyamurthy, N., Collision-induced dissociation in (He, H-2(+)(v=0-2; j=0-3)) system: A time-dependent quantum mechanical investigation. *Journal of Chemical Physics* 2012 (Jun 28), *136* (24), 244312 http://dx.doi.org/ 10.1063/1.4729255
- Viswanatha, R.; Naveh, D.; Chelikowsky, J. R.; Kronik, L.; Sarma, D. D., Magnetic Properties of Fe/Cu Codoped ZnO Nanocrystals. *The Journal of Physical Chemistry Letters* 2012 (July 12), *3* (15), 2009-2014, http://dx.doi.org/10.1021/jz300741z
- 9. Bang, A.; Gadagkar, R., Reproductive queue without overt conflict in the primitively eusocial wasp Ropalidia marginata. *Proceedings of the National Academy of Sciences* **2012 (September 4, 2012)**, *109* (36), 14494-14499, http://dx.doi.org/10.1073/ pnas.1212698109
- 10. Sharma, K.; Kumar, N., First-passage time: Lattice versus continuum. *Physical Review E* 2012 (Sep 11), *86* (3), 032104 http://dx.doi.org/10.1103/PhysRevE.86.032104
- 11. Kumar, P. A.; Mathieu, R.; Vijayaraghavan, R.; Majumdar, S.; Karis, O.; Nordblad, P.; Sanyal, B.; Eriksson, O.; Sarma, D. D., Ferrimagnetism, antiferromagnetism, and magnetic frustration in La2-xSrxCuRuO6 (0 <= x <= 1). *Physical Review B* 2012 (Sep 17), *86* (9), 094421 094421 http://dx.doi.org/10.1103/PhysRevB.86.094421
- 12. Majumder, M.; Sathyamurthy, N.; Lefebvre-Brion, H.; Vazquez, G. J., Photoabsorption of carbon monoxide: a time-dependent quantum mechanical study. *Journal of Physics B-Atomic Molecular and Optical Physics* 2012 (Sep 28), *45* (18), 185101 http:// dx.doi.org/10.1088/0953-4075/45/18/185101
- 13. Srivastava, S.; Sathyamurthy, N., Radiative lifetimes of spin forbidden  $a1\Delta \rightarrow X 3\Sigma$  and spin allowed  $A3\Pi \rightarrow X 3\Sigma$  transitions and complete basis set extrapolated ab initio potential energy curves for the ground and excited states of CH-. *Journal of Chemical Physics* **2012 (Dec 7)**, *137* (21), 214314, 214314 http://dx.doi.org/10.1063/1.4768873
- 14. Mitra, A.; Gadagkar, R., Queens and Workers of the Primitively social Wasp Ropalidia marginata do not Differ in Their Dufour's Gland Morphology. *Sociobiology* **2012** *59* (3), 875-884, http://eprints.iisc.ernet.in/id/eprint/45242
- 15. Singh, M.; Kauamanns, W.; Umapathy, G., Conservation-oriented captive breeding programs in India: Is there a perspective? *Current Science.* **2012** *103*, 1399-1400,
- Mahmoudabadi, G.; Rajagopalan, K.; Getzenberg, R. H.; Hannenhalli, S.; Rangarajan, G.; Kulkarni, P., Intrinsically disordered proteins and conformational noise Implications in cancer. *Cell Cycle* 2013 (Jan 1), *12* (1), 26-31, http://dx.doi.org/10.4161/cc.23178
- 17. Shukla, S.; Chandran, S.; Gadagkar, R., Ovarian developmental variation in the primitively eusocial wasp Ropalidia marginata suggests a gateway to worker ontogeny and the evolution of sociality. *The Journal of Experimental Biology* **2013 (January 15, 2013)**, *216* (2), 181-187,
http://dx.doi.org/10.1242/jeb.073148

- 18. Dey, S.; Das, B.; Voggu, R.; Nag, A.; Sarma, D. D.; Rao, C. N. R., Interaction of CdSe and ZnO nanocrystals with electron-donor and -acceptor molecules. *Chemical Physics Letters* **2013** (Jan 29), *556* (0), 200-206, http://dx.doi.org/10.1016/j.cplett.2012.11.046
- Majumder, M.; Mishra, B. K.; Sathyamurthy, N., CH…π and π…π interaction in benzene–acetylene clusters. *Chemical Physics Letters* 2013 (Feb 2), *557* (0), 59-65, http://dx.doi.org/10.1016/j.cplett.2012.12.027
- Sarma, D. D.; Santra, P. K.; Mukherjee, S.; Nag, A., X-ray Photoelectron Spectroscopy: A Unique Tool To Determine the Internal Heterostructure of Nanoparticles. *Chemistry of Materials* 2013 (Feb 14), *25* (8), 1222-1232, http://dx.doi.org/10.1021/cm303567d
- 21. Mangalam, M.; Singh, M., Sex and physiological state influence the rate of resource acquisition and monopolisation in urban free-ranging dogs, Canis familiaris. *Behaviour* **2013** *150* (2), 199-213, http://dx.doi.org/10.1163/1568539x-00003045
- 22. Choudhury, D.; Pal, B.; Sharma, A.; Bhat, S. V.; Sarma, D. D., Magnetization in electron- and Mn- doped SrTiO3. *Scientific Reports* **2013 (March 12)**, *3*, http://dx.doi.org/ 10.1038/srep01433
- 23. Roy, K.; Singh, M.; Singh, M., Estimation of Resource Availability with Special Reference to Nonhuman Primates in a Rainforest Region in the Central Western Ghats, South India. *Proceedings of the National Academy of Sciences India: Section B: Biological Sciences* 2013 (22/03/2013), http://dx.doi.org/10.1007/s40011-013-0173-y.
- 24. Kumar, P.; Sathyamurthy, N., An ab initio quantum chemical investigation of the structure and stability of ozone-water complexes. *Chemical Physics* 2013 (Mar 29), *415* (0), 214-221, http://dx.doi.org/10.1016/j.chemphys.2013.01.008

#### BOOK CHAPTER BY HON. PROFESSOR/HON. FACULTY

1. Gadagkar, R. (2012). The Luxury of Introspection. In: Über das Kolleg hinaus - Joachim Nettelbeck, dem Sekretär des Wissenschaftskollegs 1981 bis 2012 (Beyond the college - Joachim Nettelbeck, the Secretary of the Wissenschaftskollegs from 1981-2012) (Eds.) Diawara, M.; Günther, K., and Meyer-Kalkus, R., Wissenschaftskolleg zu Berlin, Germany, pp. 152-157.

### **AWARDS / DISTINCTIONS**

#### Prof. CNRRao

Honoris Causa D.Sc from University of Kerala

Honoris Causa D.Sc. degree from the University of St. Andrews (degree to be awarded in Sept 2013) 2012 Award for International Cooperation by The Chinese Academy of Sciences.

#### Prof. Roddam Narasimha

Padma Vibhushan (Govt. of India)

Year-of-Science Professorship, DST, Govt. of India

Semi-annual lecture series titled '*The Roddam Narasimha Distinguished Seminar Series*', instituted at IIT Gandhinagar out of an endowment made by Prof. A. V. Anilkumar, Vanderbilt University, USA. The first lecture in the series was given on 16 April 2013.

#### Prof. M M Sharma

Hari Om Ashram Sr Scientist Award, PRL Ahmadabad

Honorary Doctor of Science, I I T-Kharagpur

Indian Chemical Council (formerly Indian Chemical Manufacturers Association) Life-time Achievement Award

Institute of Chemical Technology, Mumbai -Super Star, in 80th year of the institute

AcSIR Academy Professor

#### Prof. G. U. Kulkarni

Bangalore Nano National Award, 2012

#### Prof. Tapas K Kundu

Ranbaxy Research Award, 2011 (Medical Sciences – Basic Research) First prize of India Innovation Award, Merck Millipore company

#### Prof. S.M. Shivaprasad

Dr. Raja Ramanna Science and Technology Award for Science and Education from Karnataka State Council for Science & Technology - 2013

#### Prof. Swapan K. Pati

TWAS Prize in Chemistry, 2012

#### **Prof. Umesh Waghmare**

India Citation Award 2012 from Thomson Reuters.

#### **Prof. Kaustuv Sanyal**

National Bioscience Award for Career Development 2012 from the Department of Biotechnology, GovernmentofIndia.

#### Prof. Tapas Kumar Maji

CRSI Bronze Medal, 2013

NASI-Scopus Young Scientist Awards for the year 2012 in Chemistry

#### **Prof. Meheboob** Alam

C. N. R. Rao Oration Lecture Award (2013)

#### Dr. Subi J. George

MRSI Medal, 2013

#### Prof. Govindan Rangarajan

Platinum Jubilee lecture at the Indian Science Congress.

#### Prof. Raghavendra Gadagkar

Sir M.Visvesvaraya Senior Scientist State Award, Government of Karnataka, 2011 (awarded in 2013).

#### Mr. Nadiger Nagaraj

The Most Valuable Staff Member prize, 2012

#### Mr. Sachin S Belvadi

Young Achievers Award 2012 by KKS Social Welfare Trust

#### AWARD RECEIVED BY STUDENTS

**Ms. Nisha Mammen** (Ph.D. student, TSU; Research Supervisor: Prof. Shobhana Narasimhan) received the Best Poster prize at the 2nd Gordon Research Conference on Noble Metal Nanoparticles, held at Mt. Holyoke College, USA.

**Ms. Sharmila Narendra Shirodkar**, (Ph.D. student, Materials Theory Group, TSU; Research Supervisor: Prof. Umesh Waghmare) receives "The Malhotra Weikfield Foundation - Bangalore Nano Young Scientist Award".

**Mr. M. Shivaprasad** (Ph.D. student, Bioorganic Chemistry Lab, NCU; Research Supervisor: Dr. T. Govindaraju) awarded "Best Poster" prize at Chennai Chemistry Conference (CCC 2013).

**Mr. Jiaul Hoque** (Ph.D. student, Bio-organic and Medicinal Chemistry Laboratory, NCU; Research supervisor: Dr. Jayanta Haldar) was awarded the best poster award in The first International Conference on Emerging Technologies for Clean Water-2012 at IITM, Chennai.

**Mr. Yarlagadda Venkateswarlu** (Ph.D. student, Bio-organic and Medicinal Chemistry Laboratory, NCU; Research supervisor: Dr. Jayanta Haldar) was awarded best poster award :

- by The Chemical Research Society of India at the Mid year meeting 2012, at CDRI, Lucknow.
- at the International Conference on "Current Trends in Drug Discovery Research-2013" (CTDDR-2013).

**Dr. Jeelan Basha**, (Research Associate, Transcription and Disease Laboratory, MBGU) has received best poster award in the "International symposium on chemistry and chemical biology of natural products" (CCBNP-2012) held at Indian Institute of Chemical Technology (IICT), Hyderabad during 2-4, August 2012.

ACS Chemical Biology recognizes **Mr. Dhanasekaran Karthigeyan** (Ph.D. student, Transcription and Disease Laboratory, MBGU; Research supervisor: Prof. Tapas Kumar Kundu) for "best poster" presented in the "International Symposium on Challenges in Chemical Biology-2013".

RAK-CAM Sheikh Saqr Junior Fellowship has been awarded to **Mr. Rana Saha** (Ph.D. student, CPMU; Research supervisor: Prof. A. Sundaresan and Prof. C.N.R. Rao)

#### **MEMBERSHIPS / APPOINTMENTS**

#### Prof. C.N.R. Rao

Einstein Professor of Chinese Academy of Sciences 2012 Erudite Visiting Professorship from Mahatma Gandhi University, Kottayam Academy Professor, Academy of Scientific & Innovative Research 2013.

#### Prof. M R S Rao

 $Honorary\,Visiting\,Professorship\,of\,Department\,of\,Biochemistry, I.I.Sc$ 

#### Prof. Roddam Narasimha

Hon. Distinguished Professor, ISRO Academy Professor of AcSIR (Academy of Scientific and Innovative Research)

#### Prof. M M Sharma

Academy Professor of AcSIR (Academy of Scientific and Innovative Research)

#### Prof. K. Vijay Raghavan

Appointed as Secretary to Department of Biotechnology, Govt. of India.

#### Prof. Raghavendra Gadagkar

Member, German National Academy of Sciences Leopoldina, 2012.

Chairman, Advisory Board of Council of Scientific and Industrial Research (CSIR), March 2013 – February 2016.

Member, TWAS Regional Prize – 2013 in the subject area "Public Understanding and Popularization of Science".

Member, Advisory Board, Australian Section of the International Union for the Study of Social Insects (IUSSI), Cairns, 2014.

Ex-officio Member, National Committee, International Union of Biological Sciences (IUBS), 2012-2015.

#### Prof. Meheboob Alam

Visiting Professorship Award (2013), by Yukawa Institute for Theoretical Physics, Kyoto University, Japan

#### Dr. Sebastian C. Peter

Memberships – ACS, CRSI, ASM, MRSI, IUC

#### **EDITORIAL BOARDS**

#### Dr. Jayanta Haldar

Editorial Board Member of the Journal 'Microbial Pathogenesis', published by Elsevier

#### Dr. Ranjan Datta

Editorial board member of 'Journal of Solid State Physics' published by Hindawi Publishing Corporation

#### Dr. Kanishka Biswas,

*Editorial Board Member* of the Journal 'Materials Science in Semiconductor Processing', published by Elsevier.

#### **Prof. N. Satyamurthy**

Reappointed as Editor, European Journal of Physics D (2013-2015).

#### **FELLOWSHIPS**

#### Prof. P Rama Rao

Fellowship of National Academy of Engineering, USA

#### Prof. K B Sinha

Elected as Emeritus Scientist of Indian Statistical Institute, Kolkata

#### Prof. Shobhana Narasimhan

Indo-Australia Senior Scientist Visiting Fellowship for the year 2012-2013 by INSA.

#### Prof. G. U. Kulkarni

Sheikh Saqr Senior Fellow, 2012

#### Prof. Chandrabhas Narayana

Fellow of the NASI, Allahabad.

#### Prof. S Balasubramanian

Fellow of Indian Academy of Sciences, Bangalore, 2012

#### Prof. Swapan K. Pati

DST J C Bose Fellowship from DST, Govt. of India (2013-2018).

#### Prof. Vijay Kumar Sharma

Fellow of Indian Academy of Sciences, Bangalore, 2012

Fellow of INSA, New Delhi

#### Prof. Umesh Waghmare

DSTJC Bose Fellowship

#### Prof. Tapas Kumar Maji

TWAS Young Affiliateship, 2012-2017 Sheikh Saqr Fellow, 2012

#### Prof. Ganesh Subramanian

2012-2013 Fulbright-Nehru Fellowship for Senior Researchers

### Dr. Ranjan Datta

 $\label{eq:solution} Associate of Indian\, Academy\, of\, Sciences$ 

#### Dr. Ravi Manjithaya

DBT Welcome Trust Fellowship

## FINANCIAL STATEMENTS



Name	:	JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Address	:	JAKKUR POST, BANGALORE - 560 064
Year Ended	:	31ST MARCH 2013
Assessment Year	:	2013-14

# AUDITOR'S REPORT TO THE MEMBERS OF THE GOVERNING BODY OF JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

We have audited the accompanying financial statements of Jawaharlal Nehru Centre For Advanced Scientific Research ("The JNCASR") which comprise the Balance Sheet as at March 31,2013 and the Income and Expenditure account for the year ended on that date, and a summary of significant accounting policies and other explanatory information annexed there to.

#### Management's responsibility for the financial statements

Management is responsible for the preparation of these financial statements that give a true and fair view of the financial position and financial performance and drawn up in prescribed forms as suggested by Department of Science & Technology of Government of India and are in conformity with the generally accepted accounting principles in India. This responsibility includes the design, implementation and maintenance of internal control relevant to preparation and presentation of the financial statements that give a true and fair view and are free from material misstatement whether due to fraud or error.

#### Auditor's responsibility

Our responsibility is to express an opinion on these financial statements based on our audit. We conducted our audit in accordance with auditing standards generally accepted in India. Those standards require that we comply with the ethical requirements and plan and perform the audit to obtain reasonable assurance about whether the financial statements are free of material misstatement.

An audit involves performing procedures to obtain audit evidence about the amounts and disclosures in the financial statements. The procedure selected depends on the auditor's judgment including the assessments of risks of material misstatement of the financial statements, whether due to fraud or error. In making those risk assessments, the auditor considers internal controls relevant to the JNCASR's preparation and fair presentation of the financial statements in order to design audit procedures that are appropriate in the circumstances. An audit also includes assessing the accounting principles used and significant estimates made by management as well as evaluating the overall financial statements presentation. We believe that the audit evidence we have obtained is sufficient and appropriate to provide a basis for our audit opinion

#### Opinion

In our opinion and to the best of our information and according to the explanations given to us, the financial statements have been drawn up in prescribed forms under the Department of Science & Technology of Government of India, and are in conformity with the generally accepted accounting principles in India and give a true and fair view Subject to Notes forming part of the accounts and our comments & observations:

- i) In the case of Balance Sheet, of the state of affairs of the entity as at March 31, 2013, and
- ii) In the case of Income and expenditure account, of the excess of expenditure over the income for the year ended on that date.

#### Report on other legal and regulatory requirements

1. We have obtained all the information and explanations, which to the best of our knowledge and belief were necessary for the purpose of our audit.

2. In our opinion proper books of accounts as required by law have been kept by Jawaharlal Nehru Centre for Advanced Scientific Research so for as it appears from our examination of those books.

3. The Balance Sheet, Income and Expenditure Account and Receipts and Payment account dealt with by this report are in agreement with the books of account.

4. The Balance Sheet and Income and Expenditure Account dealt with by this report are prepared in accordance with the Accounting Standards issued by the Institute of Chartered Accountants of India subject to the following observations:

a) Non-Provisions of accrued liability in respect of leave encashment which is not in conformity with the Accounting, Standard 15 [Accounting for retirement benefits in the financial statements of Employers] issued by the Institute of Chartered Accountants of India. [Refer Note No. 3 of Schedule No. 24]

b) The amount spent on acquisition of fixed assets has been deducted from the total grants/ subsidies received in the Income & Expenditure account. This is not in conformity with the Accounting Standard – 5 issued by the Institute Of Chartered Accountants of India. It has been explained that this format has been consistently used to present the accounts before the authority who grant the funds.

for P V PRABHU & CO Chartered Accountants

> Sd/-(NAGARAJA) Partner M No. 205345

Place : Bangalore Date : 16.09.2013

### JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH BALANCE SHEET AS AT 31st MARCH 2013

Description		Schedule	Current Year	Previous Year
			2012-13	2011-12
			Rs.	Rs.
LIABILITIES				
Corpus/Capital Fund		1	1,948,737,679.32	1,748,078,797.32
Reserves & Surpluses		2	(22,611,981.80)	36,041,572.19
Earmarked and Endowment Funds		3	253,237,801.82	218,031,724.82
Secured loans and Borrowings		4	-	-
Unsecured loans and Borrowings		5	-	-
Deferred Credit Liabilities		6	-	-
Current Liabilities and Provisions		7	38,401,186.43	29,029,543.04
Other funds-Cluster Studies			39,541.00	39,541.00
Scheme Balances			235,334,009.46	258,230,931.46
	Total		2,453,138,236.23	2,289,452,109.83
ASSETS				
Fixed Assets ( gross )		8	1,948,737,679.32	1,748,078,797.32
Investments-Endowment Funds		9	247,984,117.00	265,447,196.00
Investment - Others		10	-	-
Current Assets, Loans, Advances etc.		11	256,416,439.91	275,926,116.51
	Total		2,453,138,236.23	2,289,452,109.83
Significant accounting policies		24		
Contingent Liabilities & Notes on Accounts		25		

Schedule 1 to 25 form integral part of Accounts

For Jawaharlal Nehru for Advanced Scientific Research

This is the Balance sheet referred to in our report of even date.

**for P V PRABHU & CO** Chartered Accountants

Sd/-(NAGARAJA) Partner M No. 205345 ICAI. F.R. No. 050121S Sd/-Prof. M.R.S. Rao President Sd/-R.S. Gururaj Accounts Officer

### JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH INCOME AND EXPENDITURE ACCOUNT FOR THE YEAR ENDED 31 MARCH 2013

Description		Schedule	Current Year	Previous year
		No	2012-13	2011-12
Income			Rs.	Rs.
Income from services		12	0.00	0.00
Grants/Subsidies received		13	512,800,000.00	532,124,049.00
			512,800,000.00	532,124,049.00
Less: Extent of fixed assests procured			200,733,882.00	191,507,778.78
			312,066,118.00	340,616,270.22
Add:Proceeds of sale of fixed assets			75,000.00	1,750,543.00
			312,141,118.00	342,366,813.22
Income from Fees/Subscriptions etc		14	1,582,050.00	1,370,677.00
Income from investments		15	0.00	0.00
Royalty Income, Publication, Licence fee etc		16	2,985,697.05	1,133,297.69
Interest earned		17	7,207,828.00	6,549,486.00
Other income		18	44,389,619.21	37,595,352.97
Increase/decrease in stocks		19	0.00	0.00
	Total		368,306,312.26	389,015,626.88
<b>n</b>				
Expenditure		20		
Establishment expenses		20	202,993,769.00	183,487,959.00
Other administrative expenses		21	203,522,861.25	157,781,920.03
Expenditure on Grants, Subsidies etc		22	0.00	0.00
Interest & bank charges	<b>m</b> . 1	23	154,192.00	45,791.00
	lotal		406,670,822.25	341,315,670.03
P			20.264 500.00	
Excess of income over expenditure			-38,364,509.99	47,699,956.85
balance brought forward			36,041,572.19	3,341,615.34
Transformed to Cormus Fund Assount			-2,322,937.80	51,041,572.19
Palanas appried to Palanas aboat			20,289,044.00	15,000,000.00
Balance carried to Balance sneet			(22,011,901.60)	36,041,572.19
Significant accounting policies (Enclosed)		24		
Contingent Liabilities & Notes on Accounts		25		

Schedule 1 to 25 form integral part of Accounts

For Jawaharlal Nehru for Advanced Scientific Research

This is the Income & Expenditure Account referred to in our report of even date.

**for P V PRABHU & CO** Chartered Accountants

Sd/-(NAGARAJA) Partner M No. 205345 ICAI. F.R. No. 050121S

Place : Bangalore Date : 16.09.2013 Sd/-Prof. M.R.S. Rao President Sd/-R.S. Gururaj Accounts Officer

**RECEIPTS AND PAYMENT ACCOUNT FOR THE YEAR ENDED 31.03.2013** JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

OPENING BALANCES & RECEIPTS	2012-13 Rs Ps	2011-12 Rs Ps	PAYMENTS & CLOSING BALANCES	2012-13 Rs Ps	2011-12 Rs Ps
<u>L. Opening Balances:</u> a. Cash in hand & Imprest at centre	221,661.00	713,613.00	<mark>I. Expenses :</mark> a.Establishment Expenses h.A.Aministratius Exponses	202,993,769.00 203,522.861.25	183,487,959.00 157 781 920 03
b. Bank balances: In Savings Bank Accounts			c.Expenditure of endowments	2,470,822.00 408,987,452.25	2,445,760.00 343,715,639.03
At Canara bank At Union Bank of India A+ SPI	7,270,018.65 161,751.00 90,001,00	22,769,251.69 155,663.00	<u>II. Payment made against funds</u> for various projects :	0.00	0.00
ALSBI In Descrit Assessed	00,701,00	486,759.00	III. Investments and Deposits made :	0.00	0.00
At IDBI bank At IDBI bank At HDFC trust At GOI Bonds(SHCIL & SBI) At Canara Bank	47,005,500.00 0.00 217,408,000.00	34,325,000.00 11,700,000.00 124 388 000 00	<u>IV. Expenditure on Fixed assets and</u> <u>Capital Work-in-progress :</u> a. Purchase of fixed assets	200,733,882.00	191,507,778.78
	272,147,831.65	194,538,286.69			
II. Grants Received: From DST-Grant in aid	490,200,000.00	532,000,000.00	<u>V. Refund of surplus money/Loans :</u>	0.00	0.00
From Govt agencies	16,600,000.00	0.00	<u>VI. Finance charges (Bank charges) :</u>	154,192.00	45,791.00
From other agencies On behalf of Endowments	6,000,000.00 2,366,370.00	124,049.00 12,957,248.00			
	515,166,370.00	545,081,297.00			
<u>III. Income on Investments from:</u> A. Interest on FD's:					
a.From Earmarked/Endowment Funds b.From Own funds	14,184,564.00 4,499,757.00	16,863,067.10 3.083.929.00			
IV. Interest received:	18,684,321.00	19,946,996.10			
a. On Bank S.B A/c	2,708,071.00	2,431,861.00			
Balance Carried Forward	808,706,593.65	761,998,440.79	Balance Carried Forward	609,875,526.25	535,269,208.81

Contd....

(contd.) **RECEIPTS AND PAYMENT ACCOUNT FOR THE YEAR ENDED 31.03.2013** JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

OPENING BALANCES & RECEIPTS	2012-13	2011-12	PAYMENTS & CLOSING BALANCES	2012-13	2011-12
	Rs Ps	Rs Ps		Rs Ps	Rs Ps
Balance Brought Forward	808,706,593.65	761,998,440.79	Balance Brought Forward	609,875,526.25	535,269,208.81
<u>V. Other Income :</u> a.Rovalty	2,904,764.05	789,456.69	<u>VII. Other payments :</u> Earmest monev denostir returned	0.00	514,840.00
b.Licence Fee	80,933.00	343,841.00	Staff advances	0.00	1,301,199.00
c.Collections from Visitors, Guest room etc	4,082,132.00	2,786,860.00	Caution money deposit returned	0.00	0.00
d. from fee, subscription etc	1,582,050.00	1,370,677.00	TDS on interest	1,558,263.00	0.00
e. CSIR fellowships,SRFP		01 000 217 10	Other advances given	0.00	04./08/126,0
reimbersements f. Overhead recoveries	23,561,441.00 16.000.000.00	21,417,220.00	Payment to sundry creditors	0.00	U.UU
g. From services	0.00	0.00		1,558,263.00	8,337,846.40
h.From others	746,046.21	891,272.97			
	48,957,366.26	40,099,327.66			
			<u>VIII. Closing Balances</u> :		
			a. Cash in hand & Imprest at centre	68,826.00	221,661.00
			b. Bank balances:		
<u>VI. Amount borrowed</u> :	0.00	0.00	<u>In savings bank accounts :</u>		
			Canara Bank	8,615,603.05	7,270,018.65
VII. Other receipts :			Union Bank of India	168,304.00	161,751.00
From disposal of fixed assets	75,000.00	1,750,543.00	State Bank of India	1,729,686.00	80,901.00
Income tax refunds	0.00	1,389,862.00	In deposit accounts :		
From Sundry creditors	8,851,628.39	10,516,713.41	At Canara Bank	103,908,000.00	217,408,000.00
Other advances recovered	1,007,995.00		At SHCIL	61,500,000.00	
Earnest money received	11,110.00	0.00	At HDFC Trust	80,705,500.00	47,005,500.00
Recoveries from current assets	520,015.00	0.00			
	10,465,748.39	13,657,118.41		256,695,919.05	272,147,831.65
TOTAL	868,129,708.30	815,754,886.86	TOTAL	868,129,708.30	815,754,886.86

This is the Receipts and payment account referred to in our report of even date.

ed to in our report of even da for P V PRABHU & CO Chartered Accountants

For Jawaharlal Nehru for Advanced

Scientific Research

Sd/-(NAGARAJA) Partner M NO. 205345 ICALF.R.No.050121S Place: Bangalore, Dated: 16.09.2013

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Sd/-R.S.Gururaj Accounts Officer

Sd/-Prof.M.R.S.Rao President

**ANNUAL REPORT 2012-13** 

Particulars	Rs.	Rs.	Particulars	Rs.	Rs.
CONTRIBUTORY PROVIDENT FUND SUBSCRIPTION :			INVESTMENT OF FUNDS: Investments in :		
Opening Balance	E 012 011 00	39,005,634.00	Government of India 8 % Bonds ( SHCIL)	18,500,000.00	73,100,000.00
Loan coupset puotes received during the year Loan repayments Interest on subscriptions	3,038,390.00 3,530.258.00	12 481 459 00	Fixed Deposits at Canara Bank Fixed Denosit at HDFC	19,100,000.00 35 500 000 00	
Less: Loans granted during the year	3,790,415.00	51,487,093.00	Closing Cash and Bank Balance :		
Less: Amount transferred to NPS Less: Withdrawals on retirement/death	667,611.00	4,458,026.00	<u>Cash at Bank :</u>		
Closing Balance		47,029,067.00	SB A/C No.17513 Canara Bank,IISc branch		3,315,804.87
CONTRIBUTION Opening balance		30,275,367.00	TDS GOI Bonds ( 2012-13 ) receivable		148,000.00
Add : Contribution during the year Interest on total contributions	2,656,881.00 2.658.759.00	5 315 640 00	TDS GOI Bonds ( previous year ) receivable		586,492.00
Less: navments during the vear	311,630,00	35,591,007.00	Due to be remitted to bank on account of short navment during 2007 08		00.07.1
Closing Balance		35,279,377.00			00'6 / T
NEW PENSION SCHEME			Cheque related to March 2013 issued but realised on 02.04.2013		969.331.00
SUBSCRIPTION			Subscription relating to Nov 2012 not paid		497,565.00
opening balance Add : Transfer from CPF		1,039,922.00			
Add :Subscriptions received during the year Interest on subscriptions	475,350.00 166.460.00	641.810.00			
Less : Transfer to NSDL on A/c of NPS		7,681,732.00			
Closing Balance		246,984.00			
CONTRIBUTION Onening halance		6 100 570 00	<u>Accrued interest on Deposits</u> : On Fived denosite with Canara Bank	1	
Add : Contribution during the year	475,350.00				1,134,270.00
	144,904.00	620,314.00 7.029.893.00			
Less : Transfer to NSDL on A/c of NPS Closing Balance		6,810,463.00 219,430.00	Balance deficit		2,963,216.13
Total		82,774,858.00	Total		82.774.858.00
		for Jawaharla	Nehru Centre for Advanced Scientific Researc	Ч	
for P V PRABHU & CO Chartered Accountants				54 / <sup>-</sup>	
Cilai lei du ducumitante				- /nc	

**President**, **JNCASR** Prof.M.R.S.Rao -/pS

Place : Bangalore, Dated: 16.09.2013 M NO. 205345 Sd/-(NAGARAJA) Partner

R.S.Gururaj Accounts Officer -/pS

Description	2012-13	2011-12
-	Rs. Ps.	Rs. Ps.
SCHEDULE 1- Capital Fund:		
Balance as at the beginning of the year	1,748,078,797.32	1,558,321,561.54
-	1,748,078,797.32	1,558,321,561.54
Less : Depreciation up to the end of previous year	436,659,498.28	366,473,463.28
Add : Addition to Fixed Assets during current year	<b>1,311,419,299.04</b> 200,733,882.00	<b>1,191,848,098.26</b> 191,507,778.78
l f	1,512,153,181.04	1,383,355,877.04
Less : Deletion to Fixed Assets during Current Year	75,000.00	1,750,543.00
Less : Depreciation for the current year	1,512,078,181.04	<b>1,381,605,334.04</b> 70 186 035 00
	79,301,520.00 1 <b>432 776 661 04</b>	1 311 419 299 04
Add : Depreciation Reserve per contra	515,961,018.28	436,659,498.28
TOTAL	1,948,737,679.32	1,748,078,797.32
SCHEDULE 2- Reserves And Surpluses:		
General Reserve:		
Surplus In Income and expenditure Account	-22,611,981.80	36,041,572.19
F F		
SCHEDULE 3- Earmarked / Endowment Funds:		
A : Infrastructure Corpus Fund		
Opening Balance	155,909,088.64	128,460,673.54
Additions during the year	20,289,044.00	15,000,000.00
Funds-Income from Investments made	11,889,508.00	12,448,415.10
Total : Infrastructure Corpus fund	188,087,640.64	155,909,088.64
B : Other funds		
Opening Balance of the Funds	62,122,636.18	53,253,044.18
Add : Additions :		
Funds/Donations/Grants/Royalties	2,366,370.00	7,516,200.00
Funds-Income from Investments made	3.131.977.00	3,799,152.00
	67.620.983.18	64.568.396.18
<b>Less :</b> Funds-utilisation/Expenditure incurred	2.470.822.00	2,445,760,00
Total : Other Funds	65,150,161.18	62.122.636.18
Grand Total - Infrastructure Corpus and Other Funds	253,237,801.82	218,031,724.82
SCHEDULE 4-Secured Loans And Borrowings:	-	-
SCHEDULE 5-Unsecured Loans And Borrowings:	-	-
5		
SCHEDULE 6-Deferred Credit Liabilities:	-	-
SCHEDULE 7- Current liabilities and provisions:		
Sundry Creditors EMD	1 662 004 00	1,141,989.00
Sundry Creditors for others	36.739.182.43	27,887,554.04
TOTAL	38.401.186.43	29.029.543.04

Description		2012-13	2011-12
SCHEDULE 8- FIXED ASSETS		Rs. Ps.	Rs. Ps.
Land - Free Hold		17,715,351.00	17,715,351.00
Buildings :			
General		87,833,491.26	81,638,128.26
Hostel Building		15,660,055.00	15,660,055.00
New Lab Building - AMRL		25,930,339.00	25,930,339.00
Animal House		6,787,344.00	6,787,344.00
Staff Housing		4,319,353.00	4,319,353.00
ETU Building		3,091,348.00	3,091,348.00
Engineering Mechanics Unit Block		7,426,272.00	7,426,272.00
Other buildings like extn to Hostel, College etc.,		11,883,626.00	11,883,626.00
Nano Science Block		7,042,909.00	7,042,909.00
Extensions to Pauling Building - Biology Block		4,766,109.00	4,766,109.00
Dining Hall & Kitchen Block		12,404,330.00	12,404,330.00
Radio Active Lab		203,233.00	203,233.00
International Centre for Materials Science		48,077,623.00	48,077,623.00
Lecture Hall & Academic Block		9,636,712.00	9,636,712.00
Hostel Phase II		19,552,377.00	19,552,377.00
STP Building		291,699.00	291,699.00
Hostel Phase III		27,501,103.00	27,501,103.00
International House		23,142,418.00	23,142,418.00
UNK KAO HAII OF SCIENCE		10,186,569.00	10,186,569.00
Extensions to HIV lab		1,010,005.00	1,016,085.00
Animal Hausa Additional Plack		742,032.00	742,632.00
Annina House - Auditorial Diock		3 659 034 00	0,292,032.00
Child Care Contro		728 827 00	729 927 00
Now Biology Lab		25 934 842 00	25,00,635,00
Hostel Phase IV		19 424 005 00	19 424 005 00
SCADA - DG Room		240 660 00	240 660 00
President's Residence		7 080 951 00	4 457 440 00
Visiting Students Hostel		32.137.685.00	25 451 063 00
Health Centre		3.243.422.00	3 049 882 00
Nano Institute. Shivananura		3.709.242.00	3.364.466.00
EOBU Lab block		8.540.395.00	-
Post-Doc Housing-Srirampuram		1.300.000.00	-
Materials Science Lab Block		29.218.163.00	2.980.155.00
		471,005,485.26	418,819,199.26
Infrastructure Facilities:			
Roads, Streetlights, Drainage, partitions etc		89,956,110.32	84,377,350.32
Tubewells and water supply		248,912.00	248,912.00
		90,205,022.32	84,626,262.32
Plant/Machinery/Equipment:			
Scientific Equipments/Plant/Machinery		683,904,888.45	617,526,236.45
ICMS-Laboratory equipments & facilities		183,569,588.00	142,472,753.00
Equipments - Chemistry & Physics of Materials		74,041,456.00	74,041,456.00
		941,515,932.45	834,040,445.45
Others:		0 800 0 800 0	
Vehicles		2,703,373.00	2,018,246.00
Furniture and fixtures		61,286,739.87	53,919,958.87
Office equipment		15,851,946.41	12,220,675.41
Computer/peripherals		67,612,223.00	61,007,190.00
Electrical installations		112,738,560.00	112,738,560.00
Library Books		26,926,539.21	25,566,902.21
Lidrary Journais		133,486,405.80	123,807,031.80
Intensible Accete		420,005,787.29	391,2/8,564.29
Intaligible Assets:		7 690 101 00	1 500 075 00
JUILWALE	TOTAL	1 948 737 670 22	1,598,975.00
Less - Depreciation up to the end of previous year	IUIAL	436 659 498 00	366 473 463 29
Depreciation for the current year		79.301 520 00	70 186 035 00
Written down value of the assets as at the year end		1.432.776.661.32	1.311.419.299.04
Add - depreciation reserve per contra		515,961.018.00	436.659.498.00
чин на констрание и констрание и П	ΓΟΤΑΙ	1,948,737,679.32	1,748.078.797.04
			, , , , , , , , , , , , , , , , , , , ,

Sd/- R .S. Gururaj (Accounts Officer)

Description	2012-13	2011-12
	Rs. Ps.	Rs. Ps.
SCHEDULE 9- Investments - Earmarked/Endowment Funds		
Long Term Deposits		
Final Departs with UDEC Trust		
Court of India 20% Savinge Bonds 2002 [SHCIL & SBI]	80,705,500.00	47,005,500.00
Fixed Denosits with Canara hank	61.500.000.00	0.00
Interest accrued on Fixed Denosits with hanks	1,870,617.00	1,033,696.00
TOTAL	247,984,117.00	265,447,196.00
SCHEDULE 10- Investments - Others		
Short Term Deposits - SCHEMES	-	-
TOTAL	-	-
Schedule 11. Current Assets, Loans, Advances etc.		
(ash & Bank Balances ( Schemes )		
Cash in hand - Schemes Account	55 672 00	11 723 00
Cash at Bank -Schemes - Canara Bank	2 053 282 46	5.937.148.46
Interest accrued on FD	3 225 055 00	3.582.060.00
Fixed deposit with Canara Bank ( Schemes )	230.000.000.00	248,700,000.00
	235,334,009.46	258,230,931.46
Cash & Bank Balances - Centre		
Cash in hand at Centre	38,354.00	166,189.00
Cash at Bank - Canara Bank	8,615,603.05	7,270,018.65
Cash at Bank - Union Bank	168,304.00	161,751.00
Cash at Bank - SBI	1,729,686.00	80,901.00
Imprest balance	30,472.00	55,472.00
	10,582,419.05	7,734,331.65
Loans and Advances		
Advances to staff	644,120.00	1,652,115.00
Other advances & Receivables	7,430,581.40	7,441,691.40
TDS receivable	2,283,370.00	725,107.00
Amount receivable from Income Tax Department	141,940.00	141,940.00
		0.060.052.40
	10,500,011.40	9,960,853.40
TOTAL	250,416,439.91	275,926,116.51

Sd/-R.S.Gururaj Accounts Officer

Description		2012-13	2011-12
		Rs. Ps.	Rs. Ps.
SCHEDULE 12-Income from sales / services		0.00	0.00
		0.00	0.00
SCHEDULE 13-Grants/subsidies :			F22 000 000 00
Grants - DST Grants - From Governement agencies		490,200,000.00	532,000,000.00 0.00
Grants - From other Institutes		6,000,000.00	0.00
Grants - Other international agencies		0.00 512.800.000.00	124,049.00
	TOTAL	512,000,000.00	532,124,049.00
SCHEDULE 14-Income from Fee/Subscriptions etc :		4 500 050 00	1 270 (77 00
income from fee, subscriptions, medical contribution etc.,	TOTAL	1,582,050.00	1,370,677.00
	IUIAL	1,562,050.00	1,3/0,6//.00
SCHEDIHE 15 Income from investments		0.00	0.00
SCHEDOLE 13-Income from investments:		0.00	0.00
SCHEDULE 16-Royalty Income.Publication.Licence fee etc :			
From Royalty		2.904.764.05	789.456.69
Licence fee		80,933.00	343,841.00
	TOTAL	2,985,697.05	1,133,297.69
SCHEDULE 17-Interest earned:			
From Term deposits		4,499,757.00	4,117,625.00
From SB acounts with nationalised banks		2,708,071.00	2,431,861.00
	TOTAL	7,207,828.00	6,549,486.00
SCHEDULE 18-Other income:			
From Visitors house,Guest rooms,Students residense etc,		4,082,132.00	2,786,860.00
CSIR Fellowships, ICMS, SRFP reimbursement etc,.		23,561,441.00	21,417,220.00
Overhead recoveries		16,000,000.00	12,500,000.00
From others( tender fee & other fee collected)		746,046.21	891,272.97
	TOTAL	44,389,619.21	37,595,352.97
SCHEDULE 19 - Increase / Decrease in stock:		-	-

Sd/-

R.S.Gururaj Accounts Officer

Deservice til ser	2012-13	2011-12
Description	Rs. Ps.	Rs. Ps.
SCHEDULE 20- Establishment expenses:		
Salaries & Scholarship to students	144,888,858.00	134,021,801.00
Wages	39,473,208.00	33,517,514.00
Allowances (Medical reimbursements etc.,)	7,003,149.00	8,594,319.00
Bonus	221,240.00	206,069.00
Contribution to CPF	2,656,881.00	2,715,736.00
Contribution to new Pension Sceme	2,941,969.00	1,716,955.00
Contribution to Group Gratuity Scheme	1,500,000.00	1,500,000.00
Leave Encashment Benefits	258,746.00	328,671.00
Retirement & Terminal Benefits	1,128,603.00	0.00
LTC	2,921,115.00	886,894.00
TOTAL	202,993,769.00	183,487,959.00
SCHEDULE 21- Other Administrative expenses		
Electricity & Power	40,922,192.00	25,673,910.00
Water charges	5,565,111.00	5,427,788.00
Insurance	565,663.00	469,859.00
Repairs & Maintenance	38,785,984.00	29,434,199.00
Rents, Rates & Taxes	687,833.00	1,227,280.00
Vehicles Running & Maintenance	7,167,385.00	5,291,803.00
Postage, Telephone & Communication	5,416,472.00	6,182,408.00
Printing & stationery	6,754,251.64	4,812,810.24
Travelling and conveyance	6,627,980.00	7.354.701.00
Expneses on Seminars/workshops/discussion meetings	8,543,600.73	7,319,821.51
Membership & Subscriptions	414,794.00	318,026.00
Fees towards Training etc.,	769,351.00	105,274.04
Professional charges	10,805,498.00	4,937,304.00
Laboratory Consumables	48,776,565.00	38,037,529.60
Frieght Inwards	2,365,412.00	2,592,415.00
Other Consumables	2,334,326.00	539,546.00
Advertisement & Publicity	2,935,832.00	4,191,869.00
Other miscellaneous expenses	2,283,998.38	2,322,192.64
Statutory Audit fee	56,180.00	56,180.00
POBE & POCE prgramme	1,576,978.50	635.863.00
Summer Research Fellowship Programme	533,843.00	919.610.00
Fellowships - Department of Bio-Technology	-	27,262.00
ICMS - Workshops, Schools etc,.	1,050,254.00	2,094,776.00
ICMS - Visitor Programmes (National & International)	735,081.00	281,716.00
ICMS - Recurring Expenses	4,582,181.00	4,456,747.00
ICMS - Scientists & Supporting Staff	3,266,095.00	2,701,825.00
Fellowship & Honorarium to visiting Students & Scientists	-	369,205.00
TOTAL	203,522,861.25	157,781,920.03
SCHEDULE 22-Expenditure on grants, subsidies Etc:	-	-
SCHEDULE 23- Interest and Bank charges:	154,192.00	45,791.00
TOTAL	406,670,822.25	341,315,670.03

### JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

### **SCHEDULE - 24**

#### Accounting Policies:

- 1. The fixed assets are stated at cost. The Centre has identified depreciation on Fixed Assets, and since they are created out of Grant in Aid funds, they have been classified the same in the statement of affairs under Capital Fund and also under Fixed Assets schedule respectively.
- 2. Grants received and utilised for procurement of Fixed Assets have been reduced from the total grants received in the Income and Expenditure Account and the same have been included under the Capital Fund Account.
- 3. The leave encashment to the staff members is accounted as and when it is paid.
- 4. Investments of the Centre are stated at cost.
- 5. The foreign currency transactions are translated at the rates prevailing on the date of transaction.
- 6. Previous years figures have been regrouped and reclassified to read in conformity with the current year's figures.
- 7. The Centre has put in to operation a system whereby the accounting standards with respect to the above are brought in conformity with the mandatory accounting standards recommended by the institute of Chartered Accountants of India.
- 8. Royalty income has been accounted as and when received.
- 9. The Expenditure listed under Schedule 20 as Establishment Expenses include the salaries paid to Faculty, Scientific and Research Personnel. The Expenditure listed under the Schedule 21 as Administrative Expenses include the expenses towards Laboratory Consumables and Seminar/Workshops/Discussion meetings exclusively incurred for Research purposes.
- 10. In respect of fluctuation in foreign currencies on account of procurement of fixed assets are not separately shown. However, capitalized in the value of fixed assets.

for P V PRABHU & CO Chartered Accountants

Sd/-(NAGARAJA) Partner M No. 205345 ICAI. F.R. No. 050121S

Sd/-R.S. Gururaj Accounts Officer Sd/-Prof. M.R.S. Rao President

Place : Bangalore Date : 16.09.2013

### **SCHEDULE - 25**

A. Contingent Liabilities :	2012-13	2011-12
	Rs	Rs
1. Claims against the entity not acknowledged as debts	NIL	NIL
2. Letter of credit outstanding	NIL	NIL
B. Notes on Accounts :		
1. Estimated amount of contracts remaining to		
be executed on capital account and not		
provided for.	NIL	NIL

Sd/-R.S.Gururaj Accounts Officer





DAE - Raja Ramanna Lecture in Physics : Prize lecture - "Novel electronic phenomena at oxide interfaces", by Prof. R.C. Budhani, Director, National Physical Laboratory, 28th September 2012.



The Kannada Book 'NANO PRAPANCHA' has bagged the Awards for Excellence in Publishing from the Federation of Indian Publishers.



Prof. V. Ramalingaswami Memorial Lecture : "Act of observation and cancer biology", speaker : Prof. R.A. Badwe, Director, Tata Memorial Centre, Mumbai, 9th July 2012.



Visit of Delegation from Riken, Japan



The College Chemistry Kit prepared by CNR Rao Hall of Science and Education Technology Unit along with Science Outreach Programme was distributed to more than 100 Pre - University College Teachers



**Q 2000 Modulated Differential Scanning Calorimeter (MDSC)** System installed at Chemistry and Physics of Materials Unit.



Corridor near Lecture Hall, Main Building





JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH, Jakkur, Bangalore - 560 064 Editorial Assistance : Nabonita Guha, Senthil Kumar, Nanda Kumari E, Poornima Hosamani. Tel. : 91 80 22082750 Email : admin@jncasr.ac.in Fax : 91 80 22082766 Web: www.jncasr.ac.in ISSN : 0973 9319