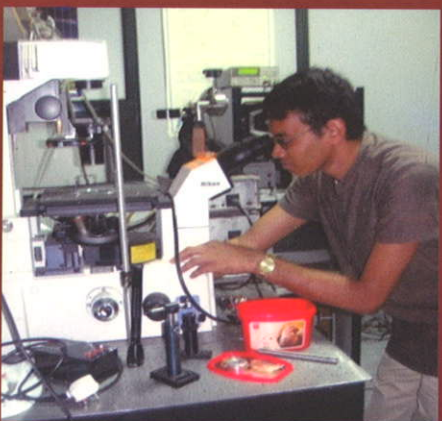
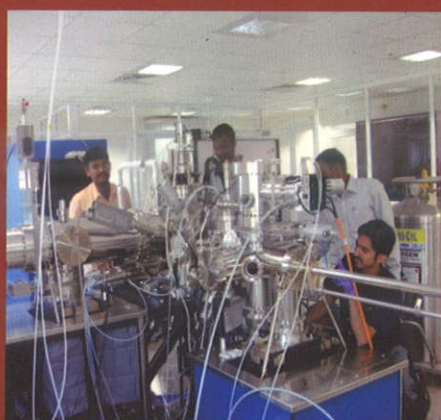
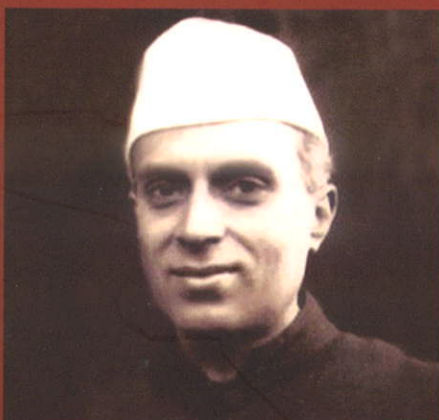
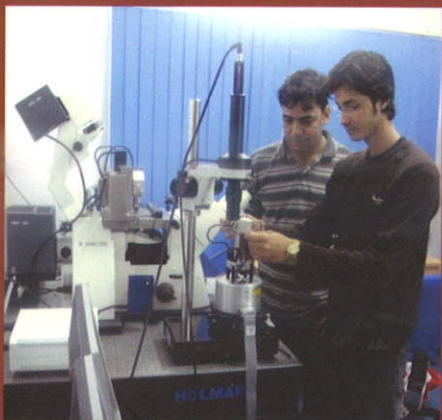
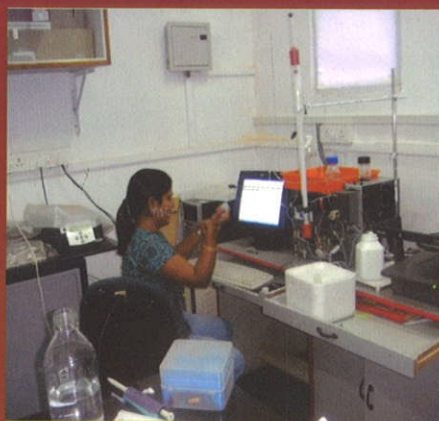
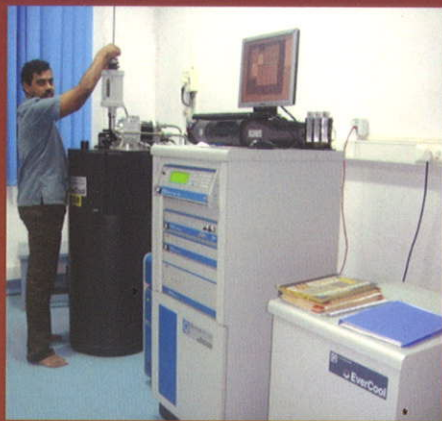


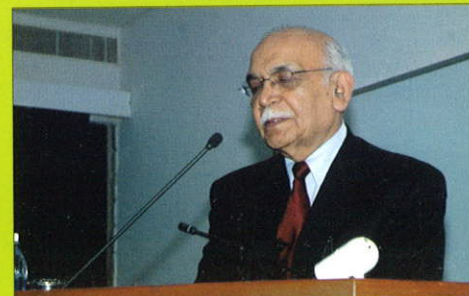


# JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH

JAKKUR, BANGALORE – 560 064



## ANNUAL REPORT 2008-2009



ISSN.0973-9319

# ANNUAL REPORT

2008-2009



**JAWAHARLAL NEHRU CENTRE FOR  
ADVANCED SCIENTIFIC RESEARCH**

**(A Deemed to be University)**

Jakkur, Bangalore – 560 064.

Website: <http://www.jncasr.ac.in>

# CONTENTS

Page No

## The Centre

1. Foreword .....	1
2. Introduction .....	2
3. Objectives .....	3
4. Progress .....	4
5. Highlights of research and other activities .....	5
6. Activities Chart .....	7
7. Organisation Chart .....	8

## The Organisation

1. Council of Management .....	9
2. Finance Committee .....	10
3. Academic Advisory Committee .....	11
4. Faculties .....	11
5. Administration .....	12

## Units, Centres, Computer Laboratory, Library and

Endowed Research Professors .....	13
-----------------------------------	----

## Academic Programmes

1. Academic Activities .....	47
2. Discussion Meetings/Workshops .....	48
3. Colloquia .....	49
4. Endowment Lectures .....	50
5. General Lecture .....	51
6. Lectures delivered at the Annual Faculty Meeting .....	51
7. Seminars .....	51
8. International Conferences/Workshops .....	54

## Extension Activities

1. Summer Research Fellowship Programme .....	55
2. JNC-TWAS-ROCASA- Summer Research Fellowship Programme .....	55
3. Academic Exchange Programme .....	56
4. Project Oriented Biological Education Programme .....	56
5. Project Oriented Chemical Education Programme .....	56
6. Science Outreach Programme .....	57
7. Visiting Fellowships .....	57
8. Intellectual Property .....	57

## Research Programmes

1. Research Areas .....	58
2. Research Facilities .....	60
3. Sponsored Ongoing Research Projects .....	61

## Publications

1. Research Publications of Units .....	65
2. Research Publications of Honorary Faculty/ Endowed Professors .....	81
3. Books authored/edited by Faculty .....	82
4. Books authored/edited by Honorary Faculty .....	82

Awards / Distinctions .....	83
-----------------------------	----

Financial Statements .....	87
----------------------------	----

# The Centre

## Foreword

With great pride the Centre is presenting its Ninteenth Annual Report for the year 2008-2009.

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 University.

There is a steady increase in the number of research students at the Centre pursuing various academic programmes. After obtaining the status of Deemed University, 57 students have obtained Ph D Degrees; 18 students M S (Engg.) and 08 students M S (Int. Ph D) degrees. The academic, research, fellowship and extension programmes have been progressing with a good pace. Many of our faculty colleagues have received various distinctions and honours including the Shanti Swarup Bhatnagar Prize of CSIR and Fellowships of Academies

It was a momentous occasion when Hon'ble Prime Minister, Dr. Manmohan Singh visited our Centre to dedicate the International Centre for Materials Science (ICMS) to the nation and inaugurate the Prof. C. N. R. Rao Hall of Science, on 3<sup>rd</sup> December 2008. This is an important milestone for the Centre.

Since then, the ICMS has made significant progress. The ICMS is taking shape and this is one of the new initiatives to expand our academic activities internationally. The ICMS organized the first International Materials Lecture by Prof. Tobin Marks, Northwestern University, on February 4, 2009. Five International Schools/Workshops were organized with the collaboration of Purdue University, ICMR-UC Santa Barbara and the Swedish Academy of Sciences. Eight seminars were held and ICMS entered into 3 MoUs.

The research activities of the Centre in materials and physical sciences, biology, and engineering mechanics continue to attract global attention and our faculty are being recognized both nationally and internationally. The progress that we are witnessing at the Centre would not have been possible but for dedicated young students pursuing various academic programmes.

The Centre is very active in several science outreach programs and continues to innovate mechanisms to attract, motivate and stimulate young students to expose to the challenges and excitements associated with scientific career. The C N R Rao Hall of Science, being established by the generous donation from Prof C N R Rao Education Foundation will be a forum for several of these programmes.

The performance on the publication front is highly appreciated by the scientific peers. In addition to publishing in high ranking journals, the faculty are also becoming aware of the importance of patenting inventions. The number of patent applications filed from the Centre is speedily increasing as also the process of licensing them to the industry.

Two inventions hit the news item this year. A group from MBGU derived two new sibling human embryonic stem (HES) cell lines from discarded human embryos, the only reported sibling HES cells in the world and the first well-characterised lines from India. Another group from the same Unit identified the gene locus causing hot water epilepsy. This is the first identification of a locus for this unusual neuro-behavioural disease.

We look forward to exciting opportunities for carrying out cutting edge research in materials science in collaboration with international scientists.

Several international collaborations have been initiated, new faculty members have joined and the campus continues to be vibrant with many discussions meetings, colloquia, seminars, workshops, etc.

It is my pleasure to thank all the community members who have supported the cause of science during the aforementioned period. We gratefully acknowledge the support of the Department of Science and Technology in all our endeavours. We hope that the present momentum of scientific achievement is not only maintained but also reach much higher levels in the years to come.

M R S RAO  
President

## INTRODUCTION

The Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), 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 eighteen years old, is creating news regularly in the scientific world with its breakthrough discoveries. The Centre has 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.

☆☆☆



## 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.

☆☆☆

## PROGRESS

The Centre has just completed 19 years encompassing several memorable and exciting moments. In addition to 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, new Unit/Centres like the International Centre for Materials Science, New Chemistry Unit, and the Centre for Computational Materials Science have been added. The new Nanoscience Centre is equipped with the state of the art facilities for advanced research in materials science.

The ICMS has established major scientific facilities like Ultra High Resolution Electron Microscope, Pulse Laser Deposition, Molecular Beam Epitaxy System, X-ray Diffractometer, FE-SEM, Technai, Plasma cleaners, Ion Millers and others. A state of the art conference facility named after Nevill Mott and a meeting room named after J C Bose have been created at ICMS. The I-house located in the same campus provides residential accommodation for the researchers visiting from various parts of the world.

The Centre is equipped with good quality 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.

The generous contributions from the C N R Rao Education Foundation and the Reliance Industries have facilitated the Centre to establish the C N R Rao Hall of Science with an amphitheatre named after Madan Mohan Malavaiya and Laboratories for Education Technology Unit and the Project Oriented Chemistry Education.

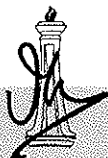
The Centre pursues excellence in research and education in frontier and interdisciplinary areas of science and engineering. It provides a stimulating academic environment to talented and motivated students to pursue scientific research. New Faculty appointments have been made in some research areas.

During the year, 15 Ph D, 8 M S (Engg.) and 2 M S (Int. Ph D) degrees have been awarded. Currently about 154 scholars are pursuing their research career. The research training at the Centre has led to the award of 64 Ph D degrees, 18 M S (Engg.) 19 M S degrees, and one M Sc (by research) degree 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.

The Centre's faculty members have received number of national and international recognitions. Prof CNR Rao, Linus Pauling Research Professor and National Research Professor, has been conferred the Order of Friendship, by the President of Russia (2009), awarded the First International Prize for Materials Science by MRSI (India) (2009), Nikkei Asia Prize For Science, Technology And Innovation from Japan (2008), First Laureate of the 21<sup>st</sup> Khwarizmi International Science Award by the Iranian Research Organization for Science & Technology (2008). Prof Roddam Narasimha has received the Trieste Science Prize of TWAS (2008). Prof Srikanth Sastry has been awarded the Shanti Swarup Bhatnagar Prize and the Sir CV Raman Young Scientist Award. Prof K S Narayan and Prof Umesh Waghmare have been awarded DAE outstanding research investigator award of the Department of Atomic Energy (Govt. of India), 2008-09. Prof Swapan K Pati has been awarded DST Swarnajayanti Fellowship, 2006-07. Prof Tapas Kumar Kundu has been awarded the National Academy of Sciences, Reliance Industries Platinum Jubilee Award for Application Oriented Innovations.

The faculty members of the Centre have published around 233 scientific papers in reputed national and international journals during the year 2008-09, some of them with very high impact factor. Many patent applications were filed for new inventions. Details are provided in a separate section on "Intellectual Property" under "Extension Activities". 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.

The ICMS conducted five International Schools/Workshops with the collaboration of Purdue University, ICMR-UC Santa Barbara and the Swedish Academy of Sciences. Eight seminars were held and ICMS





entered into 3 MoUs. Whereas researchers from leading institutions from USA, Vietnam, Iran, Philippines and Netherlands visited ICMS, the faculty and research scholars from JNC visited prestigious research institutes in Japan, Netherlands, Iran and various other places. 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, 488 completed applications were received and 131 fresh fellowships were awarded. For POCE, 238 applications from 17 states were received and 10 meritorious students from nine states were offered the fellowship. Under POBE, 351 applications were received from different parts of the country and 10 candidates were offered the fellowship. The POCE and POBE students completing their 3-year projects successfully this summer will receive a Diploma (Chemistry and Biology respectively) from JNCASR.

Eight candidates from R & D institutions have been offered Visiting Fellowships for 2008-2009. Out of the four candidates who were offered DST Postdoctoral Fellowships in Nano Science and Technology – 3<sup>rd</sup> series, three have joined and are continuing their fellowship in JNCASR and Indian Institute of Science and one has accepted and yet to join Indian Institute of Science.

Since the beginning of the financial year 2008-09, 32 Discussion Meetings/Workshops were supported, either wholly or partially. About 70 seminars, 16 Fluid Dynamics Colloquia, 9 JNC Colloquia and 5 International Conferences/Workshops/Schools were held. Five Endowment Lectures by eminent scientists were also held during the year.

## HIGHLIGHTS OF RESEARCH AND OTHER ACTIVITIES

### Research

**Chemistry and Physics of Materials Unit** : Newer methods have been developed by Rao and co-workers for large scale synthesis of graphene. Different methods have been employed- pyrolysis of camphor under reducing conditions, exfoliation of graphitic oxide, conversion of nanodiamond and arc evaporation of SiC. Developments in the fabrication and modeling of field effect transistors and solar cells based on organic and nano systems have been accomplished. Consolidated the novel photocurrent-scanning approach to gauge the transport length scales; more specifically electron vs. hole transport length scales – an important parameter in ambipolar devices such as solar cells and FETs. Oxygen nonstoichiometry on the structure, dielectric and magnetic properties of Bi-Mn-O system has been investigated. Two new phases - orthorhombic and monoclinic  $\text{BiMnO}_3$  - have been identified. The faculty have been involved in several aspects of heteroepitaxy. Adsorption of Ga, Pb and In on Si(111) monitored *insitu* by AES, XPS, LEED and EELS has been carried out and several interesting novel observations have been reported. The anomalous desorption behavior of In from Si(111) and the novel surfaces phases in the Ga/Si(111) 7x7 system have been observed. Systematically designed and synthesized novel microporous metal-organic coordination networks (MOCNs) with potential applications in gas storage ( $\text{H}_2$ ,  $\text{CH}_4$ ,  $\text{CO}_2$  etc). A hierarchically porous bioactive glass of composition 80 mol%  $\text{SiO}_2$  and 15 mol% CaO (MBGH) was synthesised using pluronic P123 and glucose-derived amorphous carbon submicron spheres as templates. The faculty have carried out Brillouin Scattering studies on pyrochlore, double walled nanotubes, hydrogels for drug delivery. High Pressure Raman studies of Zinc Selenides doped with beryllium (0 to 55% doping of Beryllium) and High Pressure Synchrotron studies of Tin Nitride were carried out in Trieste, Italy up to pressure of 25 GPa. Another major activity has been Surface Enhanced Raman Spectroscopy (SERS) for studying protein - drug interactions and diagnostics. Recently, the group has shown the use of SERS to determine the structural variations in small proteins with cationic substitution (Mg) for the first time. They have also demonstrated the sensitivity of detection of RNA up to hundreds of copies (in the case of HIV). The faculty have carried out many studies on synthesis of new nanomaterials, functionalisation and property measurements. Another activity in nanoscience is related to direct write lithography to generate nanopatterns of nanomaterials. This is being achieved using high resolution electron beam methods as well as soft lithography. Several devices containing nanowires as active elements have been fabricated. They have carried out extensive work using computer simulations. A dilute aqueous solution of the salt, 1-n-butyl,3-methylimidazolium hexafluorophosphate, has been studied using molecular dynamics simulations to investigate the effect of ions on water and vice versa.

**New Chemistry Unit** : The research activities in this unit are at the interface of chemistry and biology. Currently, this unit is involved in three different research projects which are interdependent and complementary. First chiral unnatural amino acids with metal binding properties (metal binding ligands) will be synthesized. The underlying theme of research in this unit lies at the interface between synthetic efforts on small molecules/polymers and macroscopic properties at the materials level, developing a macro-organic approach to chemistry. Currently, the Unit is working on the design of self-assembled functional systems from chromophores or p-conjugated oligomers, which are the key ingredients in the integration of electronic components for nano-sized electronics. Another focus will be on the design of supramolecular polymeric materials that are capable of sensing and reversible switching in response to external stimuli (stimuli responsive polymers).

**Education Technology Unit** had taken up the Hindi translation and production of the *Learning Science* series (four parts) both as CD-ROMs and books. The work on the translation, development of the CD-ROM and design and formatting for the print-ready copies of the books is being done simultaneously. ETU has organised science popularization programs for school children and teachers in collaboration with many institutes across the country. The programme '*Learning Science*' is organised by JNCASR in association with different institutes for students and teachers from various schools. In the program on Project Oriented Chemical Education, for undergraduate college students, a multimedia presentation from the CD-ROM '*Understanding Chemistry*' was presented by the Unit in May-June 2008. The science popularisation program "*Vignyana Kaliyona*" in Kannada was organized by Karnataka Rajya Vijnana Parishat at JCBM College Sringeri. The program called 'Nanoworld' was conducted at a few places.



In **Engineering Mechanics Unit**, it has been established that the emergence of shear-banding instabilities (for perturbations having no variation along the streamwise direction), that lead to shear-band formation along the gradient direction, depends crucially on the choice of the constitutive model. Under Geophysical Fluid Dynamics, the mean flow and the linear stability characteristics of a two-dimensional particulate suspension, driven horizontally via harmonic oscillation, have been analyzed. It is shown that the fluid-particle interaction is responsible for the onset of travelling instabilities in this flow. Spatial stability of supersonic compressible plane Couette flow, having relevance in astrophysical fluid dynamics, has been investigated. Under Computational Fluid Dynamics, a DNS study of the starting plume as a model for cumulus clouds has been initiated. Results from a 2D simulation have been published and a 3D simulation is being carried out on a powerful computing system. An ongoing analytical study focuses on the rheology of suspensions of anisotropic particles. In this regard, the formalism of vector spheroidal harmonics was used to analyze the orientation dynamics of spheroidal particles in shearing flows. A project has been started on the design of wings for aircraft driven by turbo-prop engines and propellers.

**Evolutionary & Organismal Biology Unit** continued its ongoing research in the broad areas of chronobiology, theoretical evolutionary genetics, life-history evolution and population dynamics. Members of the Unit were active in delivering invited talks at major international and national meetings and premier institutions of the country, and also participated in outreach activities aimed at students.

In **Molecular Biology and Genetics Unit**, in *Chromatin Biology Lab*, 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. Research in *Molecular Parasitology Lab* is focused towards understanding metabolism in the malaria parasite *Plasmodium falciparum*. Towards this end the enzymes involved in purine nucleotide metabolism in the parasite are being studied. This laboratory is focused towards understanding metabolism in the malaria parasite *Plasmodium falciparum*. Towards this end the enzymes involved in purine nucleotide metabolism in the parasite are being studied. In *Vascular Biology Lab*, a comparative approach has been made by using embryonic stem cell models, mouse developmental biology and transgenics, and *Drosophila* genetics, to decipher the roles of novel genes expressed early in the cardiovascular and hematopoietic systems. This approach has given useful insight into gene function as well as ontogeny of the heart, blood and blood vessels. Recently two new sibling human embryonic stem cell (hES) lines from discarded embryos have been derived and differentiated to cardiovascular derivatives that can be cultured to purity. These are called BJNh19 and BJNh20 and have been deposited in the UK Stem Cell Bank. *Parasitology Lab* is focusing its efforts on the role of *Plasmodium* kinases in host-pathogen interactions. In *Molecular Virology Lab*, significant progress took place in several projects that are presently active.

In *Human Molecular Genetics Lab*, (a) Discovery of a novel epilepsy locus at chromosome 3q13.3-q21, was followed by a detailed analysis of genes at 3q13.3-21, leading to identification of several patient-specific mutations in the extracellular calcium-sensing receptor (CaSR) gene (Annals of Neurology 2008). (b) Identification of another novel epilepsy locus at chromosome 5q12-q14, is an important finding from the laboratory. This locus, located between markers D5S641 and D5S459, is responsible for an age-related, common idiopathic generalized epilepsy (Human Genetics 2007).

Deafness genetics is another area of research in the laboratory. Studies of 500 families affected with severe-to-profound deafness wherein six deafness-causing genes have been concluded. The researchers in the *Transcription and Disease Lab* have made several original contributions in this area which include the discovery of human transcriptional coactivator PC4 a functional component of Chromatin organization, a Nucleophosmin (NPM1) as a histone chaperone and transcription regulator, hyperacetylation of histones and also NPM1 have been causally linked in the manifestation of oral cancer. They have discovered several inhibitors of Histone acetyltransferases which could serve as a lead reagent to design therapeutic agents and could be also used to study cellular functions of HATs. Most recently, by using carbon nanospheres conjugated to small molecule HAT activator CTPB (discovered by them) have been able to activate the histone acetylation both in cultured cells and in the mice brain. The researchers in *Molecular Mycology Lab* have studied centromeres of a pathogenic yeast, *Candida dubliniensis* and compared centromere sequences with those of a closely-related yeast *Candida albicans*.

The primary focus of the **Theoretical Sciences Unit** has been on understanding phase separation processes in a restricted geometry (slit pore) in which a multi-component mixture is confined while being in the miscibility gap region of the phase diagram. The emphasis has been on liquid mixtures which, compared to solid mixtures, are poorly understood because of the presence of hydrodynamic interactions. In a recent study, a symmetric exclusion process with time-dependent hopping rates was introduced. Using simulations and a perturbation theory, it was shown that if the hopping rates at two neighboring sites of a closed ring vary periodically in time and have a relative phase difference, there is a net DC current which decreases inversely with the system size. In the field of surface alloys, the research group has shown that several combinations of bulk-immiscible metals become miscible when co-deposited on a substrate of intermediate lattice constant. A broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum system were also investigated. In particular, the ground state behavior and low temperature magnetic properties of 2-D Kagome antiferromagnets with inhomogeneous spin sites have been investigated in the presence of vectorial exchange interactions (Dzyaloshinskii-Moriya interactions).

By using NEGF-DFT, finite-sized vanadium-borazine clusters are found to exhibit efficient spin filter properties when coupled to graphene. The influence of sequence on the electronic properties of DNA was studied. With regard to targeted modifications of the DNA structure, two studies, one focusing on the controlled alignment of the metal ions within the double stranded DNA helix, and the other focusing on the use of single strand DNA as scaffolds for transition metal alignment were pursued. Theoretical designing and characterization of novel organic materials like enzene, naphthalene, perylene, ocatthio-circulene, azulene, sumanene etc. were completed. The observations of remarkable charge carrier mobilities in some of those systems and their excellent agreement with experiments have been highly appreciated in many scientific communities. The electronic structure, electronic conduction and gas storage properties of graphene within both manybody and DFT formalism have been studied. The static electric field within inhome developed DMRG code have been implemented and the effect of that on one dimensional insulators was studied. For the first time they have shown the field mediated charge density wave to spin density wave phase transition which is yet to be understood experimentally. Research in the group in the past year has focussed on the following topics: (i) Liquid liquid transition in silicon, (ii) crystal nucleation in supercooled liquid silicon and other systems, (iii) the role of crystal polymorphism in determining glass forming ability, (iv) gelation in model fluids, (v) modeling protein aggregation, (vi) analyzing the role of static and dynamic length scales in glass forming liquids and the analysis of their dimensional dependence. A significant result has been to show that the relationship between dynamical heterogeneity and relaxation times are more complex than previously assumed. It has been shown that the relationship also has very interesting dependence of space dimensionality, showing peculiar behaviour in two dimensions. Interplay of multiple time scales in the lateral charge transport of polymeric semiconductors is being investigated using the model developed by the Unit. A new class of semiconducting carbon nanotubes that (a) contain a line defect consisting of octagonal and pentagonal rings, and (b) can be labeled with fractional numbers of chirality has been predicted. These nanotubes exhibit truly one-dimensional carrier states localized along the line defect.

**International Centre for Materials Science (ICMS):** During the year, the ICMS has established major scientific facilities like Ultra High Resolution Electron Microscope, Pulse Laser Deposition, Molecular Beam Epitaxy System, X-ray Diffractometer, FE-SEM, Technai, Plasma cleaners, Ion Millers and others. Besides many International Schools/Workshops were held with the collaboration of Purdue Univeristy, ICMR-UC Santa Barbara and the Swedish Academy of Sciences. ICMS entered into MoUs with leading institutions and attracted a few visitors from abroad. ICMS organized the first International Materials Lecture by the well known scientist, Prof. Tobin Marks, Northwestern University, on February 4, 2009.

**The Centre for Computational Materials Science (CCMS):** The potential energy of large clusters of ionic liquid (IL) molecules as a function of their size has been investigated using MD simulations. The behaviour of a model room temperature ionic liquid under shear is explored using non-equilibrium molecular dynamics simulations. The computational study of glass forming ability which has lead to an experimental verification of vitrification of germanium. This work is being followed up with a study of the relation between crystal polymorphism and glass forming ability. Modifications to the DNA structure which can be used as efficient scaffolds for DNA based spintronics devices have been suggested. DNA based single



molecular magnets (SMM) have been investigated. Investigated the I-V characteristics in molecular bridges in different regimes (Coulomb blockade as well as strong coupling regimes). Analyzed the effects of competing exchange interactions and lattice dimerizations for a large class of systems including Kagome antiferromagnets, 1-D spin chains and ladder structures.

Under the Visitors Programme, 4 Scientists and 3 students have visited for periods of about a week to 2 months for research / collaborative work with CCMS members during the period under report..

#### **Academic**

During the year, 41 students ( 9 Students for Integrated Ph D, 28 Students for Ph D, and 4 students for MS (Engg.) degree were admitted. Fifteen students were awarded Ph D, 8 students M S (Engg.) and 2 students were awarded M S (Int. Ph D) degree.

#### **Fellowships & Extension Programmes**

Under the Summer Research Fellowships Programme, 131 fellowships were awarded. For the JNC-TWAS-ROCOSA – Summer Research Fellowships programme, a few applications have been received. For the Project Oriented Chemical Education (POCE) Programme, 10 meritorious students from nine states were selected and about 27 undergraduate students attended the programme. The POBE programme has successfully completed three years with 28 students from various institutions in the country undergoing interactive training and for the year 2009, 10 students have been selected. While 8 candidates have been offered Visiting Fellowships for 2008-09, 4 candidates have been offered DST Postdoctoral Fellowship in Nano Science and Technology and 3 have joined and are continuing their fellowship.

#### **Vigilance**

An Orientation Workshop for Vigilance Officers of Sub-Ordinate offices and aided institutions under Department of Science and Technology was arranged on August 6-7, 2008. The Vigilance Awareness Week was celebrated during November 2008 which included a lecture to the community. The Centre informed the services, the initiatives taken for improvement of the system, procedures, complaint handling policy and the other avenues for redressal of grievances etc. All the reports and returns were submitted in time.

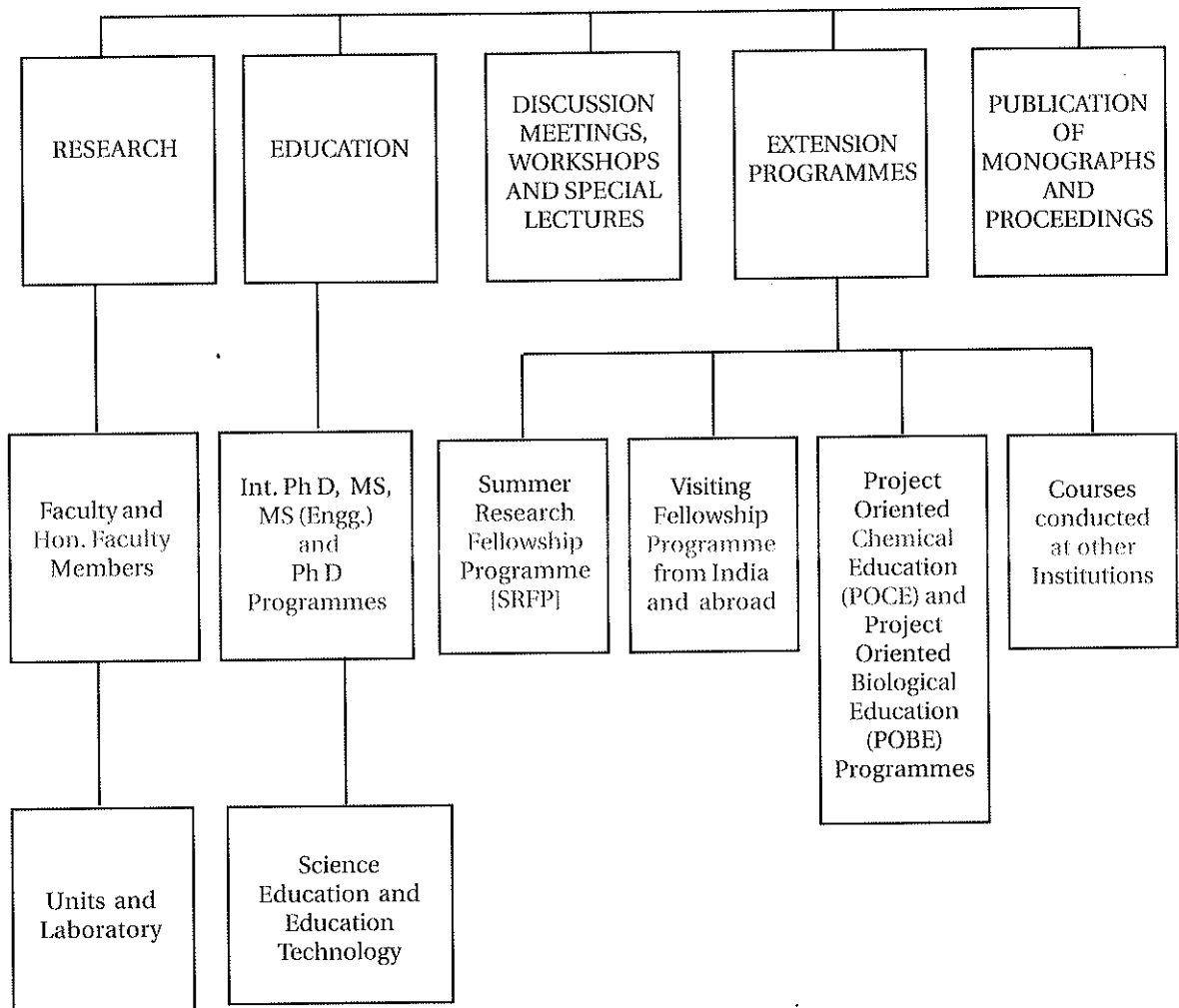
#### **Reservation, Official Language and Implementation of the judgments/orders of the CAT**

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, no cases pertaining to the Centre appeared before the CAT.

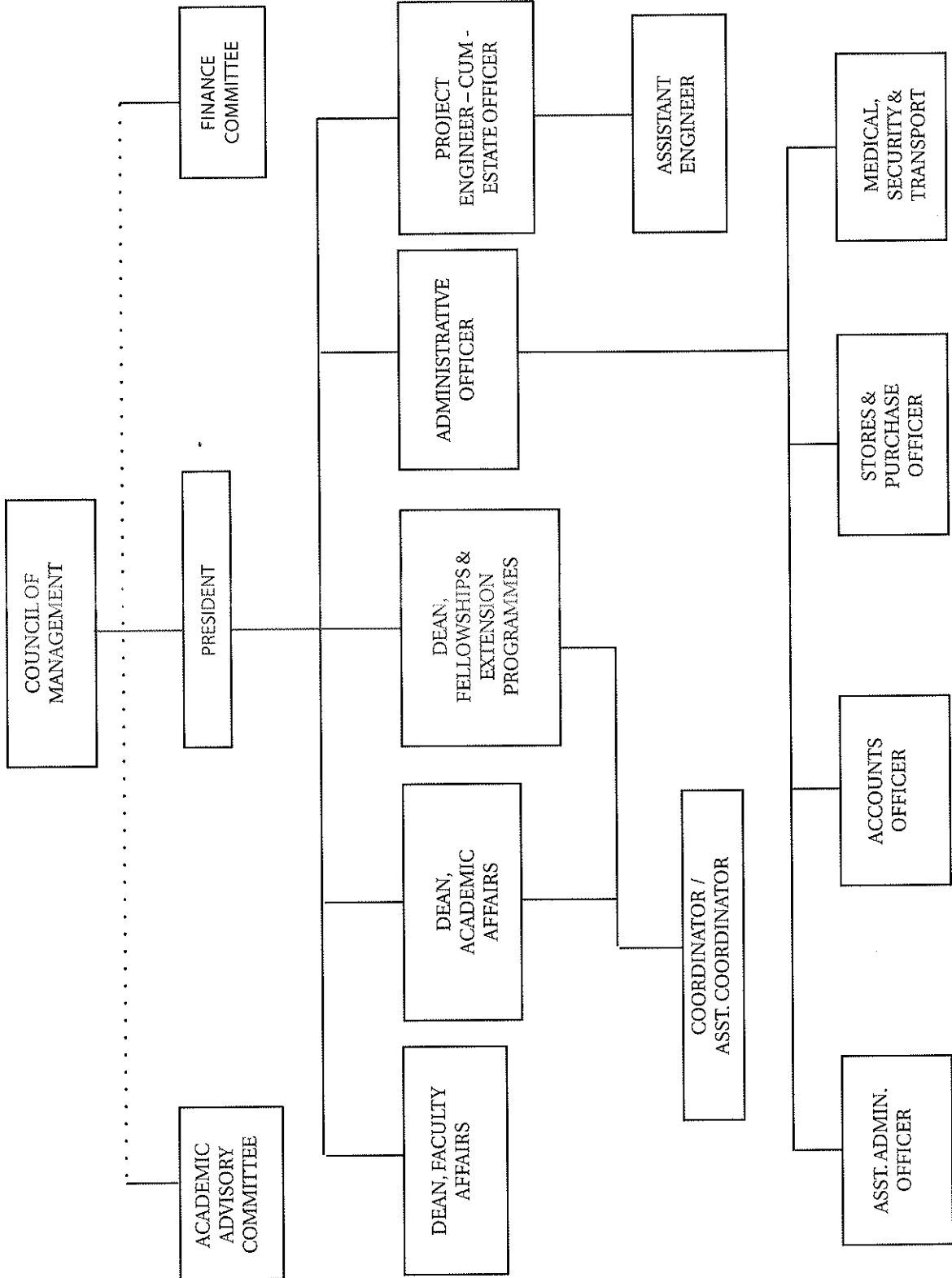
A Complaints Committee for the prohibition of Sexual Harassment of women at work place (Centre) has been constituted.

# ACTIVITIES CHART

## JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH



# ORGANISATION CHART



## THE ORGANISATION

### 1. 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>P Rama Rao</b> ISRO Brahm Prakash Distinguished Professor, ARCI, Hyderabad	Chairman
<b>M R S Rao</b> President, JNCASR	Member
<b>T Ramasami</b> Secretary Department of Science and Technology New Delhi	Member
<b>C N R Rao</b> Linus Pauling Research Professor JNCASR	Member
<b>S K Joshi</b> National Physical Laboratory New Delhi	Member
<b>K P Pandian</b> Joint Secretary & Financial Adviser Department of Science and Technology New Delhi	Member
<b>P Balaram</b> Director Indian Institute of Science, Bangalore	Member
<b>Sinha B</b> Director, VECC & Saha Institute of Nuclear Physics Kolkata	Member
<b>S Chandrasekaran</b> Indian Institute of Science Bangalore	Member
<b>A N Jayachandra</b> Administrative Officer, JNCASR	Secretary





## 2. 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>M R S Rao</b> President, JNCASR	Chairman
<b>C N R Rao</b> Linus Pauling Research Professor JNCASR	Member
<b>K P Pandian</b> Joint Secretary & Financial Adviser Department of Science and Technology New Delhi	Member
<b>S Chandrasekaran</b> Indian Institute of Science Bangalore	Member
<b>Revathi Bedi</b> Finance Officer, JNU New Delhi	Member
<b>R S Gururaj</b> Accounts Officer, JNCASR	Member
<b>A N Jayachandra</b> Administrative Officer, JNCASR	Secretary

### 3. 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>M R S Rao</b> President, JNCASR	Chairman
<b>C N R Rao</b> Linus Pauling Research Professor JNCASR	Member
<b>Chandan Dasgupta</b> IISc., Bangalore	Member
<b>Dipankar Chatterji</b> IISc., Bangalore.	Member
<b>D D Sarma</b> IISc., Bangalore	Member
<b>P Ramachandra Rao</b> Hyderabad	Member
<b>K B Sinha</b> Dean , Faculty Affairs, JNCASR	Member
<b>K VijayRaghavan</b> Director NCBS, Bangalore	Member
<b>K S Narayan</b> Head, Academic Affairs, JNCASR (up to 5.10.2008)	Member
<b>Hemalatha Balaram</b> Dean, Academic Affairs, JNCASR (from 6.10.2008)	
<b>Rama Govindarajan</b> Head, Fellowships & Extension Programmes, JNCASR (up to 5.10.2008)	Member
<b>N Chandrabhas</b> Dean, Fellowships & Extension Programmes, JNCASR (from 6.10.2008)	
<b>A N Jayachandra</b> Administrative Officer, JNCASR	Secretary



## 4. 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 2008 which included lectures by the faculty on the advances made in various research areas. Local faculty meetings were held in August 2008 and February 2009 to review the progress and provide inputs wherever required.

## 5. Administration

<b>President</b> M R S Rao	Ph D (IISc), F A Sc, F N A, F N A Sc, FTWAS
<b>Dean, Faculty Affairs</b> K B Sinha	Ph D (Univ. of Rochester), F A Sc, F N A, FTWAS
<b>Dean, Academic Affairs</b> K S Narayan (up to 5.10.2008) Hemalatha Balaram (from 6.10.2008)	Ph D (Ohio State Univ.), F N A Sc Ph D (IISc), F A Sc
<b>Dean, Fellowships and Extension Programmes</b> Rama Govindarajan (up to 5.10.2008) N Chandrabhas (from 6.10.2008)	Ph D (IISc), F N A Sc Ph D (IISc)
<b>Warden &amp; Student Counsellor</b> Umesh V Waghmare	Ph D (Yale Univ.)
<b>Associate Warden</b> Maneesha S Inamdar	Ph D (TIFR)
<b>Administrative Officer</b> A N Jayachandra	B Com (Mysore Univ.), ICWA (Inter)
<b>Assistant Administrative Officer</b> T S Vishwanath	B Sc (Bangalore Univ.)
<b>Consultant</b> G Jayaram (up to 22.10.2008)	B Com (Bangalore Univ.)
<b>Assistant Coordinator</b> Princy Jaison Pereira	Ph D (Gujarat Univ.)
<b>Accounts Officer</b> R S Gururaj	B.Sc. (Mysore Univ.) M P Ed (Bangalore Univ.)
<b>Stores &amp; Purchase Officer</b> K Bhaskara Rao	M Sc (Hyderabad Univ.), M Phil (Delhi Univ.)

<b>Library-cum-Information Officer</b>	
Nabonita Guha	MLIS (Banaras Hindu Univ.)
<b>Senior P A to President</b>	
A Srinivasan	B A (Hyderabad Univ.)
<b>Project Engineer</b>	
S Chikkappa	B E (Mysore Univ.)
<b>Junior Engineer (Civil)</b>	
Nadiger Nagaraj	DCE
<b>Junior Engineer (Elec.)</b>	
Sujeeth Kumar S	DEE
<b>Chief Medical Officer</b>	
B S Subba Rao	MBBS (Mysore Univ.)
<b>Consulting Lady Medical Officers</b>	
Kavitha Sridhar	MBBS (Bangalore Univ.)
Archana, MLV	MBBS (Bangalore Univ.)
<b>Honorary Medical Officers</b>	
G R Naghabhushan	MBBS (Mysore Univ.), FCCP, FCGP, P G Dip in M&CH
L Sharada	MBBS (DGO (Madras Univ.))
R K Nivedita	MBBS (Mysore Univ.)
C Satish Rao	MBBS (Mysore Univ.)
P K Raghupathy	MBBS (Rajiv Gandhi Univ.)
R Nirmla	MBBS (Dr. MGR Medical Univ.)
<b>Honorary Security Officer</b>	
M R Chandrasekhar	B Sc, LLB (Bangalore Univ.)



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

## 1. Chemistry and Physics of Materials Unit

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

Newer methods have been developed by Rao and coworkers for large scale synthesis of graphene. Different methods have been employed- pyrolysis of camphor under reducing conditions, exfoliation of graphitic oxide, conversion of nanodiamond and arc evaporation of SiC. Thus obtained graphene samples have been functionalized with organic molecules to induce charge transfer thereby altering the electronic structure of graphene. Binding of DNA nucleobases and nucleosides has also been carried out. Graphene has been shown to adsorb gaseous molecules such as hydrogen and carbon dioxide. The uptake with respect to the latter is ~ 38 wt%. Supercapacitors based on graphene as active element have been designed. Liquid-liquid interface has also been used in the preparation of freestanding films of various metal and semiconductor nanostructures. By using fluorine chemistry, solubilization of various nanostructures such as Au and CdSe nanocrystals, single-walled carbon nanotubes and ZnO nanorods in the most nonpolar liquid medium has been made possible. New methods have been developed to separate metallic and semiconducting carbon nanotubes. The mechanical properties of poly(vinyl alcohol) matrix composites incorporating SiC and Al<sub>2</sub>O<sub>3</sub> nanowires have been investigated. A marked increase in the elastic modulus (up to 90%) has been observed even with the addition of a small quantity (0.8 vol%) of nanowires.

Developments in the fabrication and modeling of field effect transistors and solar cells based on organic and nano systems have been accomplished by Narayan and co-workers. They have consolidated the novel photocurrent-scanning approach to gauge the transport length scales; more specifically electron vs. hole transport length scales – an important parameter in ambipolar devices such as solar cells and FETs. The approach is based on photocurrent scanning of a device with asymmetric electrodes and examining the photo-induced current decay outside the overlapping-electrode region (negligible field).

While establishing surface ferromagnetism is universal characteristic of inorganic nanoparticles, Sundaresan and coworkers have found a new way to make the classical ferroelectric material BaTiO<sub>3</sub> as multiferroic by reducing the particle size below 300 nm and forming an intrinsic bulk ferroelectric and surface ferromagnetism. The latter is associated with oxygen vacancy defects as evidenced from positron annihilation studies. Oxygen nonstoichiometry on the structure, dielectric and magnetic properties of Bi-Mn-O system has been investigated. Two new phases orthorhombic and monoclinic BiMnO<sub>3</sub> have been identified. It is found that the stoichiometric BiMnO<sub>3</sub> exhibits canted antiferromagnetic properties rather than ferromagnetism reported for BiMnO<sub>3</sub> system.

Shivaprasad and coworkers have been involved in several aspects of heteroepitaxy. Adsorption of Ga, Pb and In on Si(111) monitored insitu by AES, XPS, LEED and EELS has been carried out and several interesting novel observations have been reported. The anomalous desorption behavior of In from Si(111) and the novel surface phases in the Ga/Si(111) 7x7 system have been observed. We are also initiated collaborations with theorists to understand the formation of the 2<sup>3</sup> x 2<sup>3</sup> In/Si phase and the 2x2 quartet reconstruction of the Ni/Ru(0001) system. This group has now installed a GaN MBE system and a PVD system at ICMS to address materials' issues of GaN, InGaN and AlGaN systems such as epitaxy, doping and material stability. The system consists of insitu RHEED, Ellipsometer, Atomic Absorption, etc., to monitor growth.

Maji and coworkers have systematically designed and synthesized novel microporous metal-organic coordination networks (MOCNs) with potential applications in gas storage (H<sub>2</sub>, CH<sub>4</sub>, CO<sub>2</sub> etc). Some of the porous frameworks exhibit selective sorption of different solvent molecules like H<sub>2</sub>O, MeOH, EtOH, which have industrial applications in separation of different small molecules. We have also fabricated inorganic-

organic bifunctional hybrid nanocomposite using Prussian blue (PB) as an inorganic magnetic core which attached to the lanthanide ions ( $Tb^{III}/Eu^{III}$ ) as a luminescent probe.

Glass ceramics of composition  $CaO-P_2O_5-SiO_2-MO$  ( $M = Na, Mg, etc$ ) are highly bioactive and can be successfully used as a tissue engineering material for bone and tooth reconstruction and substitution because of their ability to form hydroxyapatite (HA) when implanted. A hierarchically porous bioactive glass of composition 80 mol%  $SiO_2$  and 15 mol%  $CaO$  (MBGH) was synthesised by Eswaramoorthy and coworkers using pluoronic P123 and glucose-derived amorphous carbon submicron spheres as templates. While the carbon spheres leave behind pores of 300 nm to a few  $\mu m$  after calcination, the walls of these pores contain orderly arranged mesopores of 3-5 nm orchestrated by the pluoronic polymer. The role of carbon spheres is not only to create pores but also to aid in increased growth rate of hydroxycarbonate apatite in simulated body fluid (SBF). The negatively charged carbon spheres favour the local enrichment of calcium ions and favours the formation of amorphous calcium phosphate around the surface. On calcination, the walls of the macropores contain a crystalline hydroxycarbonate apatite nuclei. MBGH also exhibits an accelerated growth of monoclinic-like apatite in SBF. The in vitro activity has been studied by XRD, FT-IR, FESEM and TEM. This group is active in pursuing studies related to drug delivery. A number of factors that have to be taken into account while developing intracellular drug carriers include optimal hydrophilicity and hydrophobicity which will decide its entry, surface functionalisation which will act as a chemical handle to tag the drug, fluorescent tags for their visualization and finally their cytotoxicity. We are developing 'intracellular carriers that will have no barriers' across the cell membranes and even nuclear membranes. It is of immense interest to develop materials that possess all these qualities in a single step synthesis. These carriers have been used to deliver membrane-impermeable small molecule modulators of histones within the cell nucleus and study their potential therapeutic applications in a number of diseases like cancer, diabetes etc.

Chandrabhas and coworkers have carried out Brillouin Scattering studies on pyrochlore, double walled nanotubes, hydrogels for drug delivery. The group also carried out High Pressure Raman studies of Zinc Selenides doped with beryllium (0 to 55% doping of Beryllium). This was part of the Indo-French project. High pressure synchrotron studies of Tin Nitride was carried out in Trieste, Italy up to pressure of 25 GPa. Another major activity has been Raman (surface enhanced Raman spectroscopy (SERS)) for studying protein - drug interactions and diagnostics. Recently, the group has shown the use of SERS to determine the structural variations in small proteins with cationic substitution (Mg) for the first time. They have also demonstrated the sensitivity of detection of RNA up to hundreds of copies (in the case of HIV).

Kulkarni and coworkers have carried out many studies on synthesis of new nanomaterials, functionalisation and property measurements. Another activity in nanoscience is related to direct write lithography to generate nanopatterns of nanomaterials. This is being achieved using high resolution electron beam methods as well as soft lithography. Several devices containing nanowires as active elements have been fabricated.

Balasubramanian and coworkers have carried out extensive work using computer simulations. A dilute aqueous solution of the salt, 1-n-butyl,3-methylimidazolium hexafluorophosphate, has been studied using molecular dynamics simulations to investigate the effect of ions on water and vice versa. The anion is found to diffuse faster than the cation in the solution, in contrast to observations in the pure ionic liquid. Distributions of pair energies have been employed to identify ion association, and around 13% of the ions were found to exist as pairs. The mean potential energy of water molecules present in the coordination shell of an anion is less than that of water molecules coordinated to a cation. The former kind also exhibit two distinct orientational preferences with respect to the anion. The larger diffusion coefficient of the anion is related to the faster dynamics of water molecules in its hydration layer, as evidenced from the relaxation of their residence time correlation function.

The following are the members of the Unit:

**Chair**

C N R Rao  
(up to 31.10.2008)

Ph D, D Sc, F A Sc, F N A,  
F R S, F T W A S, Hon. F R S C

**G U Kulkarni**

(from 1.11.2008)

Ph D



**Professors**

K S Narayan	Ph D, F N A Sc.
G U Kulkarni	Ph D
S M Shivaprasad	Ph D

**Associate Professors**

S Balasubramanian	Ph D
N Chandrabhas	Ph D
A Sundaresan	Ph D

**Faculty Fellows**

M Eswaramoorthy	Ph D
Tapas Kumar Maji	Ph D

**Technical Officers**

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

**Lab Assistants**

J Anil Kumar (DEE), B S Vasudev (BE), Alla Srinivasa Rao (BE)

**Research Associate**

Navneet Kaur

**Research Associates (P)**

Dattatray J Late, Sundarayya Yanamandra, Vivek Chand SRC

**Application Scientist**

Kiran Ashokrao Kulkarni

**Technical Assistant**

N R Selvi

**R & D Assistants**

Arun Dhumal Rao, Chandrababu P, Gopal K Pradhan, Gurunatha KL, Kavitha G, Madhu C, Mune Gowda A (Jr.), Pradeep J Devadig, Rajashekarayya, Sameer Y Vyasamudri, Satish Shetty, Sonia B, Thirumurugan A.

**Research Students**

Gopal Krushna Pradhan, Reji Thomas, Venkata Prasad Bhat, Manohar Rao NV, Vijay Kumar T, Jyoti Ranjan Sahu, Vengadesh Kumara Mangalam R, Soumya Saswati Sarangi, Rakesh V, Shipra, Dinesh Jagadeesan, Katla Sai Krishna, Monojit Bag, Pranab Mandal, Srinivas Raju G, Gomati A, Partha Pratim Kundu, Prakash Kanoo, Sudip Mohapatra, Radha B, Sabyasachi Mukhopadhyay, Leela Srinivas Panchakarla, Jithesh K, Manoj Kesaria, Subrahmanyam KS, Kalyan Raidongia, Narendra Kurra, Anshuman Jyothi Das, Sandeep Kumar Reddy, Satish Shetty, Venkata Srinu Bhadrani, Jaya Ramulu Kalleboyina, Shruti Badhwar

Arun N, Kumara Ramanatha Datta K, Neenu Varghese, Ramakrishna Matte H S S, Ritu Gupta, Nitesh Kumar, Urmimala Maitra, Nisha Mariam Mammen, Bivas Saha, Soumik Siddhanta, Abhay Kumar Tiwari, Piyush Kumar Chaturbedy, Vini Gautam, Arpan Hazra, Chaitanya Sharma Y SRK, Chidambar Kulkarni, Dileep Krishnan, Gayatri Kumari, Pandeewar M, Rana Saha, Sudeshna Sen, Varun Thakur.

## 2. New Chemistry Unit

The New Chemistry Unit (NCU) has been created by the Centre as part of the 11<sup>th</sup> Five Year Plan under the guidance of Prof. C. N. R. Rao. This unit will work on interdisciplinary aspects of chemical science. The most important areas that the unit will concentrate on would be chemical biology and interfaces of chemical science with materials. Some of the specific areas of research are asymmetric organic synthesis, peptide and protein chemistry, biomaterials, functional organic materials, organic and supramolecular chemistry, theoretical chemistry, carbon and oxide based materials and catalysis.

Two members of the faculty, Dr. Subi Jacob George and Dr. T. Govindaraju, have joined the unit during the academic year 2008-2009. Several faculty members from the other units of the centre are also associated with the unit. The unit is setting up excellent facilities for experimental work as well as computational and theoretical studies. As part of the infrastructure development several new instruments such as a 400 MHz NMR spectrometer, Liquid Chromatography-Mass Spectrometer (LC-MS), High Performance Liquid Chromatography (HPLC), Gas Chromatography-Mass Spectrometer (GC-MS), Gel Permeation Chromatography (GPC), Peptide Synthesizer, Digital Polarimeter and Elemental Analyzer (CHNS) are being acquired.

During the academic year 2008-2009 mid-term admission, three students have joined the unit under Ph D programme. New courses have been designed for the MS-Ph D (POCE), Integrated Ph D and Ph D in chemistry.

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

The underlying theme of research in this unit lies at the interface between synthetic efforts on small molecules/polymers and macroscopic properties at the materials level, developing a macro-organic approach to chemistry. Currently the Unit is working on the design of self-assembled functional systems from chromophores or p-conjugated oligomers, which are the key ingredients in the integration of electronic components for nano-sized electronics. Special attention will be given to the synthesis of multi-component self-assembled fibers with increased complexity and well-defined dimensions. Another focus will be on the design of supramolecular polymeric materials that are capable of sensing and reversible switching in response to external stimuli (stimuli responsive polymers). The Unit wishes to design new functional organic materials, aiming at 'Chiral Nanotechnology', wherein design of chiral polymeric/organic self-assembled nanomaterials for the enantioselective recognition, separation and asymmetric catalysis are targeted.

The following are the members of the Unit :

### Chair

Prof 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

### Faculty Fellows

Dr Subi K George

Dr T Govindaraju

Ph D

Ph D





**Associate Faculty Members**

Prof Swapan K Pati (Associate Professor)  
Prof A Sundaresan (Associate Professor)  
Dr M Eswaramoorthy, (Faculty Fellow)  
Dr Tapas Kumar Maji, (Faculty Fellow)  
Dr A Govindaraj, (Honorary Faculty Fellow)

**R & D Assistants**

Ankita Goswami, Atchutarao Pathigoolla

**Ph D Students**

Debabrata Maity  
Venkata Rao Kotagiri  
M B Avinash

### 3. Education Technology Unit

The Unit is actively involved in the concept, production and development of multimedia CD-ROM's and books especially for school students and teachers in various disciplines of science. The Unit has been involved in developing and producing CD-ROMs and books in vernacular Indian languages. The Unit organized many science popularization programs in various parts of the country.

The **C. N. R. Rao Hall of Science** was set up at the Centre. It was opened by the Hon. Prime Minister Dr. Manmohan Singh on December 3, 2008 at a ceremony held at JNCASR. ETU is now part of the C. N. R. Rao Hall of Science. ETU was actively engaged in setting up the multimedia lab., in designing and producing the panels for the Chemistry of materials Exposition. It also set up the Viewing Room to facilitate students and teachers to view lectures given by Prof. C. N. R. Rao at various venues on different topics and also the multimedia CD-ROM titles developed and produced by ETU.

The **Madan Mohan Malaviya Amphitheater** at the C. N. R. Rao Hall of Science was inaugurated in a special inaugural program held on February 3, 2009. C. N. R. Rao Hall of Science and Education Technology Unit in collaboration with Molecular Frontiers Foundation organised a one-day interactive Science Education programme as part of the formal inauguration of the Madan Mohan Malaviya Amphitheatre. The Amphitheatre was inaugurated by Prof. Richard Zare, Stanford University, USA and Prof. Bengt Norden, Chalmers University of Technology, Sweden. The Program on Learning Science in the morning session was for Junior High School students and Youth forum and for Senior High School and Pre-university students, the program was held in the afternoon. The inaugural program began with the lecture on Learning Science by Prof. C. N. R. Rao followed by multimedia presentation of excerpts from the CD-ROM title 'Learning Science'. There were short presentations on "Learning Science" by Professors Richard Zare and Bengt Norden followed by an interactive question and answer session. In the afternoon session, the keynote lecture was delivered by Prof. D. Balasubramanian of Hyderabad Eye Research Foundation. Mrs. Indumati Rao presented excerpts from the CD-ROM 'Nanoworld' developed and produced by ETU. There was a short presentation by Prof. Martin Jansen and this was followed by an interactive question and answer session. The highlight of these programs was the interactive sessions where questions posed by student participants were answered by resource participants. About 165 students and teachers participated in the morning session and 160 students and teachers participated in the afternoon session.

ETU organised and conducted the Science Education program. Prof. Krishnan gave the welcome address. Mrs. Indumati Rao presented the multimedia presentations in both the sessions. Each speaker was honoured with a shawl and presented a gift by ETU. ETU designed and printed the invitations for the inaugural program. The Chairs of the various units at JNCASR, the Deans and other dignitaries were invited for the inaugural program.

Students and teachers participating in the program were presented with Learning Science and Understanding Chemistry books.

ETU coordinated and organised the visit of the faculty and students to the Chemistry of Materials Exposition and C.N.R. Rao Archives on 20<sup>th</sup> February 2009. ETU also organised a visit for JNCASR Officers and Staff to the C.N.R. Rao Hall of Science on 3<sup>rd</sup> March 2009.

ETU had taken up the Hindi translation and production of the **Learning Science** series (four parts) both as CD-ROMs and books. The work on the translation, development of the CD-ROM and design and formatting for the print-ready copies of the books is being done simultaneously.

Part 1: **Universe, Solar System and Earth** Part 2 titled **The world of physics and energy: Learning physical principles** comprising topics in Physics and energy, Part 3 titled **The world of chemistry: Of molecules and materials, Air around us and All about water** are completed and print-ready copies have been sent to National Book trust for printing. Part 4 titled **Biology and life** will be completed shortly. The development of the CD-ROMs is being currently done with the audio work to be taken up shortly.

ETU participated in the Bangalore Nano 2008 held on 12<sup>th</sup> December 2008. ETU presented a 30-minute multimedia demonstration of excerpts from the CD-ROM 'Nanoworld' at the above function. One thousand CD-ROMs were procured by the Department of Information Technology, Biotechnology and Science &



Technology, Government of Karnataka, for distribution to the participants at the above function.

### **On-going Projects**

The Hindi translation and production of the **Learning Science** multimedia series in Hindi both as CD-ROMs and books is being done at ETU. Part 4 – Biology and Life is currently being done and will be completed shortly. The C.N.R. Rao Hall of Science and ETU will be organising several science outreach programs for both students and teachers. ETU is actively involved in popularizing science through its programs like 'A celebration of chemistry', 'Learning Science' and 'Vignyana Kaliyona'.

### **Organisation of Programs**

ETU has organised science popularization programs for school children and teachers in collaboration with many institutes across the country.

The programme '**Learning Science**' is organised by JNCASR in association with different institutes for students and teachers from various schools. It was conducted on March 22<sup>nd</sup> at IITM, Chennai, on 11<sup>th</sup> July 2008 at Institute of Himalayan Bioresource Technology, Palampur and at JNCASR, on August 22<sup>nd</sup> at JNCASR, Bangalore. At the Principals meet organised by Hindu Newspaper Education on August 29, 2008, all the participants were presented with the book Learning Science and the CD-ROM 'Learning Science' vol. 1 & 2. The Learning Science program was conducted on 13<sup>th</sup> October 2008 at Trivandrum, FCBS as part of Teacher's Orientation Workshop, on 21<sup>st</sup> November 2008 at Bhavnagar in association with Central Salt and Marine Chemicals Research Institute. It was conducted at the Inter-University Accelerator Centre (IUAC), New Delhi on 19<sup>th</sup> December 2008 as the Foundation day lecture. The program was conducted on February 3<sup>rd</sup>, 2009 at C. N. R. Rao Hall of Science, JNCASR and at Science City, Kolkata on February 10, 2009. At all the above programs Prof. C. N. R. Rao gave the theme lecture 'Learning Science' followed by a multimedia presentation using excerpts from the CD-ROMs "Learning Science Vol. 1 & 2" developed and produced by Education Technology Unit, JNCASR.

In the program on Project Oriented Chemical Education, for undergraduate college students, a multimedia presentation from the CD-ROM '**Understanding Chemistry**' was presented by the Unit in May-June 2008.

The science popularisation program "**Vignyana Kaliyona**" in Kannada was organized by Karnataka Rajya Vijnana Parishat at JCBM College Sringeri, on 7<sup>th</sup> January 2009. Prof. C. N. R. Rao gave the theme lecture in Kannada followed by a multimedia presentation of the excerpts from the Kannada CD-ROM's titled 'Vignyana Kaliyona' `Samputa 1, 2, 3 & 4' developed and produced by Education Technology Unit, JNCASR. Around 400 students attended the program.

The program called 'Nanoworld' was conducted at a few places. It was conducted on July 9<sup>th</sup> in a program called "Nano" in Bangalore and in New Delhi on 20<sup>th</sup> December 2008 at IIT Delhi. In this program Prof. Rao gave the theme lecture titled 'Nanoworld' followed by a Multimedia presentation of excerpts from the CD-ROM titled 'Nanoworld' developed and produced by ETU.

The following are the members of the Unit:

<b>Incharge</b> 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

## 4. Engineering Mechanics Unit

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

### Granular Matter:

It has been established that the emergence of shear-banding instabilities (for perturbations having no variation along the streamwise direction), that lead to shear-band formation along the gradient direction, depends crucially on the choice of the constitutive model. For any constitutive model, the onset of this shear-banding instability is tied to a *universal* criterion in terms of constitutive relations for viscosity and pressure, and the sheared granular flow evolves toward a state of lower “dynamic” friction, leading to the shear-induced band formation, as it cannot sustain increasing dynamic friction with increasing density to stay in the homogeneous state.

Using particle simulations of the uniform shear flow of a rough dilute granular gas, it is shown that the translational and rotational velocities are strongly correlated in direction, but there is no orientational correlation-induced singularity at perfectly smooth and rough limits for elastic collisions. Both the translational and rotational velocity distribution functions remain close to a Gaussian for these two limiting cases. Away from these two limits, the orientational as well as spatial velocity correlations are responsible for the emergence of non-Gaussian high velocity tails.

### Geophysical Fluid Dynamics:

The mean flow and the linear stability characteristics of a two-dimensional particulate suspension, driven horizontally via harmonic oscillation, have been analyzed. This work has been motivated to understand the topography formation on the ocean-bed and has relevance in geophysical context. Using Floquet theory, a linear stability analysis of the time-periodic mean flow indicates that the oscillatory suspension supports stationary and traveling-wave instabilities that corresponds to particle-banding patterns that are aligned parallel or orthogonal or at an oblique angle to the driving direction. It is shown that the fluid-particle interaction is responsible for the onset of travelling instabilities in this flow.

Spatial stability of supersonic compressible plane Couette flow, having relevance in astrophysical fluid dynamics, has been investigated. An analysis of the energy contained in the least-decaying mode reveals that the instability is due to the work by the pressure fluctuations and an increased transfer of energy from the mean-flow. A leading order viscous correction reveals that the neutral and unstable modes are destabilized by the no-slip enforced by viscosity. The viscosity has a dual role on the stable inviscid mode.

Studies of the Lifted Temperature Minimum (LTM) in the nocturnal atmospheric surface layer have resulted in a plausible explanation of the phenomenon based on vertical variation of aerosol concentration. It has been shown that such a layer can only arise in a heterogeneous atmosphere.

### Computational Fluid Dynamics:

A DNS study of the starting plume as a model for cumulus clouds has been initiated. Results from a 2D simulation have been published and a 3D simulation is being carried out on a powerful computing system.

Numerical Simulation of multiscale supersonic flows with low dissipative shock capturing schemes: The MKFVS method has been successfully applied to transonic and supersonic flow around 2-D airfoils. The MKFVS method captures the shocks very crisply. This is an Indo-Russian Project.

Development of TKFMG solver and its application to flutter prediction in turbomachines: The TKFMG solver has been used to predict flutter for a 2-D blade of a turbine. Energy method has been used in flutter analysis. This is a CARS Project (Jointly with CTFD, NAL).

Data assimilation for mesoscale modeling for monsoon related weather predictions – Phase II: The Ensemble Kalman Filter (EnKF) has been applied to 3-D Lorenz model problem. The EnKF does follow the truth run because of Data Assimilation. This is NIMITLI-CSIR Project.



### **Stability:**

An ongoing analytical investigation has helped characterize the modal response of a vortex column to external disturbances, and in particular, has led to the discovery of inviscid resonances.

Vortex dynamics in the presence of density stratification. The problem was studied analytically and numerically. The main result was that non-Boussinesq effects can be very important, acting sometimes to reduce vortex lifetimes drastically.

The two-dimensional stability of converging-diverging flows and of wall jets shows a number of interesting features. In particular the dependence of instability wave number on the normal coordinate is seen, which is impossible to find with traditional stability analyses. Earlier work (in 2007) at the Unit had shown that channel flow with heated walls could display large amounts of transient growth in two-dimensions. This was surprising, because all known important transient growth situations hitherto had been three-dimensional. A basic understanding of the finding was explained by a simple model how heat can take the place of the normal vorticity, i.e. of three dimensionality.

### **Complex fluids & Interfacial flows:**

An ongoing analytical study focuses on the rheology of suspensions of anisotropic particles. In this regard, the formalism of vector spheroidal harmonics was used to analyze the orientation dynamics of spheroidal particles in shearing flows.

In continuation of earlier studies on the effects of micro-scale inertia, work carried out with a summer student helped characterize the effects of inertia on the non-Newtonian rheology of a dilute emulsion. Work carried out with a second summer student helped establish the crucial effect of the disperse phase viscosity on the Nusselt number correlation applicable to dilute emulsions.

Studies carried out in collaboration with Don Koch at Cornell University examined the evolution of sedimenting particle clouds, and the structure, dynamics and stability of fibrous suspensions at finite Reynolds number.

A new mechanism of instability was identified in a dilute suspension of active particles (bacteria).

Interfacial flows : The volume-of-fluid method was studied in detail, and a new computer code for computing interfacial flows is nearing completion. Droplet shapes were studied and a new class of static stable shapes for pendant drops was found.

### **Experimental fluid dynamics:**

The focus was on (a) Laboratory simulation of magma-convection, (b) Parametric study of flapping flight to identify optimal wing kinematics and the role of wing-flexibility on lift production, and (c) study on designing green buildings with natural ventilation (in collaboration with Prof. JH Arakeri, ME, IISc).

For continuing experimental work on cloud flows, new and improved version of the apparatus used in earlier work at the Unit is being set up. First results from the new apparatus should be available during the summer 2009.

A project has been started on the design of wings for aircraft driven by turbo-prop engines and propellers. Rotor-driven aircraft have become of great interest in recent years because of their much lower fuel consumption and lower carbon foot print, which has become a major concern because of the need to counter climate change through reduction of green-house gas emissions. A study using optimization techniques has given interesting and promising results.

A Memorandum of Understanding (MoU) between Bhabha Atomic Research Centre (BARC), Department of Atomic Energy (DAE), Mumbai and JNCASR has been signed for "Development of Test Facility for Thermal Hydraulics Studies/Basic Research Salt Water/Fine Hydrogen Bubble Test Facility for Simulation

of Hydrogen Transport- Management/Fire Safety Behaviour/Containment Thermal Hydraulics/Pollution Dispersion Studies” Principal Investigator : Prof Meheboob Alam.

The following are the members of the Unit:

**Chair**

Roddam Narasimha  
(up to 31.10.2008)

Ph D, F A Sc, F N A, FTW A S, F R S

**Rama Govindarajan**  
(from 1.11.2008)

Ph D, F N A Sc

**Professor**

Rama Govindarajan

Ph D, F N A Sc

**Associate Professors**

K R Sreenivas  
Meheboob Alam

Ph D

Ph D

**Faculty Fellow**

Ganesh Subramanian

Ph D

**Senior Associate**

S M Deshpande

Ph D, F A Sc

**Research Associates**

Konark Arora, Mukund Vasudevan (P), Sarita Azad (P),  
Satya Prakash Ojha, Soumyajit Mukherjee, Vishwanath K P.

**R & D Assistants**

Ashish Malik, Vineetha Mukundan, Vivekanand Dabade

**Research Students**

Harish N Dixit, Ratul Dasgupta, Priyanka Shukla, Anubhab Roy,  
Gayathri S, Sumesh P T, Dhiraj Kumar Singh, Ponnulakshmi V K,  
Rakshith B R, Vivekanand Dabade, Vivek N Prakash, Konduri Aditya,  
Snehalatha B, Kopal Arora Dinesh Kumar, Rahul Bale, Vinay Kumar Gupta,  
Ujjayan Paul.



## 5. Evolutionary & Organismal Biology Unit

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

The faculty of the Unit continued their ongoing research in the broad areas of chronobiology, theoretical evolutionary genetics, life-history evolution and population dynamics. Two new members joined the Unit as Ramanujan Fellows of the DST and are setting up their laboratories for work on phylogeography and sociogenetics, and behavioural neurogenetics, respectively. Members of the Unit were active in delivering invited talks at major international and national meetings and premier institutions of the country, and also participated in outreach activities aimed at students. Members of the Unit have also served the broader scientific community by acting as outside reviewers for manuscripts and research proposals submitted to various national and international journals and funding agencies. In particular, significant publications during this year focused on the neuronal and molecular aspects of circadian rhythm phenotypes, theoretical evolutionary genetics and the phylogeography of Asian elephants. This work has yielded papers in top journals of biology, genetics and neurobiology.

The following are the members of the Unit:

### Chair

M K Chandrashekar (up to 31.8.2008)	Ph D, DSc, FASc, FNA, FTWAS
Amitabh Joshi (from 1.9.2008)	Ph D, FA Sc, FNA Sc

### Professor

Amitabh Joshi	Ph D, FA Sc, FNA Sc
---------------	---------------------

### Honorary Professors

Raghavendra Gadagkar	Ph D, FA Sc, FNA., FTWAS
Vidyanand Nanjundiah	Ph D, FA Sc, FNA

### Associate Professor

Vijay Kumar Sharma	Ph D
--------------------	------

### Ramanujan Fellows

T N C Vidya	Ph D
Sheeba Vasu	Ph D

### Research Associate

Punyathirth Dey	
-----------------	--

### Fellow (DBT)

B M Prakash	
-------------	--

### R & D Assistants

Aditya Rao, Deepika L Prasad, Gini C Kuriakose, Gudubasha Shaik, Joy Bose, Madhumala KS, Shantala A Hari Dass, Sudarshan R Chari, Vijay Vrajan.

### Research Students

Shampa Ghosh, Archana N, Koustubh M Vaze, Pankaj Yadav, Snigdhadip Dey, Shahnaz Rahman Lone, Nisha NK, Priya M P, Soundarya Iyer, Muzafar Beigh M

## 6. Geodynamics Unit

Identification of belts where sudden and swiftly occurring geological phenomena often destabilize the natural configuration of life and threaten the balance of ecosystems, is the principal objective and the main thrust of activities of this one-man Unit. Regions vulnerable to landslides and occurrence of earthquakes repeatedly in the central sector of the Himalayan arc (Kumaun in the Uttaranchal), the Biligirirangan Range in southeastern Karnataka, and the Sahyadri Range in western Karnataka and central Kerala are taken up for studies.

- (a) Extensive revision of the 990-page manuscript "The Making of India: Geodynamics Evolution" following copy-editing by the publisher Macmillan India Limited, New Delhi. The book is likely to be published by June or July 2009.
- (b) Writing and preparation of manuscript of an illustrated popular book in Hindi entitled "Ek Thi Nadi Saraswati". The manuscript is ready for submission to a publisher.
- (c) As Honorary Visiting Professor, delivered lectures for one week in October 2008 at the Earth Sciences Department, Indian Institute of Technology, Roorkee.

As Distinguished Guest Professor, delivered special lectures for the duration of one month each in September 2008 and February 2009 at the Earth Science Department, Indian Institute of Technology, Mumbai.

The writing of a popular book on a scientific theme in Hindi was a new programme.

**Chair**

K S Valdiya

Ph D, F A Sc, F N A,  
F N A Sc, FTWAS





## 7. Molecular Biology and Genetics Unit

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

### **Chromatin Biology Lab.**

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. 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 circular dichroism and Atomic Force microscopic analysis. Acetylation also impedes the interaction of TP2 with NPM3, a putative histone chaperone, whose expression is elevated in haploid spermatids. Colocalization studies using GC selective DNA binding dyes chromomycin A3 and 7-amino actinomycin D and AT selective dye DAPI indicate that TP2 is preferentially localized to 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 immunofluorescence experiment with anti-TP2 and anti-TP1 antibodies 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 expression 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.

### **Molecular Parasitology Lab.**

Research in this laboratory is focused towards 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. Adenylosuccinate 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.

### **Vascular Biology Lab.**

Molecular, genetic and developmental analysis of the cardiovascular system.

A comparative approach has been made by using embryonic stem cell models, mouse developmental biology and transgenics, and *Drosophila* genetics, to decipher the roles of novel genes expressed early in

the cardiovascular and hematopoietic systems. Our approach has given useful insight into gene function as well as ontogeny of the heart, blood and blood vessels. Analysis of these genes in the context of human development as well as in clinical studies with a focus on tumor angiogenesis and progression has been undertaken. Current studies are focused on understanding mechanisms that control cardiovascular development using ESCs and mutant mice.

Recently two new sibling human embryonic stem cell (hES) lines from discarded embryos have been derived and differentiated to cardiovascular derivatives that can be cultured to purity. These are called BJNhem19 and BJNhem20 and have been deposited in the UK Stem Cell Bank. The lines are also listed on the European hESC registry. The laboratory is currently involved in the International Stem Cell Initiative (ISCI) project on accumulation of genetic defects in ES cell cultures.

#### ***Parasitology Lab.***

It is focussing its efforts on the role of Plasmodium kinases in host - pathogen interactions.

#### ***Molecular Virology Lab.***

Significant progress took place in several projects that are presently active. The laboratory screened a large number of Indian clinical samples and identified an immunodominant B-cell epitope in the cysteine-rich domain of Tat only in the HIV infected people. This finding has a direct relevance for HIV vaccine design. Differential transcription factor binding to several sites in the viral promoter has been delineated in subtype-C HIV-1 promoter region.

#### ***Human Molecular Genetics Lab.***

- (a) Discovery of a novel epilepsy locus at chromosome 3q13.3-q21, was followed by a detailed analysis of genes at 3q13.3-21, leading to identification of several patient-specific mutations in the extracellular calcium-sensing receptor (*CaSR*) gene (*Annals of Neurology* 2008). The CaSR protein is proposed to sense small changes in extracellular calcium levels and integrate this information to intracellular signal transduction pathways in neuronal cells.
- (b) Identification of another novel epilepsy locus at chromosome 5q12-q14, is an important finding from the laboratory. This locus, located between markers D5S641 and D5S459, is responsible for an age-related, common idiopathic generalized epilepsy (*Human Genetics* 2007). Analysis of several candidate genes at the 5q12-q14 locus suggests that a new and diverse molecular mechanism, which functions apparently independently of the ion channel mechanisms, may underlie the pathophysiology of epilepsies.
- (c) Deafness genetics is another area of research in the laboratory. Studies of 500 families affected with severe-to-profound deafness wherein six deafness-causing genes have been concluded: *Cx 26*, *Cx 30* (connexin 26, connexin 30: cochlea-expressed genes encoding gap junction proteins); *TMPRSS3* (transmembrane serine protease 3), *TMCI* (transmembrane cochlear-expressed gene 1), *HAR* (Harmonin) and *CDH23* (cadherin 23) were analyzed. Using an efficient and cost-effective, two-step genetic analysis, the work revealed a spectrum of pathogenic mutations in these genes: 18 mutations in *Cx26*; 8 mutations in *TMCI*; 4 mutations in *TMPRSS3*; 6 mutations in *HAR*; 4 mutations in *CDH23* and one mutation in *Cx30*. Identification of a total of 41 pathogenic mutations have substantially extended allelic heterogeneity at these genes and provided a large collection of mutant alleles for potential use in cell biological, biochemical and structure-function correlation studies. A detailed cell biological and functional analysis of the *Cx26* alleles has recently been published (*European Journal of Human Genetics* 2008). Knowledge of the relative contributions of these six genes to the load of hereditary deafness has helped devise an algorithm that has important implications for early detection of this disorder and implementation of suitable intervention therapies.

#### ***Transcription and Disease Lab.***

The researchers in this Lab. have been working on the Chromatin dynamics and transcriptional regulation in humans with special emphasis on disease and therapeutics. They have made several original contributions in this area which include the discovery of human transcriptional coactivator PC4 a functional component of Chromatin organization, a Nucleophosmin (NPM1) as a histone chaperone and transcription regulator, hyperacetylation of histones and also NPM1 have been causally linked in the manifestation of



oral cancer. They have discovered several inhibitors of Histone acetyltransferases which could serve as a lead reagent to design therapeutic and could be also used to study cellular functions of HATs. Most recently, by using carbon nanospheres conjugated to small molecule HAT activator CTPB (discovered by them) have been able to activate the histone acetylation both in cultured cells and in the mice brain. Presently, the group is working on the following areas:

- a. Chromatin dynamics and transcription regulation: Role of nonhistone chromatin protein and histone chaperones:
- b. Epigenetic modifications in disease manifestation: Cancer, Diabetes and AIDS:
- c. Chemical Biology approach to probe the role of specific Chromatin modifications:
- d. Nanobiotechnology:

#### ***Molecular Mycology Lab.***

The researchers in this Lab. have studied centromeres of a pathogenic yeast, *Candida dubliniensis* and compared centromere sequences with those of a closely-related yeast *Candida albicans*. The studies indicate that centromeres are evolving at a rate faster than any other genomic region in these two species.

The laboratory also launched a new programme to study the structure-function relation of centromeres in three *Candida* species: *C. albicans*, *C. dubliniensis* and *C. tropicalis* and to investigate the mechanism of this rapid change in centromere DNA sequence.

The following are the members of the Unit:

#### **Chair**

M R S Rao

Ph D, F A Sc, F N A, F N A Sc,  
F T W A S

#### **Honorary Professors**

Dipankar Chatterji

Ph D, F N A Sc, F A Sc, F N A

H Sharat Chandra

Ph D, F A Sc, F N A

#### **Professors**

Anuranjan Anand

Ph D

Hemalatha Balaram

Ph D, F A Sc

Namita Surolia

Ph D, F A Sc, F N A Sc

#### **Associate Professors**

Maneesha Inamdar

Ph D

Ranga Uday Kumar

Ph D

Tapas Kumar Kundu

Ph D, F A Sc, F N A Sc

#### **Faculty Fellow**

Kaustuv Sanyal

Ph D

#### **Research Associates**

Anil Mukund Limayee, Benaka Prasad, Jayashree Ladha, Kiran Batta,  
Mantelingu K, Rohman Nashiour, Ravindra K C, Shritapa Dutta,  
Sunitha S N (P).

**Fellows (DBT)**

Mylarappa B N  
Chethana S.

**R & D Assistants**

Ajeesh B R, Ananad KK, Anil Babu, MHKH, , Anitha C A, Antony Augustin, Arunima Chatterjee, Ashok Reddy, Avinash, Balasiddiah A, Badi Sri Shailaja, Benaka Prasad, Bharath GN, Bindu KM, Bopanna, Chincy Thankachan, Divya Bharati, Geddam M Chowdhuri, Imitiaz Nisar Lone, Jayalaxmi Shetty, Jinal Shukla, Keerthi Nambiar T C, Manasa R, Manjunath S, Meenakshi Sharma, Mohan V, Museer Ahmad Lone, Naga Shankar G, Nandasree, Nikhil Jain, Parvathy V, Prashanta Kumar Dash, Rahul MG, Rajaguru Aradhya, Rajesh Abraham Jacob, Rajesh VM, Ramesh Reddy, Ramesh Chowdhury V, Rekha S, Rituparna Mandal, Roopa, Roshen Elsa Rajan, Sainitin, D, Sanjukta Chakraborty, Satish V, Sayali Mukherjee, Senthil Kumar T, Shivashankar TV, Siddhartha Paul, Sonali Mehrotra, Sowmya Prabhu, Sreedevi P, Sriram S, Srivatsa MS, Sujay T M, Suresh Babu V, Thanuja G R, Tariq Ahmad Najar, Uttara Chakraborty, Veda Murthy B M.

**Research Students**

Aparna G, Rahul Modak, Anand Kumar K, Rinki Ratna Priya, Subhra Prakash Chakrabarty, Vani Kulkarni, Venkatesh Prasanna K S, Arif, Vinay B, Gayatri G, Javaid Bhat Yousuf, Shrikanth Gadad, Bharat S, Jayasha Shandilya, Mamta Jain, Mangaiarkarasi A, Ruthrotha Selvi V B Vikru, Surbhi Dhar, Nishtha Pandey, Abhishek Sinha, Laxmi Narayan Mishra, Mahesh B, Jitendra Devi, Mukti Nath Mishra, Babhrubahan Roy, Varun Kumar, Karthigeyan D, Sujata Kumari, Mohan Krishna DV, Manpreet Kaur, Raju Pedabaliyarasimhuni P K, Venkateswaran G, Sanjeev Kumar, Sourav Roy, Ramachandramouli Budida, Shiva Shankar T V, Nikhil Gupta, Bhavana Mishra, Shetty Ronak Kutty, Laxmi Shanker Rai, Gautam Chatterjee, Anjali Verma, Kalpita Rashmi Karan, Deeti Shetty, Sreyoshi Mitra.



## 8. Theoretical Sciences Unit

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

The primary focus has been on understanding phase separation processes in a restricted geometry (slit pore) in which a multi-component mixture is confined while being in the miscibility gap region of the phase diagram. The emphasis has been on liquid mixtures which, compared to solid mixtures, are poorly understood because of the presence of hydrodynamic interactions. It has been attempted to understand the physics of phase-separation through atomistic simulations as well as from a coarse-grained continuum dynamical partial differential equation approach. In the more general area of phase-separation, finite-size effects during the non-equilibrium evolution and quantitative statements about them are being looked at.

- (1) ***Evolution of sex and recombination:*** It is known that an asexual population degenerates in time and may eventually go extinct. To find the time to extinction, they considered the dynamics of a non-recombining haploid population of finite size which accumulates deleterious mutations irreversibly. This ratchet like process occurs at a finite speed in the absence of epistasis, but it has been suggested that synergistic epistasis can halt the ratchet. Using a diffusion theory, explicit analytical expressions for the typical time between successive clicks of the ratchet for both non-epistatic and epistatic fitness functions have been found. The calculations show that the inter-click time is of a scaling form which in the absence of epistasis gives a speed that is determined by size of the least-loaded class and the selection coefficient. With synergistic interactions, the ratchet speed was found to approach zero rapidly for arbitrary epistasis.
- (2) ***Generating particle current by classical pumping:*** In a recent study, a symmetric exclusion process with time-dependent hopping rates was introduced. Using simulations and a perturbation theory, it was shown that if the hopping rates at two neighboring sites of a closed ring vary periodically in time and have a relative phase difference, there is a net DC current which decreases inversely with the system size. A model where hopping rates at all sites vary periodically in time was studied and shown that for certain choices of relative phases, a DC current of order unity can be obtained. The results were obtained using a perturbation theory in the amplitude of the time dependent part of the hopping rate and in a sudden approximation that assumes large modulation frequency.
- (3) ***Evolution of mutation rates:*** As most mutations are known to have deleterious effect, the spontaneous mutation rate is expected to be minimum. However, hypermutable strains in high frequency have been found in both natural isolates and laboratory. To understand these observations, an infinite asexual population with a mutator allele which can elevate mutation rates was considered. With probability  $f$ , a transition from nonmutator to mutator state occurs but the reverse transition is forbidden. It was found that at  $f = 0$ , the population is in the state with minimum mutation rate and at  $f = f_c$ , a phase transition occurs between a mixed phase with both nonmutators and mutators and a pure mutator phase. The critical probability  $f_c$  and the total mutator fraction  $Q$  in the mixed phase exactly was calculated. The predictions for  $Q$  are seen to be in agreement with those seen in microbial populations in static environments.

In the field of surface alloys, the research group has shown that several combinations of bulk-immiscible metals become miscible when co-deposited on a substrate of intermediate lattice constant. Surprisingly, a larger lattice mismatch suggests greater miscibility, in contrast to the Hume-Rothery rule for bulk alloys. Some of these systems show novel magnetic properties. The group has also studied the dissociation of NO on a variety of Rh catalysts. It was shown that strained monolayers of Rh on MgO and Rh nanoparticles promote adsorption and dissociation of NO. It was shown that a quantity called the effective coordination number can be a good predictor of adsorption energies and dissociation barriers. In another study, the

group has shown that activated carbon (modelled by defective and functionalized graphene) has good methane storage properties.

A broad spectrum of condensed matter phenomena including excitation characteristics, low-temperature thermodynamics and dynamical behavior of a range of quantum system were also investigated. Understanding the microscopic structure-property relationship for a wide spectrum of applications in transport, optical, magnetic, electrical and mechanical behavior was attempted. The systems of interest include molecules, clusters, solids, polymers and biomaterials in their isolated forms or their variants in experimental conditions. The state-of-the-art numerical methodology involves developing effective theories based on appropriate recognition of relevant states that are responsible for the particular application. With a few to a very large number of states, the effective theory considers quantum-many body interactions in the most appropriate manner through random-phase approximation, configuration interactions with one or a few reference states, non-perturbative renormalization group based on density matrix formalisms and nonequilibrium quantum manybody theory based on master equation method. Apart from numerical tools, the Unit developed analytical tools in certain limits for a host of quantum many-body models like the Heisenberg and Hubbard Hamiltonians, etc.

In particular, the ground state behavior and low temperature magnetic properties of 2-D Kagome antiferromagnets with inhomogeneous spin sites have been investigated in the presence of vectorial exchange interactions (Dzyaloshinskii-Moriya interactions).

A large number of experimental magnetic systems of different dimensionalities with a range of magnetic interactions. The quantum manybody calculations based on master equation method for coupled quantum dot systems show NDR peak in assymetric I-V characteristics for large onsite Hubbard correlation,  $U$  and Coulomb staircase behavior for small  $U$ .

By using NEGF-DFT, finite-sized vanadium-borazine clusters are found to exhibit efficient spin filter properties when coupled to graphene. The influence of sequence on the electronic properties of DNA was studied. With regard to targeted modifications of the DNA structure, two studies, one focusing on the controlled alignment of the metal ions within the double stranded DNA helix, and the other focusing on the use of single strand DNA as scaffolds for transition metal alignment were pursued.

Theoretical designing and characterization of novel organic materials like enzene, naphthalene, perylene, ocatthio-circulene, azulene, sumanene etc. were completed. The observations of remarkable charge carrier mobilities in some of those systems and their excellent agreement with experiments have been highly appreciated in many scientific communities.

The electronic structure, electronic conduction and gas storage properties of graphene within both manybody and DFT formalism have been studied. The speculations of magnetic ground state of zigzag edge graphene nano ribbons have been successfully shown within inhome developed manybody configuration interaction formalism. For the first time they predict the intrinsic room temperature half-metallic property on modified graphene nanoribbons.

The static electric field within inhome developed DMRG code have been implemented and the effect of that on one dimensional insulators was studied. For the first time they have shown the field mediated charge density wave to spin density wave phase transition which is yet to be understood experimentally. The Crank-Nicholson code to study the time evolution of wave function reflecting the dimerized BH Hamiltonian, which has been solved by the powerful numerical technique DMRG. Three types of phase transitions have been observed: conventional SF to MI, SF-BW to PI and SF-BW to MI-BW. This work has further relevance with the recent implementation of superlattice potential (SLP) in cold atom experiments.

Research in the group in the past year has focussed on the following topics: (i) Liquid liquid transition in silicon, (ii) crystal nucleation in supercooled liquid silicon and other systems, (iii) the role of crystal polymorphism in determining glass forming ability, (iv) gelation in model fluids, (v) modeling protein aggregation, (vi) analyzing the role of static and dynamic length scales in glass forming liquids and the analysis of their dimensional dependence. A significant result has been to show that the relationship



between dynamical heterogeneity and relaxation times are more complex than previously assumed. It has also been shown that the relationship also has very interesting dependence of space dimensionality, showing peculiar behaviour in two dimensions.

A collaboration with Prof. Mark Jarrel at the University of Cincinnati, USA, focuses on the quantum Monte Carlo approach to strongly correlated electronic systems. Two projects have been successfully completed. Work is progressing on "Avalanches in thermal and pressure driven hysteresis across the Mott metal-insulator transition." Codes were written, tested and have a good picture of the basic physics underlying the avalanches. They do seem to have a very good description of several recent experiments in V<sub>2</sub>O<sub>3</sub>, VO<sub>2</sub> and organic Bechgaard salts. Interplay of multiple time scales in the lateral charge transport of polymeric semiconductors is being investigated using the model developed by the Unit.

Through a combination of first-principles calculations and statistical mechanical analysis, soft shear acoustic long wave-length modes have been determined as the microscopic cause for the mechanical failure in SiC when it is used in power electronic devices. The origin of emergence of multiferroic behavior in BaTiO<sub>3</sub> at nano-scale and its magneto-capacitive coupling between the magnetism arising from oxygen vacancies at the surface of a BaTiO<sub>3</sub> nanoparticle and ferroelectric order in its core were explained. A new class of semiconducting carbon nanotubes that (a) contain a line defect consisting of octagonal and pentagonal rings, and (b) can be labeled with fractional numbers of chirality has been predicted. These nanotubes exhibit truly one-dimensional carrier states localized along the line defect. Including the dynamical corrections beyond the Born-Oppenheimer approximation, the scientists have determined effects of (i) electrochemical (ii) substitutional, and (iii) molecular doping on vibrational properties of single and a few layered graphene, and identified contributions of various mechanisms to shifts in the frequency of their Raman active modes. This work is expected to be useful in employing Raman spectroscopy for characterization of carriers and their concentration in doped graphene.

An Indo-US workshop on "Nanomaterials for energy applications" in collaboration with Purdue University in August 2008 was organized. The oxides section of the winter school on chemistry of materials in December 2008 was formulated.

New programmes launched during the year

A joint India-US centre on nanomaterials for energy applications (funded by the IUSSTF) will be started at ICMS-JNCASR.

The following are the members of the Unit:

**Chair**

Rahul Pandit (up to 31.10.2008)	Ph D, F A Sc, F N A
Shobhana Narasimhan (from 1.11.2008)	Ph D

**CSIR Bhatnagar Fellow and Hon. Professor**

Kalyan B Sinha	Ph D (Univ. of Rochester), F A Sc, F N A, FTWAS
----------------	--

**Professors**

Shobhana Narasimhan	Ph D
Srikanth Sastry	Ph D

**Associate Professors**

Swapan K Pati	Ph D
Umesh V Waghmare	Ph D

**Faculty Fellow**

N S Vidhyadhiraja	Ph D
Kavita Jain	Ph D
Subir K Das	Ph D

**Research Associates**

Anasuya Kundu, Debabrata Parihari (P),  
Hembram K P S S

**R & D Assistants**

Goutam Prasanna Kar, Manju, S T, Rajavarman K, Ramakrishna Ghosh,  
Sandeep Kumar, Shibu Saw, Snehajothi Chaterjee

**Research Students**

Bhaswati Bhattacharyya, Shibu Saw, Sairam Swaroop M, Sasmita Mohakud,  
Anil Kumar, Sudipta Dutta, Moumita Maiti, Himadri Barman, Mighfar Imam,  
Shiladitya Sengupta, Madhura Marathe Pradeep, Arup Chattopadhyay,  
Vishwas V, Prakash Parida, Arun Kumar Manna, Suman Majumder,  
Sutapa Roy, Sananda Biswas, Pramod Kumar, Ulman Kanchan Ajit,  
Gayatri Das, Arun R, Ershaad Ahamed Basheer.





## 9. International Centre for Materials Science

ICMS the first international centre devoted to research, education and extension in materials science, established in the confines of a scientific cum educational institution, envisaged by the Department of Science and Technology (DST), Government of India, was dedicated to the nation by the Hon'ble Prime Minister, Dr Manmohan Singh, on December 3, 2008. The ICMS will provide global research opportunities and supports international exchange programmes. The centre will offer a one-year (two-semester) Post-graduate Diploma in Materials Science.

A Board of Management and an International Advisory Board consisting of eminent academicians in India and abroad has been constituted to recommend policies, programmes and activities.

During the year, the ICMS has established major scientific facilities like Ultra High Resolution Electron Microscope, Pulse Laser Deposition, Molecular Beam Epitaxy System, X-ray Diffractometer, FE-SEM, Technai, Plasma Cleaners, Ion Millers and others. Besides many International Schools/Workshops were held with the collaboration of Purdue University, ICMR-UC Santa Barbara and the Swedish Academy of Sciences. ICMS entered into MoUs with leading institutions and attracted a few visitors from abroad. ICMS organized the first International Materials Lecture by the well known scientist, Prof. Tobin Marks, Northwestern University, on February 4, 2009.

### Faculty

1. Prof C N R Rao, FRS, Hon. FRSC, Hon. F Inst P, Director
2. Prof S M Shivaprasad, Ph D (Karnataka)
3. Dr Ranjan Datta, Ph D (University of Cambridge), Faculty Fellow
4. Dr Rajesh Ganapathy, Ph D (IISc.), offered position as Faculty Fellow

### Adjunct professorship and other honorary positions

1. Prof Timothy Fisher, Purdue, *Adjunct Professor*
2. Prof Vinayak Dravid, Northwestern University, *Adjunct Professor*
3. Prof Pulickel M. Ajayan, Rice University, *Adjunct Professor*
4. Prof Vinod Subramaniam, University of Twente, *Adjunct Professor*
5. Prof U Ramamurty, Indian Institute of Science, *Hon. Faculty*

### Sheikh Saqr Fellowship

1. Prof K S Narayan, Associate Professor, ICMS, *RAK-CAM Sheikh Saqr Senior Fellowship*
2. Mr S R C Vivek Chand, *RAK-CAM Sheikh Saqr Junior Fellowship*

### Schools and Workshops

1. ICMS-ICMR International Winter School – 2007, Dec 6-13, 2007
2. A joint India-US workshop on Scalable Nanomaterials for enhanced Energy Transport, convenience and Efficiency August 19-21, 2008 (with Purdue University)
3. Molecules & Materials: New Directions- Dec 4-6, 2008
4. International Winter school – 2008, Dec 8-13, 2008 with ICMR, UC Santa Barbara
5. Chemistry of Materials meeting arranged in collaboration with Swedish Academy of Sciences Feb 2-3, 2009

### Seminars and Special Lectures

1. Dr Ambrish Ghosh, Harvard University, September 2, 2008  
Title: Detection and manipulation of chiral objects
2. Dr Paralapalli Venkata Satyam, Institute of Physics, Bhubaneswar, November 5, 2008  
Title: HRTEM study of Nanostructures at Surfaces and Interfaces
3. Dr Perumal Ramasamy, Pennsylvania State University, USA, November 17, 2008  
Title: Materials Science approach to Biomaterials research
4. First International Materials Science Lecture by Prof. Tobin Marks, Northwestern University, February 4, 2009.  
Title: Transparent Conductors: New Science, Technology, and their Interface with Soft Materials
5. Prof. Arunava Gupta, University of Alabama, USA, March 5, 2009  
Title: Multiferroic Nanowire Composites and Thin Films
6. Dr Shaibal K. Sarkar, University of Colorado at Boulder, USA, March 12, 2009  
Title: Semiconductor Sensitized Solar Cells: Aspects of Different Deposition Techniques

### Visiting fellows and scientists from abroad

1. Prof Venkatesan Manivannan from USA
2. Mr Tran Duc Hoang from Vietnam
3. Mr Jafar Hoseini from Iran
4. Ms Nguyen Thi Mua from Vietnam

### Visitors from ICMS to other places

1. Ms Shipra to NIMS, Japan, Host Researcher: Dr. Kazuto Hirata
2. Mr Sandeep Ghosh to NIMS, Japan, Host Researcher: Prof. Izumi Ichinose



## 10. Centre for Computational Materials Science (CCMS)

The Centre for Computational Materials Science (CCMS) was established in 2006 and is supported through a grant provided by the Nanoscience and Technology Initiative of the Department of Science and Technology, Government of India. Members of CCMS carry out research in the broad area of computational materials science, using a variety of analytical and computational tools.

### Salient Research Achievements:

- The potential energy of large clusters of ionic liquid (IL) molecules as a function of their size has been investigated using MD simulations. Their size and shape have been characterized. Enrichment of the surface of the cluster surface with cations is observed. The difference in the mean energy of an ion pair in the cluster with that in the bulk liquid has been ascribed to the lower coordination of IL molecules present at the surface.
- The behaviour of a model room temperature ionic liquid under shear is explored using non-equilibrium molecular dynamics simulations. The external field reduces intermolecular structure in the liquid. However, orientational ordering of the molecules in the form of a nematic phase is observed under shear.
- A dilute aqueous solution of the salt, 1-n-butyl,3-methylimidazolium hexafluorophosphate, [bmim][PF6] has been studied using molecular dynamics simulations to investigate the effect of ions on water and vice versa. The anion is found to diffuse faster than the cation in the solution, in contrast to observations in the pure ionic liquid. Subtle differences between the nature of the hydration layers around the ions are observed.
- Applying density functional theory to low dimensional systems. Topics of recent and current interest include strain-stabilized surface alloys, Rh nanocatalysts and activated carbons for methane storage.
- It was found that small Rh clusters are magnetic, and that this interferes with their catalytic activity. Clusters are found to exhibit interesting scaling relations in their hardness and melting temperatures. Selenium nanowires show a slight dependence on size in their structural properties, but a strong dependence in their electronic properties.
- The computational study of glass forming ability which has led to an experimental verification of vitrification of germanium. This work is being followed up with a study of the relation between crystal polymorphism and glass forming ability.
- Liquid-liquid critical point in supercooled silicon: Extensive computational simulations have been carried out to map the location of the liquid-liquid critical point in silicon.
- Crystal nucleation in silicon has been studied near the liquid-liquid critical point. This work has shown promising evidence of the role of density fluctuations in enhancing nucleation rates.
- Modeling protein aggregation using simple statistical mechanical models.
- Development and study of a computational model for gelation.
- The study of heterogeneous dynamics in a lattice model of glass forming systems.
- The study of length scales relevant to structural relaxation in glass forming liquids.
- Modifications to the DNA structure which can be used as efficient scaffolds for DNA based spintronics devices have been suggested. DNA based single molecular magnets (SMM) have been investigated.
- Investigated the I-V characteristics in molecular bridges in different regimes (Coulomb blockade as well as strong coupling regimes).
- Analyzed the effects of competing exchange interactions and lattice dimerizations for a large class of systems including Kagome antiferromagnets, 1-D spin chains and ladder structures.
- Observations on magnetic ground state of zigzag edge graphene nano ribbons, which shows intrinsic half-metallic property on hole doping over a large temperature domain, opening up a huge application possibility in spintronics devices. Calculations that have been done also suggest two-dimensional grapheme as a promising storage material for both hydrogen and carbon dioxide.
- Research interest encompasses a broad spectrum of condensed matter phenomenon including quantum magnetism, DNA and graphene electronics, charge transfer in organic solids and polymers,

nonlinear optics and Bosonic traps in optical lattice. State-of-the-art numerical methodology involves Density functional theory, Configuration Interaction,  $T=0$  many-body perturbation theory, finite temperature methods with statistical averaging, and non-perturbative renormalization group based on density matrix formalisms.

- Multifunctional oxides: Determined the coupling between structural instabilities and magnetic ordering.
- Simulated one-dimensional nano-structures, such as carbon and BN nanotubes, Te and Se nano-wires, in complement to local experiments.
- Simulated effects of doping on vibrational properties of graphene.
- Developed further the method of first-principles model-based molecular dynamics to (a) simulate switching in ultra-thin ferroelectric films, and (b) determine numerically exact free energy landscape of ferroelectric or structural phase transitions. Using first-principles calculations, explained how multi-ferroic behavior emerges in BaTiO<sub>3</sub> at nano-scale, observed in experiment. Complemented experimental work on graphene and B, N doped graphene bilayers through computation of their Raman and electronic spectra.

#### \* New Observations:

- The emergence of a nematic order in ILs under shear.
- Effective coordination number is found to be a good predictor of catalytic activity.
- Predicted semiconducting carbon nano-tube with a line defect, that can be indexed with fractional numbers.

#### Innovations:

- Using effective coordination as a way of predicting adsorption and reaction barriers.
- The magnetic behaviors are closely correlated to the degrees of freedom of DNA basepairs and tuning this could lead to efficient SMM with high  $T_c$ .
- Intrinsic half-metallicity upon hole doping in zigzag graphene nanoribbon edges.
- A new class of nanotubes with truly one dimensional carrier states.

#### Research publications:

In the year 2008, 2007 and 2006, 55, 40 and 33 papers were published, respectively. In the first two months of 2009, 11 papers have been published.

#### Visitors Programme:

During this financial year, 4 scientists and 3 students have visited for periods of about a week to 2 months for research / collaborative work with CCMS members.

The following are the members of the Unit:

##### **Coordinator**

Balasubramanian Sundaram

##### **Members**

Shobhana Narasimhan  
Srikanth Sastry  
Swapan Pati  
Umesh Waghmare

##### **Associate Members**

**System Administrator**  
Ershaad Ahamed Basheer  
Amit Kumar Patel

##### **Programme Assistant**

Venkatesh



## 11. Chemical Biology Unit

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

MS assisted sequence determination and structural characterization of cyclodepsipeptides from fungus *Isaria*

In this work, an electrospray ionization mass spectrometer (ESI MS) coupled with an ion trap analyzer (capable of generating MS<sup>n</sup> data, n = 2, 3 etc.) and operated in positive ion mode was applied to characterize fragmentation behavior of two classes of cyclodepsipeptides, namely *isariins* (possessing one b-hydroxy acid and five a-amino acids) and *isaridins* (composed of one a-hydroxy acid, four a-amino acids and one b-amino acid) isolated from a fungus, *Isaria*. Changes in fragmentation pattern of these cyclic peptides in the presence of different metal ions (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Ag<sup>+</sup>) were also studied. The objectives were to get information about

1. Extent of sequence coverage from MS<sup>2</sup> as well as from MS<sup>n</sup> type experiments
2. Quality of spectra (by measuring peak intensity), generated in the presence of different metal ions
3. Fragmentation pattern for generating consensus of sequencing

Considering the spectral information of different metal ion adducts with the cyclodepsipeptides it can be concluded that in MS<sup>2</sup> as well as in MS<sup>n</sup> mode, Ag<sup>+</sup> adduct gives best sequence coverage. A consensus made for sequence coverage from MS<sup>2</sup> as well as from MS<sup>n</sup> data is as follows: Ag<sup>+</sup> > H<sup>+</sup> > Li<sup>+</sup> > Na<sup>+</sup> >> K<sup>+</sup>.

On the basis of quality of spectra, Ag<sup>+</sup> adducts and protonated molecules produce more information with readily assignable daughter ion peaks. The consensus made from MS<sup>2</sup> and MS<sup>n</sup> data is as follows: Ag<sup>+</sup> e<sup>-</sup> H<sup>+</sup> > Li<sup>+</sup> > Na<sup>+</sup> >> K<sup>+</sup>.

Analysis of fragmentor ions in the tandem mass spectrometry experiments shows that for *Isariins* in the presence of all metal ions, back bone cleavage occurs at the ester-bond and the observed fragmentor ions belong to 'b-ion' series (according to Biemann's nomenclature). Even in the acyclic methyl-ester derivatives obtained from the cleavage of cyclic-ester bond (treating the cyclic compound with absolute MeOH at 55 °C), identical trend is followed. However for *isaridins*, ring opening occurs at different positions either at the ester linkage or at the amide linkage or at both the positions depending on the types of metal adducts. Further, the MS/MS data of the metal adducted cyclodepsipeptides show fragmentor ions belong to both b and y ion series. But in the case of acyclic methyl-ester derivatives of isaridins, only y-ion series is generated irrespective of the metal ions.

Further, *de novo* approach was followed to get sequence information of four new cyclodepsipeptides with measured molecular masses at m/z, 526, 612, 626 and 596, isolated from *Isaria* chloroform extract.

### Studies on cytosolic chaperones SecA and SecB

In *Escherichia coli*, the cytosolic chaperone SecB is responsible for the selective entry of a subset of precursor proteins into the Sec pathway. *In vitro*, SecB binds to a variety of unfolded substrates without apparent sequence specificity, but not native proteins. Selectivity has therefore been suggested to occur by kinetic partitioning of substrates between protein folding and SecB association. Evidence for kinetic partitioning is based on earlier observations that SecB blocks the refolding of the precursor form of maltose-binding protein (preMBP) and slow-folding maltose-binding protein (MBP) mutants, but not faster-folding mature wild-type MBP. In order to quantitatively validate the kinetic partitioning model, we have independently measured each of the rate constants involved in the interaction of SecB with refolding preMBP (a physiological substrate of SecB) and mature MBP. The measured rate constants correctly predict substrate folding kinetics over a wide range of SecB, MBP, and preMBP concentrations. Analysis of the data reveals that, for many substrates, kinetic partitioning is unlikely to be responsible for SecB-mediated protein export. Instead, the ability of SecB-bound substrates to continue folding while bound to SecB and their ability to interact with other components of the secretory machinery such as SecA may be key opposing determinants that inhibit and promote protein export, respectively.

### Studies on cationic lipids and DNA binding ligands

The effect of the headgroup variation on the gene transfer properties of cholesterol based cationic lipids possessing ether linkage has been worked out. Structure-activity investigation on the gene transfection properties of cardiolipin mimicking gemini lipid analogues have been studied. Photophysical and duplex-DNA-Binding properties of distamycin dimers based on 4,4'- and 2,2'-dialkoxybenzenes as the core have been investigated.

### Soft/nano materials

Physical gelation of binary mixtures of hydrocarbons mediated by n-lauroyl-L-alanine and characterization of their thermal and mechanical properties has been made. Novel nanocomposites made of single-walled carbon nanotubes and low molecular mass organogels and their thermo-responsive behavior triggered by near IR radiation have been studied. Structural and Rheological Properties of Aqueous Viscoelastic Solutions and Gels of Tripodal Cholamide-Based Self-Assembled Supramolecules have been investigated in detail. Facially amphiphilic bile thiol capped silver nanoparticles have been synthesized.

### Synthesis of bioactive molecules

- The total synthesis of a number of complex bioactive molecules such as ( $\pm$ )-frondosins A & B and (+)-hexacyclinol have been achieved. Synthetic methodology has been developed towards the polycyclic core units of several other bioactive molecules.

The following are the members of the Unit:

#### Chair

Uday Maitra

Ph D, FA Sc.

#### Professor

V Krishnan

(Hindustan Lever Research Professor)

Ph D, FA Sc, FNA, FTWAS

#### Honorary Professors

P Balaram

G Mehta

Ph D, FA Sc, FNA, FTWAS

Ph D, FA Sc, FNA, FTWAS

#### Honorary Faculty

Raghavan Varadarajan

Santanu Bhattacharya

Ph D, FA Sc, FNA

Ph D, FA Sc



## 12. Condensed Matter Theory Unit

### Significant Research Accomplishments

The members of the Condensed Matter Theory Unit (CMTU) are engaged in theoretical research on a wide variety of topics in the general area of Condensed Matter Science. During the period from 2008-09, they achieved significant progress on several problems in this area in which support from JNCASR has been acknowledged, and these are summarized below. More details can be gleaned from the publications of CMTU.

### Quantum Condensed Matter, especially Strongly correlated Systems:

- A new theory for time resolved Photo emission experiments and other pump-probe experiments in condensed matter was developed.
- A new strong-coupling expansion technique for calculating Greens functions, self energies and correlation functions in strongly correlated models including the effects of confining potentials, and thermal effects that will be of value for cold atom systems was developed.
- Non-classical rotational inertia of superfluids in complex geometry. Soft Condensed Matter and Nonequilibrium Statistical Physics :
- Finite-size scaling studies of growing length and time scales in glass-forming liquids.
- Dynamics of water molecules in narrow carbon nanotubes.
- The study of the dynamic multiscaling of time-dependent structure functions in different models of passive-scalar and fluid turbulence for both statistically steady and decaying turbulence was systematized by carrying out extensive analytical and numerical studies of models for such turbulence. This work shows, in particular, that dynamic multiscaling exponents are related *via* bridge relations to equal-time multiscaling exponents and that these exponents are the same for statistically steady and decaying turbulence.
- It has been shown that the use of a high power of the Laplacian in the dissipative term of hydrodynamical equations leads asymptotically to truncated inviscid conservative dynamics with a finite range of spatial Fourier modes. Those at large wave numbers thermalize, whereas modes at small wave numbers obey ordinary viscous dynamics. The energy bottleneck observed for finite dissipativity may therefore be interpreted as incomplete thermalization.
- Extensive studies of spiral-wave dynamics in four partial-differential-equations for cardiac tissue have been carried out which establish that such dynamics depends very sensitively on the shape, size, and properties of inhomogeneities.

The following are the members of the Unit:

#### Chair

HR Krishnamurthy

Ph D, F A Sc, F N A

#### Hon. Professors

Biman Bagchi

Ph D, F A Sc, F N A, FTWAS

Chandan Dasgupta

Ph D, F A Sc, F N A

N Kumar

Ph D, F A Sc, F N A, FTWAS

S Ramasesha

Ph D, F A Sc.

D D Sarma

Ph D, F A Sc, F N A

#### Hon. Faculty

G Ananthakrishna

Ph D, F A Sc

Binny J Cherayil

Ph D

Diptiman Sen

Ph D, F A Sc

Rahul Pandit

Ph D, F A Sc, F N A

K L Sebastian

Ph D, F A Sc

Sriram Ramaswamy

Ph D, F A Sc

S Yashonath

Ph D, F A Sc

#### Research Associate

Sarika Bhattacharya

#### R & D Assistants

Abhijit Hazarika, Ganapati Sahoo, Nandan Pakhira, Srijan Kumar Saha

### 13. Computer Laboratory

During the year 2008-2009 the CompLab was involved in upgrading and enhancing the IT infrastructure in the campus. With the procurement of an additional bandwidth of 2Mbps from Sify (this effort was initiated during the tenure of Prof. Umesh Wagmare, previous Head of CompLab), the current internet bandwidth has been raised to 4Mbps. This additional bandwidth has helped to increase the internet speed significantly as well as to extend the internet facility to other buildings. The LAN backbone facility has recently been extended to the "Hostel-Office" and the "Health-Center" which makes the respective staffs to interact with their office work through LAN also. Wi-Fi facility has been provided to the new Dining Hall. We plan to extend this Wi-Fi connection to the Students' Hostel during 2009-2010. The Gigabit LAN facility was also extended to new "Stores and Purchase section" and the scholar room at the AMRL building.

A spam-controller, IronPortC150, was installed in the CompLab to block malicious, unwanted mails. It has been licensed for 600 users. This prevented the mail server and individual mailboxes from a lot of spams. 3TB of data which is critical has been backed up on hard disks which were procured this year. Hundred licenses for windows-vista (50) and office-2007 (50) have been procured. LAN cabling has been upgraded from CAT-V to CAT-VI standard.

ICMS (International Centre for Material Science) facility which was dedicated to the nation during this year went with full fledged Gigabit networking and wireless facilities which was accomplished by the CompLab. The same network-facility was provided to the International-House (I-House) which is a guest house for all visiting researchers at JNCASR. Programs such as POCE (Project Oriented Chemical Education), POBE (Project Oriented Biological Education) which were shifted to C.N.R Rao Hall Of Science, and the related gigabit networking LAN along with internet-facilities were provided by the CompLab.

For the CompLab printing facility, a new Xerox-printer (model 7345) has been procured which supports both colour and black-and-white printing as well as high quality posters on A3-size papers. This printer also supports scanning and xeroxing.

The following are the members of the CompLab:

**Head**

Meheboob Alam

PhD

**R & D Assistants**

B Dharmasena, R Ravikumar, Vikas Mohan Bajpai

**Engineer (Facility Management from Locuz/Enterprise Solutions)**

K Nishaj





## 14. Library

The Library presently has a collection of 5625 books and subscribes to 130 Scientific Journals. We continued to acquire, organize and disseminate information resources to render need based information services to faculty, students and researchers. Following are the initiatives taken in the year 2008-09:

### 1. Document Delivery Service (DDS)

Document Delivery Service has been launched to facilitate JNC community to get easier and faster access to the resources which are not available in JNCASR library. Journal articles which are requested by the faculty and students are procured from IISc library or the libraries across India in the form of hard or soft copy. The library also provides an inter-library loan facility with neighbouring institutes such as IISc, RRI, NCBS and NIAS.

### 2. Joining DST-CSIR E-journal Consortium

The Department of Science and Technology (DST) has initiated the move to get all DST Institutions associated with the existing CSIR E-journal Consortium. This is enabling DST institutions to access the resources which are available in CSIR consortium. In this process the institute is getting access to all the journals from the publishers in addition to our subscribed ones. The publishers which are presently available through the consortium are: Nature, IEEE, Cambridge University Press, Oxford University Press, and Sage Publishing whereas Elsevier, American Chemical Society, Taylor & Francis, Royal Society of Chemistry and several others are there in the pipeline. JCCC is a Document Delivery Portal which has been subscribed by the consortium. This portal provides search option to the journal holdings of all the participating libraries of CSIR and DST and further enables to send online requests for articles to the nearest library.

### 3. Digital Library Initiative

The work of digitization is in progress. A high-end HP Server and an Optical Channel based storage box has been procured which is capable to storing and providing instant access to the huge data of the upcoming JNCASR digital repository.

### 4. Collection Development

#### 4.1 Books Acquisition and Budget spent

In the financial year 2008-09, 1,487 books worth Rs. 23,82,990/- have been procured so far in the library based on the recommendations of JNCASR Faculty members. With the procurement of books for the current year the total books in stock has reached 5929 (Five thousand Nine Hundred and Twenty Nine) books.

#### 4.2 Journal Subscription and Budget

Since 2007 most of the print journals are made accessible online. Rs. 1.5 crore is the journal budget approved for the year 2009.

#### 4.2.1 New Journal Titles

Following are the new titles added in 2009 to our e-journal collection, cost approx. Rs. 2,83,000/- (Rs. Two Lakhs Eighty Three Thousand Only):

1. American Journal of Primatology (Wiley Blackwell Publication)
2. Nature Neuroscience (Nature Publishing Group)

The following are the members of the Library:

**Library In-Charge**

YM Patil

Ph D

**Library-cum-Information Officer**

Nabonita Guha

MLIS (Banaras Hindu Univ.)

**Library Assistant**

Nandakumari, Hadimani Nagesh

**Library Trainee**

Jaiprakash HL

**Helper**

Rajeeva J.

## Endowed Research Professors

**DS Kothari Chair**

M M Sharma

FRS, FASc, FNA

**Hindustan Lever Chair**

TV Ramakrishnan

FASc, FNA, FTWAS

**Linus Pauling Research Professor**

CNR Rao

FASc, FNA, FRS, FTWAS,  
Hon.FRSC



## ACADEMIC PROGRAMMES

### 1. Academic Activities

The Centre offers regular Ph D, Integrated Ph D, M S (by research) and M S Engg. (by research) degree programmes in Science and Engineering. The Integrated Ph D programme in Materials Science is available to those with a B Sc degree. The regular Ph D programme is available to graduates and post-graduates in science and engineering, who have successfully completed GATE/UGC-CSIR-NET, JRF, ICMR JRF/JEST/ equivalent examinations. The Centre selects candidates on an all-India basis, offers course work, provides research facilities, administers the programme and awards the degree.

#### (a) Research Admissions

Nineteen students under the MS/Ph D programme and 9 students under the Integrated Ph D programme were selected for the August 2008-09 semester and 12 students were selected during mid-year admissions for January 2008-09 semester. The student strength at the Centre is now 154.

The Unit-wise students' strength are as follows:

Unit	Int. PhD	PhD	MS/MS Engg.	Total
CPMU	22	32	01	55
NCU	00	03	00	03
EMU	00	07	11	18
EOBU	00	09	01	10
MBGU	00	44	01	45
TSU	00	19	04	23
<b>Total</b>	<b>22</b>	<b>114</b>	<b>18</b>	<b>154</b>

#### (b) Degrees awarded

During the year 2008-09, 15 Ph D, 8 M.S (Engg.) and 2 M S (Int. Ph D) students have been awarded degrees. Details of degrees awarded during the year are as given below:

Sl. No.	Units	Degree	Name of the Students
1	Chemistry & Physics of Materials	Ph D	Moumita Saharay, Bhargava B L, Pavan Kumar GV, A Thirumurugan, G Kavitha, Ved Varun Agrawal, Chandrasekhar Rout.
		MS (Engg.) (by research)	Leela Srinivas Panchakarla, Kalyan Raidongia, K S Subrahmanyam
		MS (Int. Ph D) in Chemical Sciences	Neenu Varghese, Shrinwantu Pal
2	Molecular Biology & Genetics	Ph D	Prasanth Kumar Dash, Kiran Batta, Debjani Das, Sonali Mehrotra
3	Theoretical Sciences	Ph D	Mousumi Upadhyay Kahaly, Prasenjit Ghosh, Gargi Dutta
4	Engineering Mechanics	Ph D	Mukund Vasudevan
		MS (Engg.)	Kaushik Srinivasan, Pinaki Bhattacharya, Bishakhdatta Gayen, Vijayakumar K Chikkadi, A Rajapandian

## 2. Discussion Meetings/Workshops

1. *Frontier Lectures in Chemistry*, April 12-13, 2008, at Mangalore University, Prof Uday Maitra, IISc.
2. *Bangalore Area Statistical Mechanics Meeting*– 2008, April 12-13, 2008, Dr Subir K Das, JNCASR.
3. *Futuristic Aspects & Directions in Advanced Materials (FADAM)*, April 16-19, 2008 at Shimla.
4. *Managing Complexity in a Distributed World*, May 27-31, 2008, Prof H P Khincha, IISc.
5. International Conference on “*Aerospace Science & Technology*”, June 26-28, 2008, Dr A R Upadhyaya, Director, NAL.
6. *Electrochemical Science and Technology, NSEST-2008*, July 18-19, 2008, Dr J R Mudakavi, IISc.
7. *Twelfth Asian Congress of Fluid Mechanics*, August 18-21, 2008, Prof G S Bhat, IISc.
8. *JNC-Purdue Meeting*, August 19-21, 2008, Prof G U Kulkarni, JNCASR.
9. *4<sup>th</sup> Kannada Vijnana Sammelana*, September 15-17, 2008, Swadeshi Vijnana Andolana.
10. *JNC Research Conference on Chemistry of Materials*, September 27-29, 2008 at Alleppy, Kerala, Dr M Eswaramoorthy, JNCASR.
11. *JNCASR-FCBS Workshop for Postgraduate students*, October 13-15, 2008 at Trivandrum, Prof S Chandrasekaran, IISc
12. *Annual Meeting of Trendys-2008*, November 14-15, 2008, Prof H S Savithri, IISc.
13. *Indo-US Conference on Translational Medicine and Infectious Diseases*, November 17-20, 2008 at National Institute of Technology, New Delhi, Dr Akhil C Banerjee,
14. *JNC-Frontier Lecture Series*, November 20-21, 2008 at Bhavnagar, Prof V Krishnan, JNCASR.
15. International Symposium on ‘*Current Trends in Organic Synthesis*’, November 20-22, 2008, Prof Uday Maitra, IISc.
16. *Satellite Meeting to 2<sup>nd</sup> Asian Forum of Chromosome & Chromatin Biology Meeting. “Chromatin and Transcription Regulation”*, November 25, 2008, Prof Tapas Kumar Kundu, JNCASR.
17. *Winter School*, December 2-15, 2008, Prof Swapan K Pati, JNCASR
18. International Conference on “*Molecules & Materials: New Directions*”, December 4-6, 2008, Prof G U Kulkarni, JNCASR.
19. Conference on “*Eighty Years of Raman Effect: Reflections & Future*”, December 8-10, 2008, Prof S Umapathy, IISc.
20. National Conference on *Some Major National Problems and Solutions*, December 12-14, 2008, Mr A P Deshpande, NCSC, Mumbai.
21. *6<sup>th</sup> Asian Young Geotechnical Engineers Conference*– 2008, December 20-21, 2008, Prof T G Sitharam, IISc.
22. *High School Science Teachers programme at Bijapur District*, December 22-31, 2008, Prof Arun M Umarji and Prof S Ramakumar, IISc.
23. International Conference on “*Hydrogen & Hydrogen Storage- Methods and Materials*”, January 3-6, 2009, Dr B P Jagiradar and Prof A G Samuelson, IISc; Sponsor : JNCASR
24. International Workshop “*Strong Frontier 2009*” January 12-18, 2009, Prof N D Hari Dass, Poorna Prajna Institute of Scientific Research.
25. International Conference on Hampi on “*Tangible & Intangible Heritage Issues of Hampi*”, January 16-18, 2009, Prof S Ranganathan, IISc
26. *Theoretical Chemistry Meeting (National Meeting)*, January 18-23, 2009, Prof Biman Bagchi, IISc
27. *18<sup>th</sup> International Science and Engineering Conference*, January 19-23, 2009 at Kolkata, Prof A K Barma



28. International conference on "Germ Cell Development – Function", January 22-24, 2009, Prof P B Seshagiri, IISc
29. International Conference and School on "Emergence in Genomic Matter: An interdisciplinary approach to understand the human genome organization", February 8–16, 2009, Prof N Chandrabhas and Prof T K Kundu, JNCASR.
30. 20<sup>th</sup> AGM (AGM 2009) of Materials Research Society of India (MRSI), February 10-12, 2009, Prof N R Bandyopadhyay, MRSI Kolkata Chapter
31. International Conference on "Tissue Engineering & Stem Cell Research using Nanomaterials", February 17-19, 2009, Prof Shantikumar Nair, Director, Amrita, Kerala
32. Malaria Meeting, March 3-5, 2009, Dr Swati Patankar, IIT Bombay; and Prof Namita Surolia JNCASR.

### 3. Colloquia

The following JNCASR Colloquia were held during the period under the series:

- *Democracy as Common Sense: Can the "Right to Information" bring Rationality and Ethics into Democratic Decision Making*, Smt. Aruna Roy, Mazdoor Kisan Shakti Sanghatan, National Campaign for People's Right to Information (NCPRI), April 22, 2008.
- *An atomistic view of the initial stages of interface formation*, Prof S M Shivaprasad, April 29, 2008.
- *Toxicity inherent with RNA polymerases and transcription*, Dr. J. Gowrishankar, Centre for DNA Fingerprinting & Diagnostics, Hyderabad, August 5, 2008
- *How good is the scientific evidence for global climate change?*, Prof J Srinivasan, Indian Institute of Science, Bangalore, August 26, 2008
- *Computer Simulation of Protein Dynamics*, Jeremy C. Smith, Governor's Chair and Director, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, USA., September 30, 2008.
- *Between Three Hard Places: India's Energy and Climate Change Policies*, Mr MV Ramana, Centre for Interdisciplinary Studies in Environment and Development, Institute for Socio Economic Change, Bangalore, October 14, 2008.
- *Fluid dynamics from gravity*, Prof. Shiraz Minwalla, Theoretical Physics, TIFR Mumbai, December 2, 2008.
- *The queen of the tropical sky: The cumulus cloud as a problem in fluid dynamics*, Prof Roddam Narasimha, JNCASR, February 24, 2009.
- *Protein complexes that modify chromatin for transcription*, Prof Jerry L. Workman, Stowers Institute for Medical Research Kansas City, Missouri, USA, March 9, 2009.

### Fluid Dynamics:

The following colloquia were held during the period :

- *Channel flow mode of extrusion of higher Himalayan shear zone, NW Himalaya and salt diapirs of Hormuz & Namakdan, Persian Gulf - Tectonic insights*, Dr Soumyajit Mukherjee, JNCASR, April 9, 2008.
- *A wave driver theory for vortical waves propagating across alternate rigid and compliant panels*, Prof P K Sen, Centre for Applied Mechanics, IIT Delhi, April 18, 2008.
- *Minimal molecular dynamics*, Dr. Santosh Ansumali, Assistant Professor, School of Chemical and Biomedical Engg, Nanyang Technological University, Singapore, June 19, 2008
- *Experimental Diagnostics for Aerospace Applications*, Dr. Jürgen Kompenhans, Head, Experimental Methods, Institute of Aerodynamics and Flow Technology, German Aerospace Center, Göttingen, Germany, June 25, 2008.
- *Aeroacoustics of high-speed jets: role of linear and nonlinear mechanisms*, Dr. Sanjiva Lele, Associate Professor, Department of mechanical engineering, Stanford University, June 26, 2008.

- *Unsteady simulation of turbine blade cooling*, Prof. Paul Durbin, Aerospace engineering, Iowa State University, June 27, 2008.
- *Structure and dynamics of fluids confined at the nanoscale*, Prof K Ganapathy Ayappa, Dept. of Chemical Engineering, Indian Institute of Science, Bangalore, July 2, 2008.
- *Mechanical design in cardiovascular systems*, Dr Namrata Gundiah, August 4, 2008.
- *Direct/adjoint analysis of non-normal thermoacoustic systems*, Dr. Mathew Juniper, Engineering Department, Trumpington Street, Cambridge, November 25, 2008.
- *CFD study in benchmark problem - backward facing step*, Dr. H.P.Rani, Lecturer, Department of mathematics and humanities, National Institute of Technology, Warangal, December 3, 2008.
- *Mean momentum balance analysis of rough-wall turbulent boundary layers*, Dr Faraz Mehdi, Department of mechanical engineering, University of New Hampshire, USA, December 16, 2008.
- *Numerical simulations of miscible channel flow with viscosity and density stratifications*, Dr. Kirti Chandra Sahu, Post-Doctoral Research Associate, Department of Chemical Engineering, Imperial College London, January 7, 2009.
- *Polymeric turbulence and time scales of turbulence*, Dr. Dhruvhaditya Mitra, School of Mathematical Sciences, Queen Mary College, University of London, January 12, 2009.
- *Characterizing magnetic particle transport for microfluidic applications*, Dr. Ashok Sinha, Virginia Polytechnic Institute and State University, January 21, 2009.
- *Plasma climatology: key issues in tokamak turbulence and fusion research*, Dr. Tyagarajan, Theory and Modelling, Culham Science Centre, EURATOM/UKAEA Fusion Association, Abingdon, OX14 3DB, UK, February 26, 2009.
- *Elastohydrodynamic phenomena in viscous and viscoelastic liquids*, Prof. V.Shankar, department of chemical engineering, IIT Kanpur, March 25, 2009.

#### 4. Endowment Lectures

##### AV Rama Rao Foundation Lectures in Chemistry :

*Atomic and molecular clusters: Designer materials for the nanoworld*, Prof N Satyamurthy, Director, IISER, Mohali;

*Photoresponsive Soft Materials (Prize Lecture)* Prof Suresh Das, National Institute for Interdisciplinary Science and Technology, CSIR, Trivandrum, on May 15, 2008.

##### ISRO Satish Dhawan Lecture 2008:

*The Sense of Wonder: The Indian Painter and his Work*, Prof. B.N. Goswamy, Punjab University, Chandigarh, July 14, 2008.

##### Prof. V. Ramalingaswami Memorial Lecture :

*How Structural Biology is driving information-based Innovation*, Sir. Tom Blundell FRS FMedSci, Professor and Head of Bio Chemistry, University of Cambridge, August 12, 2008.

##### C N R Rao Oration Award Lecture:

*Multiple Approaches to Fight Malaria*, Prof Namita Surolia, August 13, 2008 followed by welcome to new students.

##### DAE Raja Ramanna Lectures in Physics:

*Low-dimensional physics using nanomaterials*, Prof Milan K Sanyal, Saha Institute of Nuclear Physics, Kolkata;

*Morphotropic Phase Transitions in Ferroic and Multiferroic Oxide Perovskites*, (Prize Lecture) Prof Dhananjai Pandey, School of Materials Science and Technology, Institute of Technology, BHU, Varanasi, , September 9, 2008.



## 5. General Lecture

### Guest Lectures

*Host catalyzed capsid assembly: From novel paradigm to a new generation of anti-viral drugs*, Prof Vishwanath R. Lingappa M.D., Ph.D, Professor Emeritus Department of Physiology University of California, San Francisco, December 19, 2008.

*Molecular biology of virus mediated cancer: Understanding the role of Epstein Barr virus (EBV) latency protein in cancer metastasis*, Dr. Rajeev Kaul, University of Pennsylvania School of Medicine, January 21, 2009.

*Genetic and functional characterization of HIV-1 genes from north India and gene therapeutic approaches*, Prof Akhil C. Banerjee, Chief - & Staff-Scientist, Lab- Virology, National Inst Immunology, JNU Campus, New Delhi-110067, March 31, 2009.

## 6. Lectures delivered at the Annual Faculty Meeting by Faculty/ Hon. Faculty

*What have we learnt about the organization of membranes and proteins from Slow solvent relaxation* by Dr Amit Chattopadhyay

*Challenging materials issues in GaN optoelectronics for solid state lighting* by Prof S M Shivaprasad

*Two problems in Evolutionary Biology* by Dr Kavita Jain

*Understanding collective behaviour in cellular slime mould development* by Prof V Nanjundiah

*Growing length and time scales in glass forming liquids* by Prof Chandan Dasgupta

## 7. Seminars

The following seminars/workshops were held during the period:

1. *Steady States of Passive Particles Sliding on Fluctuating Surfaces*, Dr Apoorva Nagar, Korea, Institute for Advanced Studies, Korea, April 2, 2008.
2. *Vibrational spectral diffusion in aqueous solutions*, Dr Amalendu Chandra, Department of Chemistry, IIT Kanpur, Kanpur, April 9, 2008.
3. *Invariant solutions and visualization of state-space dynamics in plane Couette flow*, Prof John Gibson, School of Physics and Center for Nonlinear Science, Georgia Institute of Technology, USA, April 21, 2008.
4. *Metal and Metal Oxide Particles in Nanometer Length scale*, Prof Tarasankar Pal, Department of Chemistry, Indian Institute of Technology, Kharagpur, April 21, 2008.
5. *Studies on p300 auto-acetylation and its protein-protein interactions (journey from Jakkur to Johns Hopkins)*, Dr Balasubramanyam K, Johns Hopkins University, USA, April 28, 2008.
6. *Quantum entanglement – mystery element of quantum information science*, Dr AR Usha Devi, Bangalore University, April 30, 2008.
7. *Self Organized Substrates as Templates for Magnetic Nanostructures*, Dr Yann Girard, Laboratoire Matériaux et Phénomènes Quantiques Université Paris 7- CNRS, France May 1, 2008.
8. *Hierarchical materials: bridging structure and properties across length scales*, Dr Erika Merschrod, Memorial University of Newfoundland, May 2, 2008.
9. *Conduction in Metal Hydrides*, Dr Timothy S. Fisher and Dr Kyle C. Smith, Purdue University Department of Mechanical Engineering, May 2, 2008.
10. *Micro/Nano Technologies for Bioengineering Applications*, Dr. Javeed Shaikh Mohammed, Department of Bioengineering, University of Illinois at Chicago, Chicago, IL, May 6, 2008.
11. *Some Transport Anomalies in Two Dimensional Electron Systems*, Dr V. Pai, Technion, Israel, May 6, 2008.
12. *Structure and Dynamics of Fluids Confined at the Nanoscale*, Prof Ganapathy Ayappa, Chemical Engineering Dept, IISc, May 7, 2008.

13. *Transport properties of low dimensional systems*, Dr V Pai, Technion, Israel, May 12 and 13, 2008.
14. *Some simple models of classical heat and particle pumps*, Dr Rahul Marathe, Raman Research Institute, Bangalore, May 14, 2008.
15. *Technology Talk*, Dr B S Adiga, Consultant, TCS, May 28, 2008.
16. *Time-dependent density-functional approaches for optical excitations in semiconductors*, Prof Carsten A. Ullrich, University of Missouri, May 29, 2008.
17. *Simulation of Bacteriorhodopsin Proton Transfer Process using Multi-scale approach*, Dr Prasad Phatak, TU-BS, Germany, July 10, 2008.
18. *Stability analysis of double diffusive system with time varying temperature and salinity profiles*, Mr Niranjana S Ghaisas, Dept. of Mechanical Engg., Indian Institute of Science, Bangalore, July 15, 2008.
19. *Meiotic crossing over: characterizing the role of the MSH-MLH complex*, Dr. Nishant T. Koodali, Department of Molecular Biology and Genetics, Cornell University, Ithaca, NY 14853-2703, July 16, 2008.
20. *Thermo-fluid-dynamic aspects of vapour-droplet and gas-particle flows*, Dr Abhijit Guha, Dept. of Aerospace Engineering, University of Bristol, Bristol, U K, July 22, 2008.
21. *Novel phenomena in low dimensional systems*, Dr Sumathi Rao, HRRI, Allahabad, July 23, 2008
22. *The complexity of gene regulation: computational methods and a recent example*, Dr. Rahul Siddharthan, Reader, Institute of Mathematical Science, Chennai, July 29, 2008.
23. *Transport Processes in Polymer Electrolyte Membrane*, Prof Ajay K Prasad, Department of Mechanical Engineering, University of Delaware, Newark-DE, USA, August 4, 2008.
24. *Metal/Semiconductor Superlattices as Thermoelectric Metamaterials*, Prof. Timothy D. Sands, Purdue University, West Lafayette, IN, August 22, 2008.
25. *Stress relaxation in a colloidal glass: strain induced jamming and microscopic viscosities*, Dr Ranjini Bandyopadhyay, Raman Research Institute, Bangalore, August 27, 2008.
26. *Understanding and Controlling Cavitation in Biomedical Applications*, Dr. Manish Arora, Institute for Biomedical Engineering, Oxford University, September 2, 2008.
27. *Detection and manipulation of chiral objects*, Dr. Ambarish Ghosh, Rowland Institute at Harvard University, USA, September 2, 2008.
28. *Electron transport at the mesoscale*, Prof Mukunda Das, Australian National University, September 5, 2008.
29. *Single molecule and Single chain magnets*, Prof J P Sutter, LCC, Toulouse, France, September 12, 2008.
30. *Wires, Reporters and Information Capsules: Cellular journalism with DNA*. Prof Yamuna Krishnan, NCBS, Bangalore, September 17, 2008
31. *Phases and Excitations of Cold Atoms in Optical Lattices*, Dr. Venkateswara Pai, Physics, Technion Univ, Israel, September 18, 2008
32. *Pattern Formation in Kinetics of Phase Transitions*, Prof Sanjay Puri, School of Physical Sciences, JNU, New Delhi, September 26, 2008.
33. *The Human Circadian Clock in Daily Life*, Prof. Dr. Till Roenneberg, Centre for Chronobiology, Institute for Medical Psychology, Medical Faculty, Ludwig-Maximilians-University, Munich, October 3, 2008.
34. *Global stability and control of flow over a cavity*, Prof Peter Schmid, Department of Applied Mathematics, University of Washington, Seattle, October 23, 2008
35. *New Challenges in Disseminating Science*, Prof Sami Mitra, American Physical Society, November 6, 2008.





36. *Dynamics of polymers in shear flow*, Prof. Sanjib Sabhapandit, Raman Research Institute, Bangalore, November 12, 2008.
37. *Materials Science approach to biomaterials research*, Dr. Perumal Ramasamy, November 17, 2008.
38. *Driven out of equilibrium: Using colloids to model atomic epitaxial processes, sheared solvent-free fluids and Rheochaos*, Dr. Rajesh Ganapathy, November 18, 2008.
39. *Green-Kubo formula for heat conduction in open systems*, Prof. Abhishek Dhar, Raman Research Institute, Bangalore, November 19, 2008.
40. *Novel role of a Dynamin-related protein in the nuclear remodeling of Tetrahymena*, Dr Abdur Rahaman, MGCB, University of Chicago, November 24, 2008.
41. *Spin supersolid phase*, Dr. Pinaki Sengupta, Los Alamos National Laboratory, New Mexico, USA, November 26, 2008.
42. *Interaction between heterochromatin and RNAi in fission yeast*, Dr. Jagmohan Singh, Institute of Microbial Technology, Chandigarh, December 1, 2008.
43. *Analytical challenges in mapping complex genetic traits*, Dr. Saurabh Ghosh, Human Genetics Unit, Indian Statistical Institute, Kolkata, December 11, 2008.
44. *Origin and reduction of threading dislocations in GaN and its alloys*, Dr. Ranjan Datta, December 15, 2008.
45. *Homeostasis and flexibility in the large scale genetic regulatory network controlling E. coli metabolism*. Prof. Sanjay Jain, Delhi University, December 17, 2008.
46. *What is Quantum correlation? What are its implications?* Dr. Aditi Sen De, Assistant Professor, School of Physical Sciences, Jawaharlal Nehru University, New Delhi, December 30, 2008.
47. *Protein folding: Revisiting a long unsolved problem with MD and statistical analysis tools*, Dr Aruna Rajan, University of Illinois, Urbana-Champaign, January 2, 2009.
48. *Metallasupramolecular network structures derived from reduced Schiff base ligands*, Dr. Bellam Sreenivasulu, National University of Singapore, January 9, 2009.
49. *'Supersolid' Helium-4: A new state of matter?*, Dr Vikram Gadagkar, Physics Department, Cornell University, Ithaca NY 14853, USA, January 13, 2009.
50. *Routes to helicity*, Dr. Dwaipayan Chakrabarti, Research fellow, Department of Chemistry, University of Cambridge, Cambridge, January 23, 2009.
51. *Phase ordering processes and different ways to remain out of equilibrium*, Prof. Marco Zannetti, Salerno, Italy, January 27, 2009.
52. *Membrane-based action of antimicrobial oligomers: an atomistic view from simulations*, Dr. Jerome Henin, Department of Chemistry, University of Pennsylvania, January 28, 2009.
53. *Evolution of the code of life*, Dr. Supratim Sengupta, Centre for Computational Biology & Bioinformatics, School of Information Technology, Jawaharlal Nehru University, New Delhi, January 28, 2009.
54. *Environmentally benign chemical process with high-pressure carbon dioxide and high-temperature water*, Dr. Masayuki Shirai, AIST, Sendai, Japan, February 4, 2009.
55. *Population dynamics, genomic evolution, and the emergence of drug resistance during HIV infection*, Prof. Narendra Dixit, Department of Chemical Engineering, IISc, February 4, 2009.
56. *Survival of Cryptococcus neoformans at 37C depends on the integrity of the septin protein complex*, Dr Lukasz Kozubowski, Department of Molecular Genetics and Microbiology, Duke University Medical Center, Durham, North Carolina 27710, USA February 4, 2009.
57. *Self Propelled Particles: From microdynamics to hydrodynamics*, Dr. Aparna Baskaran, Post doctoral research associate, Physics Dept, Syracuse University, Syracuse, NY, February 5, 2009.
58. *Sedimentation of small particles*, Professor Elisabeth Guazzelli, IUSTI CNRS 6595, Polytech'Marseille, Aix-Marseille Universite, France, February 6, 2009.

59. *Structural phase transitions from first-principles*, Dr. Varadharajan Srinivasan, Berkeley Nanoscience and Nanoengineering Institute, University of California, Berkeley, CA 94720, USA, February 13, 2009.
60. *Phonon anomalies in superconductors studied by inelastic X-ray scattering*, Prof. Matteo d'Astuto, IMPMC - Université Pierre et Marie Curie Paris, February 16, 2009
61. *Organic synthesis in supramolecular chemistry and drug discovery*, Dr. Pinaki Talukdar, February 17, 2009
62. *Dynamics of water molecules in narrow carbon nanotubes*, Prof. Chandan Dasgupta, Dept of Physics, IISc, February 18, 2009.
63. *Multiferroic nanowire composites and thin films*, Prof. Arunava Gupta, University of Alabama, USA, March 5, 2009.
64. *Semiconductor sensitized solar cells: aspects of different deposition techniques*, Dr. Shaibal K Sarkar, University of Colorado at Boulder, March 11 and 12, 2009.
65. *Admixture mapping and related ideas: a tale of two ethnicities*, Dr. Analabha Basu, Institute for Human Genetics, University of California, San Francisco, March 11, 2009.
66. *Finding "HITS" against Bromodomain and SIRT1*, Dr. Sachidanand, Institute of Life Sciences, March 16, 2009.
67. *Implementing quantum gates using the Heisenberg ferromagnetic quantum spin chain*, Dr Jaideep Mulherkar, Department of Mathematics, UC Davis, March 18, 2009.
68. *Combining high resolution experiments and theory to study local environment: Core-level spectroscopy*, Prof. Stefano de Gironcoli, SISSA, Italy, March 24, 2009.
69. *Infectious diseases: the ways to tackle*, Dr. Jayanta Haldar, MIT, March 26, 2009.

## 8. International Conferences/Workshops

1. JNC-Purdue Meeting, August 19-21, 2008, Prof G U Kulkarni, JNCASR.
2. Satellite Meeting to 2<sup>nd</sup> Asian Forum of Chromosome & Chromatin Biology Meeting. "Chromatin and Transcription Regulation", November 25, 2008, Prof Tapas Kumar Kundu, JNCASR.
3. Winter School, December 2-15, 2008, Prof Swapan K Pati, JNCASR
4. International Conference on "Molecules & Materials: New Directions, December 4-6, 2008, Prof G U Kulkarni, JNCASR.

International Conference and School on "*Emergence in Genomic Matter: An interdisciplinary approach to understand the human genome organization*", February 8 – 16, 2009, Prof N Chandrabhas and Prof T K Kundu, JNCASR.



## EXTENSION ACTIVITIES

1. Summer Research Fellowships/ Department of Science Technology Fellowships/ Rajiv Gandhi Science Talent Research Fellowships

### Summer Research Fellowships Programme

The Centre offers summer fellowships for two months to bright undergraduate and M.Sc students (renewable for a second year for select students). This programme has proved to be popular and competitive with students all over India applying for the 120 -130 fellowships awarded. Of the 125 fellowships awarded in 2008, Seventy five fellowships are supported by the Department of Science & Technology, Government of India, fifteen by the Rajiv Gandhi Institute for Contemporary Studies, New Delhi, and the rest by the Centre. Students are placed with research groups at the Centre or with scientists elsewhere in India and they are paid a monthly stipend of Rs 5000 during their stay and also reimbursed their travel expenses.

For Summer Research Fellowships Programme 2009, the advertisement was released in seven newspapers in the country. This year, the minimum eligibility criteria was raised to 80% and above in science and mathematics subjects in 10<sup>th</sup> and 12<sup>th</sup>(PUC) and first class and above in bachelor's or master's degree(as applicable).

**Completed Applications Received – 2488**

Break up of applications received and fellowships offered:

	No. of Applications Received (for 2009)	No. of Fellowships Offered (in 2008)	No. of Fellowships utilized (in 2008)
Life Science	1135	38	23
Engineering Science	330	30	24
Atmospheric Science	47		
Physical Science	381	22	16
Chemical Sciences	339	25	17
Mathematics	98	05	04
Materials Science	158	05	05
Total	2488	125	89
Renewal for the second year		30	09
		<b>155</b>	<b>98</b>

### 2. JNC-TWAS-ROCASA – SRFP Programme

The below mentioned are the details of the students selected under the TWAS-ROCASA – SRFP-2008 fellowship :

No	Name	Country	Guide
1.	Mr YPYP Ariyasinghe	Sri Lanka	Prof K S Narayan
2.	Mr Yub Raj Sapkota	Nepal	Prof C N R Rao
3.	Ms Madeeha Afzal	Pakistan	Prof Maneesha Inamdar
4.	Ms Asima Shoukat	Pakistan	Prof M R S Rao
5.	Mr Syed Waqar Ahmed	Pakistan	Prof Amitabh Joshi
6.	Mr Jagaran Acharya	Nepal	Prof Umesh Waghmare
7.	Mr Rafi Ullah	Pakistan	Prof KV Ramanathan

### 3. Academic Exchange Programme

As part of the academic exchange programme, the following scientists/scholars carried out collaborative work with scientists of the Centre and of the Indian Institute of Science for varying periods during the year.

Visiting Professor  
Prof Garry L Brown

Visiting Scientists  
Dr Suparna Mukhopadhyay  
Kalyani Govt. Engineering College,  
Nadia, West Bengal

Dr Tarun K Mondal  
Haldia Institute of Technology  
East Midnapur, West Bengal

Dr Sharmin Kharrazi  
Shahid Behesti University  
Tehran, Iran

Dr Indrani Bose  
Western Carolina University  
USA

Visiting Scholars  
Mr Tapan Naskar  
University Centre for Astronomy &  
Astrophysics, Pune

Ms Shaista Ahmad  
School of Sciences  
JNU, New Delhi

Mr L Nsika Dlamini  
University of Johannesburg  
South Africa

### 4. Project Oriented Biological Education (POBE)

Advertisement for the POBE-2009 has been placed in several newspapers and on the website of JNCASR. Date of receiving the applications is till the end of February 2009 for the batch that shall come to the Centre during mid-May 2009 and stay here for about 8 weeks.

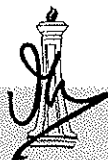
In addition, POBE second batch (2007) and third batch (2008) students will be returning back for their training at the Centre wherein they spend about two months, mostly in laboratories in MBGU and EOBU, in addition to attending special lectures and seminars at the Centre. The students of the POBE 2007 batch who successfully complete the programme will receive a Diploma in Biology from the Centre.

### 5. Project Oriented Chemical Education (POCE)

In order to reach more number of students, POCE-2009 programme was advertised in all major national newspapers. In addition, information about the activities of POCE (along with a copy of the advertisement and application form) was sent to top 125 colleges all over the country.

Two students of POCE-2008 returned during mid semester break of 2008 to work with faculty of the Centre.

Two of the POCE students were selected for Ph.D. Programme of JNCASR –one in Integrated Ph.D (2008) and another in regular Ph.D. (mid - year 2008-09), and they have joined the Centre. Two of POCE students are doing their Ph.D. in USA. The students of the POCE 2007 batch who successfully complete the programme will receive a Diploma in Chemistry from the Centre.



## 6. Science Outreach Programmes

Three workshops on, "Experiments using the College Chemistry Kit" were conducted for students of Jawahar Navodaya Vidyalaya, Doddaballapur and the response was very good.

As a part of "National Science Day" programme, along with Biosciences, a two days workshop/lecture-cum-demonstration was conducted where 20 participants were selected from the top students of various Jawahar Navodaya Vidyalaya.

## 7. Visiting Fellowships

The following Visiting Fellows were selected for 2008-09. and they have been placed under faculty from JNC and IISc for their 2-3 month tenure.

### Physics / Chemistry / Material Sciences : Non- Biological Sciences

Sl No.	Name & Present Position / Employment	Proposed to work With ( Name of the Faculty)
01	Dr R Balagurunathan	Prof G U Kulkarni
02	Dr Debajyoti Ghoshal	Dr Tapas Kumar Maji
03	Dr S Balaji	Dr M Eswaramoorthy
04	Dr Mohd. Ikram	Prof C N R Rao
05	Dr Altaf Hussain Pandit	Prof Swapan K Pati

### Life Sciences / Biological Sciences

01	Dr Raja Banerjee	Prof P Balaram
02	Dr Dharani Dhar Dubey	Dr Kaustuv Sanyal
03	Dr M B Bharathi	Prof Maneesha Inamdar

## 8. Intellectual Property

JNCASR values the creative and innovative research being carried out by its faculty. The Intellectual Property Management Committee of JNCASR fosters IPR culture and addresses all issues concerned with securing, protecting, maintaining and valorizing the Intellectual Property. The Committee facilitates the scientific community in securing patents and in post patent actions.

During the year, the IPM Committee met three times, reviewed a number of inventions and approved filing of patent applications for fifteen inventions. Out of these, eight national and three international patent applications have already been filed, whereas the remaining four are in the process of being filed. The Centre received three patents, granted by the Indian Patent Office and the US Patent and Trademark Office for the inventions made by Prof. Tapas Kundu and his group, and Prof. Ranga Udaykumar. Most of the inventions are in the licensing stage. A couple of inventions was licensed to Companies in India, Switzerland and USA. Nominal royalty on the licensed products viz. *Anacardic Acid* and *CTPB* was received. Negotiations are on with many Companies for further licensing of the inventions.

### Applications Filed

#### International Patent Applications under PCT

- PCT/IN2008/000632, filed on 30/09/2008 for the invention *Intrinsically fluorescent Carbon nanospheres and a process thereof*, Inventors being Kundu TK, Eswaramoorthy M, Selvi BR, Dinesh Jagadeesan.
- PCT/IN2008/000771, filed on 14/11/2008 for the invention *Nanoparticles composition and a process thereof*, Inventor being Chandrabhas N.
- PCT/IN2008/000760, filed on 7/11/2008 for the invention *Polynucleotide sequences and processes thereof*, Inventor being Sanyal K, Sreedevi P, Jitendra T.

## National Phase Applications

### India

- *A template free metal nanosponge and a process thereof*, Inventors being Eswarmoorthy M, Saikrishna K
- *A Tat vaccine, a process and an expression cassette*, Inventor being Ranga U
- *Polynucleotide sequences and processes thereof*, inventor being Sanyal K, Sreedevi P, Jitendra T.
- *SERS active paper substrate and a process thereof*, Inventors being Kulkarni GU, Gupta A, Karthick B, Applicants: JNCASR and M/s. YashNanotech Ltd.

### USA

- No. 12/203,185 filed on 3/9/2008 for the invention *A mirror adapted in microscope to perform surface enhanced Raman Spectroscopy, a microscope and methods thereof*, inventors being Chandrabhas N, Pavan Kumar GV.

### USA, Europe and Japan

- USA Application No. 12/306,675 filed on 24/12/2008, European Application No. 07805629.8-1211 filed on 23/12/2008 and Japanese Application filed on 24/12/2008 for the invention *Site specific inhibitors of histone methyltransferase (HMTase) and process of preparation thereof*, inventors being Kundu TK, Selvi BR, Kishore AH, Mantelingu K.

### Letters Patent Received

- The US Patent (No. 7,402,706 B2 on 22/7/2008) and an Indian Patent was issued (No. 223720, on 19/9/2008) for the invention *'Polyisoprenyl benzophenones as inhibitors of histone acetyltransferases and uses thereof*, Inventors being Kundu TK, Balasubramanyam K, Mantelingu M, Mohammad A, Swaminathan V, Radhika AV.
- An Indian Patent was issued (No. 221411 on 23/6/2008) for the invention *'A novel composition to be used in the field of Molecular Biology'*, Inventor being Ranga U.

### IPR Awareness Program

To update the knowledge of scientific community on the state of the art in the field of IPR, two lectures were held by inviting Experts viz, (a) *Developing Intellectual Property Policy for Public Funded Research Institutions* by Shri R. Saha, Adviser, Ministry of Science and Technology, Dept. of Science and Technology, Govt. of India, New Delhi on 12/11/2008 and (b) *Issues Beyond Patent, With Focus On Patent Commercialisation* by Mr. Vinod Khurana, Executive Director, Institute of Intellectual Property Research and Development, Greater Noida, U.P. on 17/3/2009.



# RESEARCH PROGRAMMES

## 1. 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:

- Chemistry of Materials
- Molecular Modelling of Materials
- SERS, Raman Spectroscopy, Brillouin Scattering and High-Pressure Research
- Nanomaterials: Synthesis and Applications
- Experimental Nonoscillation, Electronic Charge Density from Molecular Crystals
- Organic Electronics and Optoelectronic Device
- Physics and Photophysics
- Solution processing and Patterning
- Soft Matter and Hard Properties
- Biophotonics
- Study of Novel Functional Oxides
- Magnetism, Superconductivity, and Ferroelectricity
- Surface Science, Heteroepitaxy and Nanostructures
- Self Assembled Molecular Materials based on Metal-Organic Coordination Networks
- Aerospace and Atmospheric Fluid Mechanics
- Complex Fluids : From 'Microscopic' to 'Hierarchical' Modelling
- Flow Instabilities and Discontinuities
- Transition to Turbulence
- Fluid Mechanics and Heat Transfer
- Dynamics and Rheology of Complex Fluids
- Hydrodynamic Stability
- Vortex Dynamics
- Nonlinear Dynamics and Electronic Circuits
- Computational Fluid Dynamics
- Chronobiology and Animal Behaviour
- Evolutionary Genetics and Population Ecology
- Circadian Rhythms in Fruit Flies, Ants and Mice
- Neotectonic and Environmental Geology
- Chromatin Biology and Genomics
- Molecular and Cellular Mechanisms of Human Genetic Disorders
- Protein Engineering and Molecular Parasitology
- Molecular, Genetic and Developmental Analysis of the Cardiovascular System
- Transcription Regulation in Humans by Histone Chaperones,
- Epigenetic Modifications
- Altered Chromatin Dynamics (by nonhistone chromatin proteins)
- Small Molecule Modulators of Chromatin Modifying Enzymes
- HIV-1 Subtype-C Strain: Success Story of the Fittest Viral Subtype
- Mechanism of Chromosome Segregation: A Molecular Approach
- *Plasmodium falciparum* : Functional Genomics of Metabolic Pathways

- Antimalarial Drug Development and Molecular Epidemiology Equilibrium and Nonequilibrium Statistical Mechanics of Condensed-Matter Systems
- Condensed Matter Theory : *Ab initio* Investigations of Low-Dimensional Systems
- Advanced Quantum Theory: From Molecules to Extended Materials
- Dynamics and Phase Transformations in Disordered Systems: Liquids, Glasses and Biomolecules
- Computational Materials Theory: From Electronic Motion to Macroscopic Properties of Materials
- Strongly Correlated Electron Systems
- Statistical Physics of Equilibrium and Nonequilibrium Condensed Matter Systems
- Nonequilibrium Statistical Mechanics
- Isolation and Structure Determination of Unusual Peptides from Fungal Sources
- Effect of Signal Peptide on the Stability and Folding Kinetics of Maltose Binding Protein
- Design of Temperature Sensitive Mutants
- Total Synthesis of Complex Bioactive Natural Products
- Cationic Surfactants, Novel Lipids and Nucleic Acid Analogs
- Bile Acid Chemistry
- Electronic Structure, Especially Strongly Correlated Electron Systems
- Equilibrium and Non-equilibrium Statistical Mechanics of Soft Condensed Matter and Other Complex Systems

## 2. Research Facilities

The Centre has procured the following research equipment/facilities during the year 2008-09 :

Incubation & Cell Cultivation System  
 Ultra High Resolution Transmission Electron Microscope  
 7890 Gas Chromatograph  
 70micron Flat Scanner  
 Micro Calorimeter  
 Digital Polarimeter  
 Protein Purifier 10 Core System  
 Peptide Synthesizer  
 NMR Spectrometer  
 Gas Chromatograph Mass Spectrometer  
 Single Prealigned Laser System  
 Independent Station Surface Area Analyzer  
 Advanced Plasma System  
 Carbon Nitrogen Hydrogen Sodium Analyzer  
 Analytical Gel Permeation Chromatography - GPC  
 Liquid Chromatography Mass Spectrometer - LCMS  
 High Pressure Liquid Chromatography – HPLC





### 3. Sponsored Ongoing Research Projects

Sl.No	Investigator	Title	Funding Agency	Duration
1.	Ranga Uday Kumar	Efficacy and safety evaluation of siddha Medicines HIVS-2003 for HIV/AIDS	DST and Vedic Drugs Ltd.	2 years
2.	R Narasimha	Research Programme on Flow Instabilities	DRDO	3 years
3.	Co-ordinated by JNCASR	Postdoctoral Fellowship in Nano Science and Technology	DST	2 years
4.	C N R Rao	The Science Outreach Programme	DAE/BRNS	3 years
5.	C N R Rao	Publication of series on Learning Science in English	INSA	
6.	S Balasubramanian	Computer simulation studies of room temperature ionic liquids	DST	3 years
7.	R Narasimha	Novel Transition	DRDO/IDS	5 years
8.	S Balasubramanian	Simulation studies of structure, Dynamics and solute-solvent interactions in super-critical carbon dioxide	CSIR	3 years
9.	Tapas Kumar Kundu	Role of multifunctional human transcriptional coactivator PC4 in Chromatin Organization, cell cycle and apoptosis in vivo" National Bioscience Award 2004-05"	DBT	3 years
10.	Tapas Kumar Kundu	Chromatin modifications (Methylation, Acetylation, Deacetylation) – a new target for Cancer therapy and diagnostics	DBT	3 years
11.	Shobhana Narasimhan	Effect of Local Environment on Catalytic Activity – Indo-Italian Research project Under the AEGIS of Indo-Italian POC in S&T 2005-07	DST	3 years
12.	Tapas Kumar Kundu	Functional genomics of Human Transcriptional cofactors and histone deacetylases-A special reference to cancer	ICMR	3 years
13.	Ranga Udaykumar	Pathogenic relevance of Extracellular tat in the body fluids of HIV-I seropositive subjects to disease progression	DBT	3 years
14.	Tapas Kumar Kundu	The Role of Anti-Cancer DNA Binding Drugs on Chromatin Organization and Function	DAE	3 years
15.	Maneesha S Inamdar	Training and research facility for human embryonic stem and human embryonic carcinoma cells	DBT	3 years
16.	Namita Surolia	X-ray Crystallographic Analysis of the Proteins involved in the Fatty Acid Biosynthesis of <i>Plasmodium falciparum</i>	DBT	3 years
17.	A Sundaresan	Atomic Engineering of High to Super-conductors by layer by-layer deposition of $AuO_2$ (A=Ba, Sr, Ca) infinite layers	CSIR	3 years

18.	M R S Rao	NMITLI Project on "A prospective study to correlate gene signatures with clinical outcome of astrocytomas and identification of potential therapeutic target(s) under the New Millennium Indian Technology Leadership Initiative Scheme	CSIR	3 years
19.	Anuranjan Anand	Whole Genome-based Studies to Identify Novel Molecular Genetic Pathways Causing Human Epilepsy Syndrome - DAE-SRC Outstanding Research Investigator Award	DAE	5 years
20.	S Balasubramanian	Centre for Computational Materials Science	DST	5 years
21.	C N R Rao	CSIR-COE	CSIR	5 years
22.	C N R Rao	Collaborative projects between JNCASR and DRDO	DRDO	5 years
23.	Namita Surolia	Genetic manipulations and apcoplast targeting studies with Plasmodium Type II FAS Proteins	DBT	3 years
24.	Namita Surolia	National facility for screening drugs and their biological effects for Cancer, AIDS and Malaria	DBT	3 years
25.	M R S Rao	J C Bose Fellowship to Prof M R S Rao	DST/JCB	5 years
26.	C N R Rao	Spectroscopic Investigation of dip pen nanolithography pattern – Indo-Italian Project	DRDO	3 years
27.	Ranga Uday Kumar	Delineating viral determinants of HAD using SCID mice	AECOM	2 1/2 yrs
28.	Ranga Uday Kumar	Design and characterization of stable folded fragments/derivatives of HIV env for use as Immunogens	DBT	3 years
29.	Tapas Kumar Kundu	Structure function analysis of Tumor suppressor, p53 interacting proteins: structural basis of p53 activation	DBT	3 years
30.	Maneesha S Inamdar	Gene targeting of the mouse asrij locus to generate knockout mice for functional analysis	DST	3 years
31.	Kaustuv Sanyal	Characterization of an evolutionarily conserved kinetochore protein Mtwlp: A tool to analyse kinetochore structure of the human fungal pathogen candida albicans	CSIR	3 years
32.	Namita Surolia	Development of triclosan for treating human malaria and inhibitors of fatty acid synthesis especially enoyl-ACP reductases as anti-malarial agents	DBT	2 years
33.	Swapan K Pati	Quantum magnetic mixing effects in fully frustrated magnets – India-Japan Cooperative Science Programme	DST	2 years
34.	Namita Surolia	Structure-activity relationship of <i>Plasmodium falciparum</i> B-Ketoacyl-ACP reductase (FabGO)	DST	3 years
35.	K B Sinha	Bhatnagar Fellowship – 2005 "Quantum mechanics – A Mathematical tool to study non-equilibrium Processes and dissipative systems in Physical Sciences, Geometry and Information Theory"	CSIR	5 years
36.	K R Sreenivas	Investigation of Lift and Thrust in Asymmetric Flight	DST	3 years

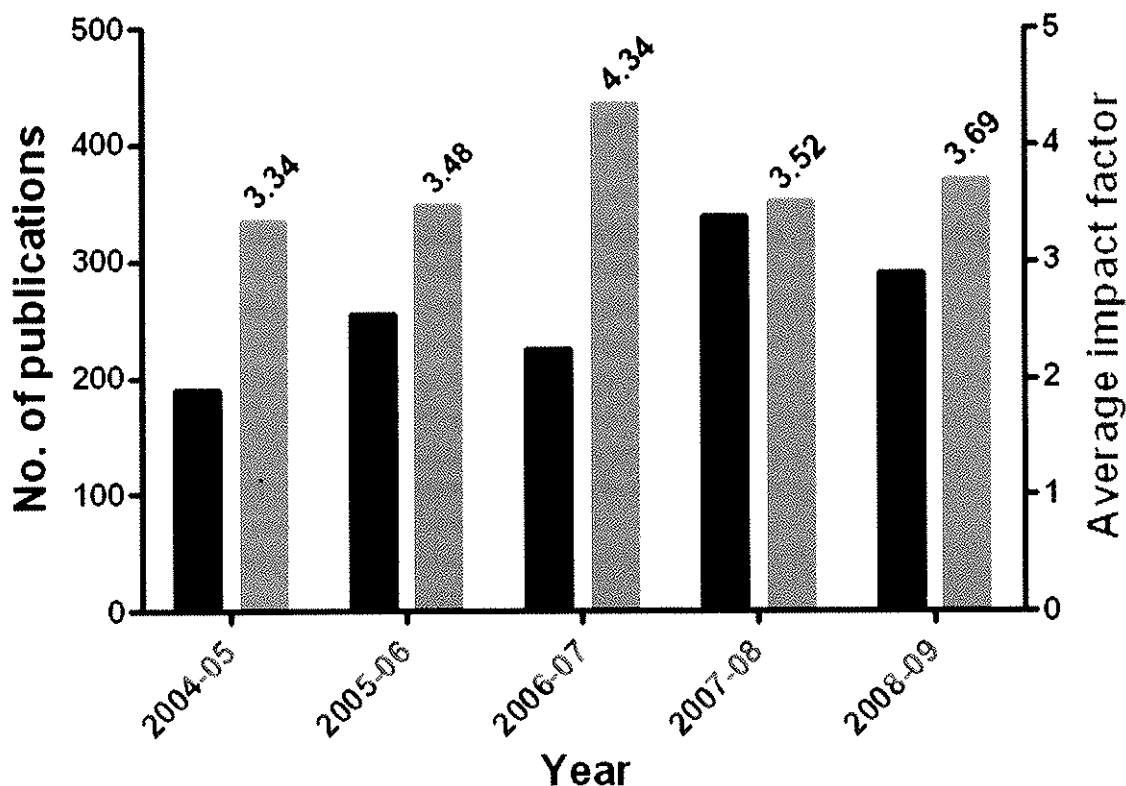


37.	Namita Surolia	Functional Genomics based approach to novel anti-malarial targets and agents	ICMR	3 years
38.	S M Deshpande	NMITLI Project on "Mesoscale modeling for monsoon related weather predictions Phase II"	CSIR	2 ½ yrs
39.	Shobhana Narasimhan	Self-organized nanostructures at surfaces	IFCPAR	3 years
40.	Shobhana Narasimhan	MOU between MIPL & JNCASR - Consultancy and Research	MIPL	3 years
41.	Umesh V Waghmare	MOU between MIPL & JNCASR Consultancy and Research	MIPL	3 years
42.	S Balasubramanian	Swarnajayanthi Fellowship	DST	5 years
43.	Swapn K. Pati	Opto-Electronic Properties of conducting Polymers	CSIR	3 years
44.	S.M. Deshpande	Development of TKFMG solver and its application to flutter prediction in turbo Machines	GTRE	3 years
45.	S Balasubramanian	DST-DAAD (German Academic Exchange Service) joint research Project entitled "Computer Simulation of Ionic liquids"	DST	2 years
46.	Mehaboob Alam	Contract to establish a partner group of the MPI-MM "Partner Group for Topography Formation"	MPI	2 years
47.	K S Narayan	Studies of organic FETs and 3-terminal structures for switching memory and imaging Applications	DST	3 years
48.	Kaustuv Sanyal	Characterization of factors required for determining centromere identity using human pathogenic yeast <i>candida albicans</i> as a model system	DST	3 years
49.	Tapas Kumar Kundu M Eswaramoorthy	Cellular Interaction of Nanoparticles; Effect on epigenetics and thereby its role in gene expression: Implications from Drug delivery to diagnosis	DBT	3 years
50.	G U Kulkarni	Design fabrication of an injection system for patterning of metal cup structures	YNDYM	One year
51.	Tapas Kumar Maji	Microporous metal-organic coordination networks(MOCNs): Application towards H <sub>2</sub> -storage – SERC fast track scheme	DST	3 years
52.	K B Sinha	Evaluation of Impact of DST-FIST Scheme	DST	One year
53.	Umesh V. Waghmare	Density functional theory calculations	Procter & Gamble	One year
54.	Swapn K. Pati	Molecular Electrocnics and its Application (AOARD-08-4008)	US Airforce Lab, Dayton	One year
55.	M R S Rao	Chromatin Biology: Epigenomics of chromatin and chromatin remodelling during male germ cell differentiations and glioma progression	DBT	3 years
56.	Tapas Kumar Kundu	Structure-Function analysis of histone chaperones: Role in chromatin dynamics and transcriptional regulation	IFCPAR	3 years

57.	K R Sreenivas	Lift Generation Mechanisms in Flapping Flight	AOARD	2 years
58.	M K Chandra-shekar	Ramanna Fellowship	DST	3 years
59.	T N C Vidya	Ramanujan Fellowship	DST	5 years
60.	A Sundaresan (Dr Y Tanaka- NIAIS, Japan)	India-Japan co-operative program mme (DST-JST) 2007 - joint Project entitled" Feasibility study on the application of multiple order parameters in materials to information processing.	DST-JST	3 years
61.	K B Sinha	British Council Grant "Quantum probability, Noncommutative Geometry and Quantum information	LANCAS	3 years
62.	G U Kulkarni	ICPC Nano Net Coordination and support action	ICPNN	2 years
63.	Swapan K Pati	Swarnajayanthi Fellowship	DST	5 years
64.	Kaustuv Sanyal	Functional Analysis of Dynamic Kineto chore-Microtubule Interaction in the human Pathogen Candida albicans	DBT	3 years
65.	S M Deshpande	Numerical simulation of multiscale supersonic flows with low dissipative shock capturing schemes	DST	2 years
66.	Tapas Kumar Kundu	Bovine Mastitis: Unraveling molecular details of host microbe interaction and development of molecular diagnostic methods	ICAR	3 years
67.	Sheeba Vasu	Ramanujan Fellowship	DST	5 years
68.	G U Kulkarni Hemalatha Balaram M Eswaramoorthy	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	Yash Nanotech Ltd.	1 year
69.	Santosh Ansumali	Ramanujan Fellowship	DST	5 years
70.	Umesh V Waghmare	DAE-SRC Outstanding Research Investigator Award for R/P "Multi scale modeling and simulations of functional Materials	DAE	5 years
71.	K S Narayan	DAE-SRC Outstanding Research Investigator Award for R/P "Electronic, optoelectronics and photonic properties in soft matter and device exploration	DAE	5 years
72.	C N R Rao	Collaborative projects between JNCASR/ICMS & DST	DST-ICMS	5 years

## 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:



### 1. Research Publications of Units

#### (i) Chemistry and Physics of Materials Unit

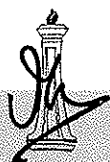
- 1) Bhargava BL, Krishna AC, Balasubramanian S. Molecular dynamics simulation studies of CO<sub>2</sub>-[bmim][PF<sub>6</sub>] solutions: Effect of CO<sub>2</sub> concentration. *AIChE Journal*, 54, 2971-2978, 2008.
- 2) Bhargava BL, Saharay M, Balasubramanian S. Ab initio studies on [bmim][PF<sub>6</sub>]-CO<sub>2</sub> mixture and CO<sub>2</sub> clusters. *Bulletin of Materials Science*, 31, 327-334, 2008.
- 3) Bhargava BL, Balasubramanian S, Klein ML. Modelling Room Temperature Ionic Liquids. *Chemical Communications*, 3339-3351, 2008 (Feature Article).
- 4) Bhargava BL, Balasubramanian S. Ab Initio Molecular Dynamics Simulation Studies of 1-ethyl-3-methylimidazolium fluoride - hydrogen fluoride mixture. *Journal of Physical Chemistry B*, 112, 7566-7573, 2008.
- 5) Zhao W, Leroy E, Balasubramanian S, Muller-Plathe F. The shear viscosity of the ionic liquid 1-n-butyl,3-methylimidazolium hexafluorophosphate [bmim][PF<sub>6</sub>] computed by reverse non-equilibrium molecular dynamics. *Journal of Physical Chemistry B*, 112, 8129-8133, 2008.
- 6) Datta KRK, Srinivasan B, Balaram H, Eswaramoorthy M. Synthesis of agarose-metal/semiconductor nanoparticles having superior bacteriocidal activity and their simple conversion to metal-carbon composites. *J. Chem. Sci.*, 120, 1-8, 2008.
- 7) Pal S, Jagadeesan D, Gurunatha KL, Eswaramoorthy M, Maji T. Construction of bi-functional inorganic-organic hybrid nanocomposites. *J. Mater. Chem.*, 18, 5448-5451, 2008.

- 8) Raveendran P, Eswaramoorthy M, Bindu U, Chatterjee M, Hakuta Y, Kawanami H, Mizukami E. Template-free formation of meso-structured anatase TiO<sub>2</sub> with spherical morphology. *J. Phys. Chem. C*, 112, 20007–20011, 2008.
- 9) Ruthrotha Selvi B, Jagadeesan D, Nagashankar G, Suma BS, Arif M, Balasubramanyam K, Eswaramoorthy M, Kundu TK. Intrinsically fluorescent carbon nanospheres as a nuclear targeting vector: Delivery of membrane impermeable molecule to modulate gene expression in vivo. *Nano Lett.*, 8, 3182 - 3188, 2008.
- 10) Jagadeesan D, Mansoori U, Mandal P, Sundaresan A, Eswaramoorthy M. Hollow Spheres to Nanocups: Tuning the Morphology and Magnetic Properties of Single Crystalline  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Nanostructures. *Angew. Chem. Int. Ed.*, 47, 7685 - 7688, 2008.
- 11) Jagadeesan D, Deepak C, Kavitha Siva, Inamdar M, Eswaramoorthy M. Carbon spheres assisted synthesis of porous bioactive glass containing hydroxycarbonate apatite nanocrystals: A material with high invitro bioactivity. *J. Phys. Chem. C.*, 112, 7379 - 7384, 2008.
- 12) Gupta D, Bag M, Narayan KS. Area dependent efficiency in organic solar cells. *Applied Phys. Lett.*, 93, 163301, 2008.
- 13) Shruti Badhwar, Narayan KS. Optimum Design of Organic Electrochemical Type Transistors for Applications in Biochemical Sensing. *Journal of Sensors*, 702161, 2008.
- 14) Rao M, Narayan KS. Evaluation of Electrode-Semiconductor Barrier in Transparent Top -Contact Polymer FETs. *Applied Phys. Lett.*, 92 223308, 2008.
- 15) Kabra D, Verma J, Vidyadhiraja NS, Narayan KS. Model for Studies of Lateral Photovoltaic Effect in Polymeric Semiconductors, *IEEE Sensors journal*, 8, 1663, 2008.
- 16) Maitra U, Gomati A, Rao CNR. Covalent and non-covalent functionalization and solubilization of nanodiamond. *J. Expt. Nanosci.*, 3, 27, 2008.
- 17) Voggu R, Kumar N, Rao CNR. Dependence of the properties of magnetic nanoparticles on the interparticle separation. *J. Phys. Chem. C. (Letter)*, 112, 17775, 2008.
- 18) Voggu R, Das B, Rout CS, Rao CNR. Effects of the charge-transfer interactions of graphene with electron-donor and -acceptor molecules examined by Raman spectroscopy and cognate techniques. *J. Phys. Condens. Matter.*, 20, 472204, 2008.
- 19) Bera MK, Sanyal MK, Banerjee R, Kalyanikutty KP, Rao CNR. Effect of vibrations on the formation of gold nanoparticle aggregates at the toluene-water interface. *Chem. Phys. Lett.*, 461, 97, 2008.
- 20) Rao CNR. Science and Technology Policies: The case of India, *Technology in Society*. 30, 242, 2008.
- 21) Sanyal MK, Agarwal VV, Bera MK, Kalyanikutty KP, Daillant J, Blot C, Kubowicz S, Konovalov O, Rao CNR. Formation and ordering of gold nanoparticles at the liquid-liquid interface. *J. Phys. Chem. C (Letter)*, 112, 1739, 2008.
- 22) Serrao CR, Sahu JR, Ramesha K, Rao CNR. Magnetoelectric effect in rare earth ferrites, LnFe<sub>2</sub>O<sub>4</sub>. *J. Appl. Phys.*, 104, 016102, 2008.
- 23) Serrao CR, Sahu JR, Sundaresan A, Rao CNR. Charge-order driven magnetoelectric effect in rare earth ferrites and manganites. *AIP Proceedings*, 1003, 115, 2008.
- 24) Chitara B, Bhat SV, Vivekchand SRC, Gomati A, Rao CNR. White-light sources based on composites of GaN nanoparticles with conducting polymers and nanophosphors. *Solid State Commun.*, 147, 409, 2008.
- 25) Ghosh A, Dan M, Rao CNR. Hybrid compounds with chain and layered structures formed by beta-alanine. *Solid State Sci.*, 10, 998, 2008.
- 26) Thirumurugan A, Rao CNR. Supramolecular organization in lead bromide salts of imidazolium -based ionic liquids. *Crystal Growth & Design*, 8, 1640, 2008.
- 27) Ghosh A, Rao CNR. Chiral and achiral malate frameworks of different dimensionalities. *Z. Anorg. Allgem. Chem.*, 634, 1115, 2008.



- 28) Padmanabhan M, Joseph JC, Thirumurugan A, Rao CNR. Maleate-fumarate conversion and other novel aspects of the reaction of a Co(II) maleate with pyridine and bipyridine. *Dalton Trans. (Communication)*, 2809, 2008.
- 29) Thirumurugan A, Rao CNR. Hybrid structures formed by homo- and hetero-leptic aliphatic dicarboxylates of lead with 2D-inorganic connectivity. *J. Solid State Chem.*, 181, 1184, 2008.
- 30) Murugavel R, Choudhury A, Walawalkar MG, Pothiraja R, Rao CNR. Metal complexes of organophosphate esters and open-framework metal phosphates: Synthesis, structure, transformations and applications. *Chem. Rev.*, 108, 3549, 2008.
- 31) Pati SK, Rao CNR. Kagome network compounds and their novel magnetic properties, *Chem. Commun. (Feature article)*, 4683, 2008.
- 32) Varghese N, Biswas K, Rao CNR. Investigations of the growth kinetics of capped CdSe and CdS nanocrystals by a combined use of small angle x-ray scattering and other techniques. *Chem.-Asian J.*, 3, 1435, 2008.
- 33) Biswas K, Varghese N, Rao CNR. Investigations of the growth kinetics of nanocrystals and nanorods by employing SAXS and other techniques. *J. Mater. Sci. Tech.*, 24, 615, 2008.
- 34) Pal A, Chikkara BS, Govindaraj A, Bhattacharya S, Rao CNR. Synthesis and properties of novel nanocomposites made of SWNTs and low molecular mass organogels and their thermo responsive behaviour triggered by near IR radiation. *J. Mater. Chem.*, 18, 2593, 2008.
- 35) Voggu R, Rout CS, Franklin AD, Fisher TS, Rao CNR. Extraordinary sensitivity of the electronic structure and properties of single-walled carbon nanotubes to molecular charge-transfer. *J. Phys. Chem. C (Letter)*, 112, 13053, 2008.
- 36) Das B, Voggu R, Rout CS, Rao CNR. Changes in the electronic structure and properties of graphene induced by molecular charge transfer. *Chem. Commun.*, 5155, 2008.
- 37) Ghosh A., Subrahmanyam KS, Krishna, Dutta S, Govindaraj A, Pati SK, Rao CNR. Uptake of H<sub>2</sub> and CO<sub>2</sub> by graphene, *J. Phys. Chem. C*, 112, 15704, 2008.
- 38) Raidongia K, Rao CNR. Study of the transformation of elemental nanowires to nanotubes of oxides and chalcogenides through Kirkendall effect. *J. Phys. Chem. C*, 112, 13366, 2008.
- 39) Biswas K, Varghese N, Rao CNR. Growth kinetics of gold nanocrystals: A combined small angle x-ray scattering and calorimetric study. *Small*, 4, 649, 2008.
- 40) Ahmed J, Ramanujachary KV, Lofland SE, Furiato A, Gupta G, Shivaprasad SM, Ganguli AK. Bimetallic Cu-Ni nanoparticles of varying composition (CuNi<sub>3</sub>, CuNi, Cu<sub>3</sub>Ni), *Colloids and Surfaces A: Physicochemical and Engineering Aspects* 331, 206, 2008.
- 41) Aruna BR, Mehta LK, Malhotra, Shivaprasad SM. Size dependence of core and valence binding energies in Pd nanoparticles: Interplay of quantum confinement and co-ordination reduction. *Journal of Applied Physics*, 104, 064308, 2008.
- 42) Sharma SN, Sharma H, Singh G, Shivaprasad SM. Studies of interaction of amines with TOPO/TOP capped CdSe quantum dots: Role of crystallite size and oxidation potential. *Materials Chemistry and Physics*, 110, 471, 2008.
- 43) Kumar A, Singh F, Govind, Shivaprasad SM, Avasthi DK, Pivin JC. X-ray photoelectron and X-ray Auger electron spectroscopy studies of heavy ion irradiated C60 films. *Applied Surface Science*, 254, 7280, 2008.
- 44) Khanuja M, Mehta BR, Shivaprasad SM. Geometric and electronic changes during interface alloy formation in Cu/Pd bimetal layers. *Thin Solid Films*, 516, 5435, 2008.
- 45) Jagadeesan D, Mansoori U, Mandal P, Sundaresan A, Eswaramoorthy M. Hollow Spheres to Nanocups: Tuning the Morphology and Magnetic Properties of Single-Crystalline  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Nanostructures. *Angew. Chem. Int. Ed.*, 47, 7685 – 7688, 2008.

- 46) Madhu C, Sundaresan A. Magnetocaloric effect across the coupled structural and ferro-magnetic transition in  $\text{Pr}_{0.1}\text{Ce}_{0.4}\text{Sr}_{0.5}\text{MnO}_3$ . *J. Chem. Sci.*, 120, 595–598, 2008.
- 47) Chaudhuri AR, Mandal P, Krupanidhi SB, Sundaresan A. Magnetocapacitive  $\text{La}_{0.6}\text{Sr}_{0.4}\text{MnO}_3/0.7\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.3\text{PbTiO}_3$  epitaxial hetero-structure. *Solid State Commun.*, 148, 566–569, 2008.
- 48) Mua NT, Serrao CR, Shipra A, Sundaresan A, Hien TD, Man NK. High critical current density in Ag-doped Bi-2212 thin films. *Supercond. Sci. Technol.*, 21, 105002, 2008.
- 49) Pal S, Jagadeesan D, Gurunatha KL, Eswaramoorthy M, Maji TK. Construction of bi-functional inorganic-organic hybrid nanocomposite. *J. Mater. Chem.*, 18, 5448-5451, 2008.
- 50) Gurunatha KL, Uemura K, Maji TK. Temperature and Stoichiometry Controlled Dimensionality in a Magnesium 4,5-Imidazolecarboxylate System with Strong Hydrophilic Pore Surfaces. *Inorg. Chem.* 47, 6578-6580, 2008.
- 51) Vijaykumar T, Raina G, Heun S, Kulkarni GU. Catalytic Behavior of Individual Au Nanocrystals in the Local Anodic Oxidation of Si Surfaces. *J. Phys. Chem. C*, 112, 13311–13316, 2008.
- 52) Bhuvana T, Kulkarni GU. Polystyrene as a zwitter resist in electron beam lithography based electroless patterning of gold. *Bull. Mater. Sci.* 31, 201–206, 2008.
- 53) Raju SG, Balasubramanian S. Intermolecular correlations in an ionic liquid under shear. *Journal of Physics: Condensed Matter*, 21, 035105, 2009.
- 54) Raju SG, Balasubramanian S. Aqueous Solution of [bmim][PF6]: Ion and Solvent Effects on Structure and Dynamics. *Journal of Physical Chemistry B*, 113, 4799-4806, 2009.
- 55) Raju SG, Balasubramanian S. Emergence of nanoscale order in room temperature ionic liquids: Simulation of symmetric 1,3-didecylimidazolium hexafluorophosphate, *Journal of Materials Chemistry*, 19, 4343–4347, 2009.
- 56) Saharay M, Balasubramanian S. Ab initio molecular dynamics investigations of structural, electronic and dynamical properties of water in supercritical carbon dioxide, *Indian Journal of Physics*, 83, 13–29, 2009.
- 57) Singh P, Shivaprasad SM., Lal M, Husain M. Angle-dependent XPS analysis of silicon nitride film deposited on screen-printed crystalline silicon solar cell. *Solar Energy Mat. and Solar Cells*, 93, 19, 2009.
- 58) Mangalam RVK, Nirat Ray, Waghmare UV, Sundaresan A, Rao CNR. Multiferroic Properties of Nanocrystalline  $\text{BaTiO}_3$ , *Solid State Commun. (Fast Track)*, 149, 1–5, 2009.
- 59) Sahu JR, Serrao CR, Ghosh A, Sundaresan A, Rao CNR. Charge-order-driven multiferroic properties of  $\text{Y}_{1-x}\text{Ca}_x\text{MnO}_3$ . *Solid State Commun.*, 149, 49–51, 2009.
- 60) Sundaresan A, Rao CNR. Ferromagnetism as a universal feature of nanoparticles. *Nanotoday*, 4, 096–106, 2009.
- 61) Mangalam RVK, Sundaresan A. Crystal structure and dielectric properties of ordered perovskites  $\text{Ba}_2\text{BiSbO}_6$  and  $\text{BaSrBiSbO}_6$ . *Physica B*, 404, 154–157, 2009.
- 62) Mandal P, Sundaresan A. Dielectric and Impedance studies on the double perovskite  $\text{Ba}_2\text{BiTaO}_6$ . *Solid State Sciences*, 11, 861–864, 2009.
- 63) Mangalam RVK, Sundaresan A. Itinerant ferromagnet to insulating spin glasses in  $\text{SrRu}_{1-x}\text{Cu}_x\text{O}_3$ , *Mater. Res. Bull.*, 44, 576–580, 2009.
- 64) Gurunatha KL, Maji TK. Three isomorphous threefold interpenetrated 2D supramolecular frameworks: Synthesis, structure and sorption properties. *Inorg. Chim. Acta*, 362, 1541-1545, 2009.
- 65) Bhuvana T, Subramaniam C, Pradeep T, Kulkarni GU. Conducting Nanocrystal Patterns Using a Silver Organic Complex Blended with Polystyrene as e-Beam Resist. *J. Phys. Chem. C*, 113, 7038-7043, 2009.
- 66) Radha B, Kulkarni GU. Dewetting Assisted Patterning of Polystyrene by Soft Lithography to Create Nanotrenches for Nanomaterial Deposition. *ACS Appl. Mater. Interfaces*, 1, 257–260, 2009.





- 67) Bhuvana T, Kulkarni GU. Femtoliter silver cups as surface enhanced Raman scattering active containers. *Nanotechnology*, 20, 045504 (5 p), 2009.
- 68) Bhuvana T, Gregoratti L, Heun S, Dalmiglio M, Kulkarni GU. Electron Resist Behavior of Pd Hexadecanethiolate Examined Using X-ray Photoelectron Spectroscopy with Nanometric Lateral Resolution. *Langmuir*, 25, 1259 - 1264, 2009.
- 69) Reji Thomas, Lakshmi S, Pati SK, Kulkarni GU, Mallajyosula, SS. Conjugation in 1,4-diphenylbutadiyne and 1,2-diphenylacetylene: A combined experimental and theoretical study. *J. Mol. Struct.*, 922, 46 - 50, 2009.
- 70) Chattopadhyay S, Mukherjee R, Datta A, Saha A, Sharma A, Kulkarni GU. Self-Assembly of a two-dimensional Au-nanocluster superlattice and its photoluminescence spectra. *J. Nanosci. Nanotech.* 9, 190 - 194, 2009.
- 71) Sarangi SS, Balasubramanian S. Nanoclusters of room temperature ionic liquids: A molecular dynamics simulation study, *Physical Chemistry Chemical Physics*, 2009. (in Press).
- 72) Reji Thomas, Varghese S, Kulkarni GU, The influence of crystal packing on the solid state fluorescence behavior of alkyloxy substituted phenyleneethynylenes, *J. Mater. Chem.*, (2009). In Press.
- 73) Sharma H, Sharma SN, Kumar U, Singh VN, Mehta BR, Singh G, Shivaprasad SM, Kakkar R. Formation of water-soluble and biocompatible TOPO-capped CdSe quantum dots with efficient photoluminescence. *Journal of Mat. Science: Materials in Medicine*, 2008 Article (in Press)
- 74) Praveen Kumar, Nair L, Bera S, Shivaprasad SM, Formation of SiC at room temperature by ion bombardment. *Appl. Surf. Sci.*, 2009 (in Press).
- 75) Khanuja M, Sharma H, Mehta BR, Shivaprasad SM,. XPS depth-profile of the suboxide distribution at the native oxide/Ta interface. *Journal of Electron Spectroscopy and Related Phenomena*, 2009 (in Press).
- 76) Kanoo P, Madhu C, Mostafa G, Maji TK, Sundaresan A, Pati SK, Rao CNR. A Planar Cu<sup>2+</sup> (S = ½) kagomé Network Pillared by 1,2- bis(4-pyridyl)ethane with Interesting Magnetic Properties. *Dalton. Trans.*, 2009 (In Press, accepted for Cover page in July Issue).
- 77) Gurunatha KL, Dutta S, Mostafa G, Pati SK, Maji TK. A Novel 3D Chiral Supramolecular Framework of Cu(II): Synthesis, Structure and Magneto-Structural Correlations. *Inorg. Chim. Acta*, 2009 (in Press).
- 78) Maji TK, Pal S, Gurunatha KL, Govindaraj A, Rao CNR. A Bimetallic Pillared-Layer Metal-Organic Coordination Framework with a 3D Biporous Structure. *Dalton. Trans.* 2009 (in Press).
- 79) Gurunatha KL, Mostafa G, Ghoshal D, Maji TK. Single-Crystal-to-Single-Crystal Structural Transformation in a 3D Bimetallic (4f-3d) Supramolecular Porous Framework. *Cryst. Growth. Des.*, 2009 (in Press).
- 80) Vyasamudri SY, Maji TK. Six-fold Interpenetrated Diamondoid Network of Cu(I): Synthesis, Structure, Selective anion Exchange and Luminescence Properties. *Chem. Phys. Lett.*, 2009 (in Press).
- 81) Uemura K, Maeda A, Maji TK, Kanoo P, Kita H. Syntheses, Crystal Structures, and Adsorption Properties of Ultramicroporous Coordination Polymers Constructed from Hexafluorosilicate Ion and Pyrazine. *Eur. J. Inorg. Chem.*, 2009 (In Press, accepted for Cover page).
- 82) Gurunatha KL, Maji TK. Structural Flexibility and selective guest accommodation in two Metal-Organic Coordination Frameworks of Cu(II). *Eur. J. Inorg. Chem.*, 2009 (in Press).
- 83) Gupta D, Vidyadhiraja NS, Narayan KS. Transport of Photogenerated Charge Carriers in Polymer Semiconductors. *Proc. of IEEE* (to be published).
- 84) Bag M, Gupta D, Arun N, Narayan KS. Deformation of Metallic-Liquid Drop by Electric Field for Contacts in Molecular-Organic Electronics. *Royal Society Proc. A* (to be published).
- 85) Vijaykumar T, Kulkarni GU. Local Anodic Oxidation Patterning of Au Deposited Si Surfaces, *J. Nanosci. Nanotech.* , 2009 (accepted)

(ii) **Engineering Mechanics Unit**

- 1) Alam M, Khalili A. Instabilities and patterns in horizontally oscillating particulates suspension. *Physical Review E*, 77, 041305, 2008.
- 2) Alam M, Shukla P, Luding S. Universality of shear-banding instability and crystallization in sheared granular fluid. *Journal of Fluid Mechanics*, 615, 293 – 321, 2008.
- 3) Sahu KC, Sameen A, Govindarajan R. The relative roles of divergence and velocity slip in the stability of plane channel flow. *The European Physical Journal, Appl. Phys.* 44, 101–107, 2008.
- 4) Victor S. L'vov, Anna Pomyalov, Itamar Procaccia, Govindarajan R. Random Vortex-Street Model for a Self-Similar Plane Turbulent Jet. *Physical Review Letters*, 101, 094503, 2008.
- 5) Subramanian G, Koch DL. Evolution of clusters of sedimenting low-Reynolds- number particles with Oseen interactions. *Journal of fluid mechanics*, 603, 63-100, 2008
- 6) Sreenivas KR, Singh OP, Srinivasan J. On the relationship between finger width, velocity, and fluxes in thermohaline convection. *Physics of Fluids*, 21, 026601, 2009.
- 7) Brent Daniel W, Robert E. Ecke, Subramanian G, Koch DL. Clusters of sedimenting high-Reynolds- number particles, *J. Fluid Mech.*, 2008. (In Press.)

**Articles/Chapters in Books and Papers Presented at Conferences:**

- 1) Alam M, Shukla P. Nonlinear Stability of Granular Shear Flow: Landau Equation, Shearbanding and Universality, 2<sup>nd</sup> International Congress of Theoretical and Applied Mechanics, (ICTAM2008, 24-30 August 2008, Adelaide, Australia), p. 1-2, ISBN 978-0-9805142-0-9.
- 2) Alam M. Dynamics of Sheared Granular Fluid, 12<sup>th</sup> Asian Fluid Mechanics Conference (ACFM2008, 18-21 August 2008, Daejeon, Korea), p. 1-6 (Ed. H.J. Sung), 2008.
- 3) Malik A, Alam M. Large-scale Structures and Fluctuations in 3D granular Poiseuille Flow. 12<sup>th</sup> Asian Fluid Mechanics Conference (ACFM2008, 18-21 August 2008, Daejeon, Korea), p. 1-4 (Ed. H.J. Sung), 2008.
- 4) Shukla P, Alam M. Nonlinear Stability of Granular Shear Flow: Landau Equation and Shearbanding, 12<sup>th</sup> Asian Fluid Mechanics Conference (ACFM2008, 18-21 August 2008, Daejeon, Korea), p. 1-4 (Ed. H.J. Sung), 2008.
- 5) Malik M, Dey J, Alam M. Spatial Stability of Compressible Plane Couette Flow, 12<sup>th</sup> Asian Fluid Mechanics Conference (ACFM2008, 18-21 August 2008, Daejeon, Korea), p. 1-4 (Ed. H.J. Sung), 2008.
- 6) Anil N, Rajan NKS, Rishi O, Deshpande SM. A low dissipative discrete adjoint m-KFVS method. The Fifth International Conference on Computational Fluid Dynamics (ICCFD5), Seoul, Korea, July 7-11, 2008.
- 8) Rishi O, Deshpande SM. The Fifth International Conference on Computational Fluid Dynamics (ICCFD5), Seoul National University, Seoul, Korea, July 7-11, 2008.
- 9) Arora K., Rajan NKS, Deshpande SM. On the Robustness and Accuracy of Least Squares Kinetic Upwind Method (LSKUM), Proceedings of the 12<sup>th</sup> Asian Congress of Fluid Mechanics 18-21 August 2008, Daejeon, Korea.
- 10) Narasimha R. How green could Tomorrow's Aircraft be? Climate Change, Environment and Aviation, Pt. Govind Ballabh Pant Memorial Lecture: XIV Kosi-Katarmal, Almora, 2008.
- 11) Narasimha R, Bhattacharya P, Govindarajan R. In what sense is a low-Reynolds number mixing layer stable? *Proceedings of the 12th Asian Congress of Fluid Mechanics, Daejeon, Korea*, 2008.
- 12) Aditya K, Deshpande SM, Sreenivas KR, Narasimha R. Numerical simulation of a starting-plume cloud-flow ERCOFTAC workshop on Direct and large-Eddy Simulations 7, 8-10 September 2008 Trieste, Italy.



- 13) Aditya K, Deshpande SM, Sreenivas KR, Narasimha R. Numerical Simulation of a Starting-Plume Cloud-Flow, Proceedings of the Direct and Large-Eddy Simulation, 9-11 September 2008, Trieste, Italy.
- 14) Samanta D, Sreenivas KR. Parametric dependence of lift in a flapping flight, 7th Euromech Fluid Mechanics Conference -September, 14-18, 2008, Manchester, UK. 2008.
- 15) Mukund V Sreenivas, KR. Effect of radiation on temperature profiles in a radiatively participating medium, 7th EUROMECH Fluid Mechanics Conference - September, 14-18, 2008, Manchester, UK, 2008.
- 16) Vivek N. Prakash, Sreenivas KR, Jaywant H. Arakeri. High rayleigh number high prandtl number natural convection mimicking mantle convection, 7th EUROMECH Fluid Mechanics Conference - September, 14-18, 2008, Manchester, UK. 2008
- 17) Srikanth Rao, Rao Tatavarti, Govindarajan R. Two-Dimensional Flow Field in the Vicinity of an Oscillating Body, OSICON-2, National Conference of the Ocean Society of India, Vishakapatnam, March 19-21, 2009.
- 18) Sreenivas KR. Characteristics of Double Diffusive Finger-convection. Invited talk at the National Conference of the Ocean Society India, OSICON-2, Vishakapatnam, March 19-21, 2009, 2009.
- 19) Rao Tatavarti, Rajapandiyan A, Sreenivas KR. Wakes and Jets in Stratified Medium, National Conference of the Ocean Society of India, OSICON-2, Vishakapatnam, March 19-21, 2009.

#### (iii) Evolutionary and Organismal Biology Unit

- 1) Jain K. Loss of least-loaded class in asexual populations due to drift and epistasis. *Genetics*, 179, 2125, 2008.
- 2) Joshi A, Mueller LD.. Evolutionary genetics: 150 years of natural selection. Preface to a Special Issue. *Journal of Genetics*, 87, 319-320, 2008.
- 3) Lone SR, Sharma VK. Exposure to light enhances pre-adult fitness in two dark-dwelling sympatric species of ants. *BMC Developmental Biology*, 8, 113, 2008.
- 4) Manjunatha T, Hari Dass S, Sharma VK. Egg laying rhythm in *Drosophila melanogaster*. *Journal of Genetics*, 87, 495-501, 2008.
- 5) Nagar A, Jain K. Exact phase diagram of quasispecies model with mutation rate modifier. *Physics Reviews Letters*, 102, 38101, 2008.
- 6) Sheeba V. The *Drosophila melanogaster* circadian pacemaker circuit. *Journal of Genetics*, 87, 485-493, 2008.
- 7) Sheeba V, Fogle KJ, Kaneko M, Rashid S, Chou YT, Sharma VK, Holmes TC. Large ventral neurons modulate arousal and sleep in *Drosophila*. *Current Biology*, 18, 1537-1545, 2008.
- 8) Vidya TNC, Sukumar R, Melnick DJ. A range-wide phylogeography of the Asian elephant (*Elephas maximus*) based on mitochondrial DNA. *Proceedings of the Royal Society of London, Series B* 276: 893-902, 2009.

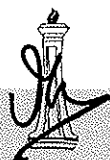
#### (iv) Geodynamics Unit

- 1) Valdiya KS. Sinking of ancient Talakad temples on the Kaveri bank, Mysore Plateau, Karnataka. *Current Science*, 95, 1675-1676, 2008
- 2) Valdiya KS, Pande K. Behaviour of basement-cover decoupling in compressional regime, northern Kumaun (Uttarakhand) Himalaya, *Proc. Indian National Science Academy*, 106, March issue, 2009.

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

- 1) Kapoor A, Satishchandra P, Ratnapriya R, Reddy RJ, Kadandale J, Shankar SK, Anand A. An idiopathic epilepsy syndrome linked to 3q13.3-q21 and missense mutations in the extracellular calcium sensing gene. *Annals of Neurology*, 64, 158-167, 2008.

- 2) Mani RS, Aparna G, Jalvi R, Srikumari CR, Malhotra V, Chadha S, Agarwal A, Ramesh A, Rangasayee R, Anand A. Functional consequences of novel *connexin 26* mutations associated with hereditary hearing loss. *European Journal of Human Genetics*, 1-8, 2008.
- 3) Chatterjee A, Jalvi R, Pandey N, Rangasayee R, Anand A. A novel locus *DFNA59* for autosomal dominant nonsyndromic hearing loss maps at chromosome 11p14.2-q12.3. *Human Genetics*, 124, 669-675, 2008.
- 4) Ram Shankar M, Aparna G, Jalvi R, Srikumari SCR, Malhotra V, Chadha S, Agarwal A, Ramesh A, Rangasayee R, Anand A. Functional consequences of novel connexin 26 mutations associated with hereditary hearing loss, *European Journal of Human Genetics*, 1 – 8, 2008.
- 5) Mehrotra S, Balaram H. Methanocaldococcus jannaschii adenylosuccinate synthetase: studies on temperature dependence of catalytic activity and structural stability. *Biochim Biophys Acta*, 1784, 2019-28, 2008.
- 6) Gayathri P, Sujay Subbayya IN, Ashok CS, Selvi TS, Balaram H, Murthy MR. Crystal structure of a chimera of human and Plasmodium falciparum hypoxanthine guanine phosphoribosyltransferases provides insights into oligomerization. *Proteins*, 73, 1010-20, 2008
- 7) Chakrabarty SP, Saikumari YK, Bopanna MP, Balaram H. Biochemical characterization of Plasmodium falciparum Sir2, a NAD<sup>+</sup>-dependent deacetylase. *Mol Biochem Parasitol*. 158, 139-51, 2008. (Highly Accessed)
- 8) Datta KKR, Srinivasan B, Balaram H, Eswaramoorthy M. Synthesis of agarose-metal/semiconductor nanoparticles having superior bacteriocidal activity and their simple conversion to metal-carbon composites. *Journal of Chemical Sciences*, 120, 579 – 586, 2008.
- 9) Bhat JY, Shastri BG, Balaram H. Kinetic and biochemical characterization of *Plasmodium falciparum* GMP synthetase. *Biochemical Journal*, 409, 263 – 273, 2008.
- 10) Dinesh J, Deepak C, Kavitha S, Inamdar M, Eswaramoorthy M. Carbon spheres assisted synthesis of porous bioactive glass containing hydroxycarbonate apatite nanocrystals: A material with exceptionally high in vitro bioactivity. *J. Phys. Chem. C*, 112, 7379 – 7384, 2008.
- 11) Robyn MB, Loureiro, Kelli-Ann Monaco, Joseph B. Kearney, Courtney E. Blickarz-Durand, Suzanne L. Kirby, Inamdar M, Victoria L. Bautch. CSF-1 is Required for Early Embryonic Macrophage Development: Characterization of the csfnop/csfmop Mutation in ES cell-derived Macrophages, *British Journal of Hematology*, 141, 739 – 742, 2008.
- 12) Karmodiya K, Modak R, Sahoo N, Sajad S, Surolia N. Deciphering the key residues in Plasmodium falciparum beta-ketoacyl acyl carrier protein reductase responsible for interactions with Plasmodium falciparum acyl carrier protein. *FEBS J*. 275(19),4756-66, 2008.
- 13) Gratraud P, Surolia N, Besra G. Surolia A, Kremer L. Antimycobacterial activity and mechanism of action of NAS-91. *Antimicrob. Agents Chemother*. 52(3), 1162-1166, 2008.
- 14) Mishra S, Karmodiya K, Surolia N, Surolia A. Synthesis and exploration of novel curcumin analogues as anti-malarial agents. *Bioorg. Med Chem.*, 16(6),2894-902. 2008.
- 15) Mishra S, Karmodiya K, Parasuraman P, Surolia A, Surolia N. Design, synthesis, and application of novel triclosan prodrugs as potential antimalarial and antibacterial agents. *Bioorg. Med Chem.*, 16(10),5536-46, 2008.
- 16) Pradeepa MM, Manjunatha S, SathishV, Agrawal S, Rao MRS. Involvement of importin 4 in the transport of transition protein 2 into spermatid nucleus. *Mol. Cell Biol.*, 28(13), 4331-4341, 2008.
- 17) Reddy PS, Britoo R, Katyayni V, Aparna H, Sreepathi HK, Samuel C, Shetty M., Tandon A, Hegde S, Hegde AS, Santosh V, Kondaiah P, Somasundaram K, Rao MRS. Novel glioblastoma markers with diagnostic and prognostic value identified through transcriptome analysis. *Clin. Cancer Res*. 14 (10), 2978-2987, 2008.
- 18) Reddy PS, Umesh S, Thota B, Tandon A, Pandey P, Hegde AS, Balasubramaniam A, Chandramouli BA., Santosh V, Rao MRS, Kondaiah P, Somasundram K. PEBF1/NAmpRTse/Visfatin: A potential



- malignant astrocytoma/glioblastoma serum marker with prognostic value. *Cancer Biology and Therapy* 7, 665-670, 2008.
- 19) Gayatri G, Rao MRS. A novel non-coding RNA processed by Drosha restricted to nucleus in mouse. *RNA*, 14, 1399-1410, 2008.
  - 20) Vimalaswaran KS, Radha V, Ramya, K, Satish Babu HN, Savitha N, Roopa V, Monalisa D, Deepa R, Ghosh S, Majumdar PP, Rao MRS, Mohan V. A novel association of a polymorphism in the first intron of adiponectin gene with Type 2 Diabetes, Obesity and Hypoadiponectinemia in Asian Indians. *Human Genetics*, 123(6) 599-605, 2008
  - 21) Rao VR, Sas AR, Eugenin EA, Siddappa NB, Nelson HB, Berman JW, Ranga U, Tyor WR, Prasad VR. Human Immunodeficiency Virus-1 Clade-Specific Differences in the Induction of Neuropathogenesis. *The Journal of Neuroscience*, 28, 10010-16, 2008.
  - 22) Mishra M, Vetrivel S, Siddappa NB, Ranga U, Seth P. Clade Specific Neurotoxicity of HIV Tat: Significance of the Dicysteine C30C31 Motif, *Annals of Neurology*, 63, 366 – 376, 2008.
  - 23) Kishore AH, Vedamurthy BM, Mantelingu K, Agrawal S, Reddy BA, Roy S, Rangappa KS, Kundu TK. Specific small-molecule activator of Aurora kinase A induces autophosphorylation in a cell-free system. *J Med. Chem.*, 51(4), 792-7, 2008.
  - 24) Kumar GV, Selvi BR, Kishore AH, Kundu TK, Narayana C. Surface enhanced Raman spectroscopic studies of coactivator-associated arginine methyltransferase 1. *J Phys Chem B.*, 112(21):6703-7, 2008.
  - 25) Padmanabhan S, Thakur J, Siddharthan R, Sanyal K. Rapid evolution of Cse4p-rich centromeric DNA sequences in closely related pathogenic yeasts, *Candida albicans* and *Candida dubliniensis*. *Proc. Natl. Acad. Sci., USA*, 105: 19797- 19802, 2008
  - 26) Selvi R, Jagadeesan D, Suma BS, Nagashankar G, Arif M, Balasubramanyam K, Eswaramoorthy M, Kundu TK. Intrinsically Fluorescent Carbon Nanospheres as a Nuclear Targeting Vector: Delivery of Membrane-Impermeable Molecule to Modulate Gene Expression In Vivo, *Nano lett.*, 8(10):3182-8, 2008.
  - 27) Ratnapriya R, Satishchandra P, Kumar D, Gadre G, Reddy R, Anand A. A locus for autosomal dominant reflex epilepsy precipitated by hot water maps at chromosome 10q21.3-q22.3. *Human Genetics*, doi 10.1007/S00439-009-0648-3, 2009.
  - 28) Bulusu V, Srinivasan B, Bopanna MP, Balaram H. Elucidation of the substrate specificity, kinetic and catalytic mechanism of adenylosuccinate lyase from *Plasmodium falciparum*. *Biochim Biophys Acta.*, 1794, 642-54, 2009.
  - 29) Sharma AK, Sharma SK, Surolia A, Surolia N, Sarma SP. Solution structures of conformationally equilibrium forms of holo-acyl carrier protein (PfACP) from *Plasmodium falciparum* provides insight into the mechanism of activation of ACPs. *Biochemistry*, 45, 694-6916, 2009.
  - 30) Karmodiya K, Surolia N. Analyses of co-operative transitions in *Plasmodium falciparum* beta-ketoacyl acyl carrier protein reductase upon co-factor and acyl carrier protein binding. *FEBS J*, 273, 4093 – 4103, 2009.
  - 31) Kumar G, Parasuraman P, Sharma SK, Banerjee T, Karmodiya K, Surolia N, Surolia A. Discovery of a Rhodanine Class of Compounds as Inhibitors of *Plasmodium falciparum* Enoyl-Acyl Carrier Protein Reductase. *J Med. Chem.*, 50, 2265 – 75, 2009.
  - 32) Modak R, Sinha S, Surolia N. Isothermal unfolding studies on the apo and holo forms of *Plasmodium falciparum* acyl carrier protein. Role of the 4'-phosphopantetheine group in the stability of the holo form of *Plasmodium falciparum* acyl carrier protein. *FEBS Journal*, 274, 3313 – 3326, 2009.
  - 33) Arif M, Pradhan SK, Thanuja GR, Mantelingu K, Vedamurthy M, Dasgupta D, Kundu TK. Mechanism of p300 specific histone acetyltransferase inhibition by small molecules. *J Med. Chem.*, 52(2), 267-77, 2009.

- 34) Kiran Batta, Masatoshi Yokokawa, Kunio Takeyasu, Kundu TK. Human Transcriptional coactivator PC4 stimulates DNA end joining and activates DSB repair activity. *J Mol. Biol.*, 385(3),788-99, 2009.
- 35) Sunil K Noothi, Mamata Kombrabail, Kundu TK, Krishnamoorthy G, Basuthkar J Rao. Enhanced DNA dynamics due to cationic reagents, topological states of dsDNA and high mobility group box 1 as probed by PicoGreen. *FEBS J.*, 276,541-551, 2009.
- 36) Selvi R, Pradhan S, Shandilya J, Das D, Sailaja BS, Nagashankar G, Gadad SS, Reddy A, Dasgupta D, Kundu TK. Putative anticancer therapeutic, Sanguinarine interacts with chromatin; modulates epigenetic modifications and chromatin transcription. *Chem. Biol.*, 16(2), 203-216, 2009.
- 37) Selvi BR, Kundu TK. Reversible acetylation of Chromatin: Implication in regulation of gene expression, disease and therapeutics. *Biotechnol. J.*, 4(3),375-390, 2009.
- 38) Gadad SS, Shandilya J, Swaminathan V, Kundu TK. Histone chaperone as coactivator of chromatin transcription: Role of acetylation. *Chromatin Protocols (Humana Press)* 523(2),263-278, 2009.
- 39) Inamdar M, Venu P, Rao K, Srinivas MS, VijayRaghavan K. Derivation and characterization of two sibling human embryonic stem cell lines from discarded Grade III embryos. *Stem Cells and Development* (In Press).
- 40) Banerjee T, Sharma SK, Surolia N, Surolia A. Epigallocatechin gallate is a slow-tight binding inhibitor of enoyl-ACP reductase from *Plasmodium falciparum*. *Biochem Biophys Res Commun*, 2009. (In Press).
- 41) Gupta S, Modak R, Surolia N, Surolia A. Partial molar volumes of acyl carrier proteins are related to their states of acylation. *Biochem. Biophys. Res. Commun.*, 2009, (In Press).
- 42) Misra A, Surolia N, Surolia A. Catalysis and mechanism of malonyl transferase activity in type II fatty acid biosynthesis acyl carrier proteins. *Mol. Biosyst.*, 2009, (In Press).
- 43) Sharma S, Sharma SK, Surolia N, Surolia A. Beta-Ketoacyl-ACP synthase I/II from *Plasmodium falciparum* (PfFabB/F)-Is it B or F? *IUBMB Life*, 2009, (In Press).

#### Articles/Chapters in Books and Papers Presented at Confernces

Bulusu V, Bhat JY, Mehrotra S, Balaram H. Purine nucleotide metabolism in *Plasmodium falciparum*, in Antimicrobial resistance – The modern epidemic, Current status and research issues, The 9<sup>th</sup> Sir Dorabji Tata Symposium, Eds. Rangunath D, Nagaraja V, Durga Rao C., pp 53-72, 2009.

#### (vi) Theoretical Sciences Unit

- 1) Kurt Binder, Das SK, Juergen Horbach, Sanjay Puri. Simulation of surface-controlled phase separation in slit pores: Diffusive Ginzburg-Landau kinetics versus Molecular Dynamics. *Computer Physics Communications*, 179, 1, 2008.
- 2) Das SK, Juergen Horbach, Thomas Voigtmann. Structural relaxation in a binary metallic melt: Molecular dynamics computer simulation of undercooled Al80Ni20. *Physical Review E*, 78, 064208, 2008.
- 3) Jain K. Loss of least-loaded class in asexual populations due to drift and epistasis. *Genetics*, 179, 2125, 2008.
- 4) Marathe R, Jain K, Dhar A. Particle current in symmetric exclusion process with time-dependent hopping rates. *J. Stat. Mech.* 11014, 2008.
- 5) Imam M, Marathe M, Narasimhan S. Competition between elastic and chemical effects in the intermixing of Ag and Co on Rh(111). *J. Chem. Sci.* 120, 621, 2008.
- 6) Ghosh P, Pushpa R, Gironcoli S de, Narasimhan S. Interplay between bonding and magnetism in the binding NO to Rh clusters. *J. Chem. Phys.*, 128, 194708, 2008.
- 7) Sinha KB. Semigroups of Maps on Operator Algebras, their Dilations and Applications. *TWAS Science Frontiers, Current Science*, 95(9),1268-1276, 2008.



- 8) Kabra D, Verma J, Vidhyadhiraja NS, Narayan KS. Model for studies of lateral photovoltaic effect in polymeric semiconductors. *IEEE Sensors Journal*, Vol.8, No.10, Oct. 2008.
- 9) Parihari D, Vidhyadhiraja NS. Interplay between strong correlations and magnetic field in the symmetric periodic Anderson model. *Physical Review B*, 78, 035128, 2008.
- 10) Lakshmi S, Sudipta Dutta, Pati SK. Molecular Electronics: Effect of Electric Field. *J. Phys. Chem. C. (Feature Article)*, 112, 14718, 2008.
- 11) Pati SK, Rao CNR. Kagome network compounds and their novel magnetic properties. *Chem. Comm. (Feature Article)*, 4683, 2008.
- 12) Sairam SM, Lin JC, Cox DL, Pati SK, Singh, RRP. Sequence Dependent Electron Transport in Wet DNA: Ab-initio and Molecular Dynamics. *Phys. Rev. Lett.*, 101, 176805, 2008.  
(Selected for the Virtual Journal of Nanoscale Science and Technology, 3 (2008) and Virtual Journal of Biological Physics Research, 1 (2008).  
(Selected for the Virtual Journal of Nanoscale Science and Technology, 17 (11) 2008)).
- 13) Sairam SM, Pati SK. Benzimidazole modified Single Stranded DNA: Stable Scaffolds for 1-Dimensional Spintronics Constructs. *J. Phys. Chem. B*, 112 (51), 16982, 2008.
- 14) Dutta S, Lakshmi S, Pati SK. Comparative Study of The Electron Conduction in Azulene and Naphthalene. *Bulletin of Material Science*, 31, 353, 2008.
- 15) Ghosh A, Subrahmanyam KS, Sai Krishna K, Dutta S, Govindaraj A, Pati SK, Rao CNR. Uptake of H<sub>2</sub> and CO<sub>2</sub> by Graphene. *J. Phys. Chem. C*, 112 (40), 15704, 2008.
- 16) Pal S, Manna AK, Pati SK. The role of H-bonding and dipole-dipole interactions on the electrical polarizations and charge mobilities in linear arrays of urea, thiourea and their derivatives. *J. Chem. Phys.*, 129(20), 204301, 2008.
- 17) Reji Thomas, Pal S, Ayan Datta, Mariusz K. Marchewka, Henryk Ratajczak, Pati SK, Kulkarni GU. Charge density analysis of two proton transfer complexes: Understanding hydrogen bonding and determination of in-crystal dipole moments. *J. Chem. Sciences*, 120(6), 613, 2008.
- 18) Sairam SM, Usha H, Ayan Datta, Pati SK. Molecular Modeling of a chemodosimeter for the selective detection of As(III) ion in water. *J. Chem. Sciences*, 120(6), 627, 2008.
- 19) Chaudhuri P, Sastry S, Walter Kob. Tracking heterogeneous dynamics during the alpha-relaxation of a simple glass-former. *Phys. Rev. Lett.* 101, 190601, 2008.
- 20) Burton BP, Silvia Tinte, Eric Cockayne, Waghmare UV. The effect of nearest neighbor [Pb-O] divacancy pairs on the Ferroelectric-relaxor transition in Nano-ordered Pb(Sc<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub> Integrated Ferroelectrics. 101,37, 2008.
- 21) Jaita Paul, Nishimatsu T, Kawazoe Y, Waghmare, UV. Polarization Switching in Epitaxial Films of BaTiO<sub>3</sub>: A Molecular Dynamics Study. *Appl. Phys. Lett.*, 93 242905, 2008
- 22) Sanyal S, Waghmare UV, Subramanian PR, et al. Effect of dopants on grain boundary decohesion of Ni: A first-principles study. *Appl. Phys. Lett.*, 93, 22, 223113, 2008
- 23) Saha SK, Waghmare UV, Krishnamurthy HR, et al. Phonons in few-layer graphene and interplanar interaction: A first-principles study. *Physical Review B*, 78, 16, 165421, 2008.
- 24) Kahaly MU, Waghmare UV. Electronic Structure of Carbon Doped Boron Nitride Nanotubes: A First-Principles Study. *Journal of NanoScience and Nanotechnology*, 8, 8, 4041-4048, 2008.
- 25) Dutta G, Waghmare UV. Ti-doped ThO<sub>2</sub>: a first-principles study of dielectric properties. *Journal of Physics D-Applied Physics*, 41, 20, 205414, 2008.
- 26) Nishimatsu T, Waghmare UV, Kawazoe Y, et al. Fast molecular-dynamics simulation for ferroelectric thin-film capacitors using a first-principles effective Hamiltonian. *Phys. Rev. B*, 78, 10, 104104, 2008.
- 27) Kahaly MU, Waghmare UV. Effect of curvature on structures and vibrations of zigzag carbon nanotubes: A first-principles study. *Bulletin of Materials Science*, 31, 3, 335-341, 2008.

- 28) Dutta G, Waghmare UV. Dielectric response in Ce-doped ThO<sub>2</sub>. *Physica B-Condensed Matter*, 403, 13-16, 2197-2199, 2008.
- 29) Lee JH, Waghmare UV, Yu JJ. First-principles effective Hamiltonian for ferroelectric polarization in BaTiO<sub>3</sub>/SrTiO<sub>3</sub> superlattices. *Journal of Applied Physics*, 103, 12, 124106, 2008.
- 30) Datta A, Waghmare UV, Ramamurty U. Structure and stacking faults in layered Mg-Zn-Y alloys: A first-principles study. *Acta Materialia*, 56, 11, 2531-2539, 2008.
- 31) Nabarro FRN, Luyckx SB, Waghmare UV Slip in tungsten monocarbide I. Some experimental observations. *Materials Science and Engineering A*, 483, 139-142, 2008
- 32) Ray N, Waghmare UV. Coupling between magnetic ordering and structural instabilities in perovskite biferroics: A first-principles study. *Physical Review B*, 77, 13 134112, 2008.
- 33) Das A, Pisana S, Chakraborty B, et al. Monitoring dopants by Raman scattering in an electrochemically top-gated graphene transistor. *Nature Nanotechnology*, 3, 4, 210-215, 2008.
- 34) Thomas T, Pandey D, Waghmare UV. Soft modes at the stacking faults in SiC crystals: First-principles calculations. *Physical Review B*, 77, 12, 121203, 2008.
- 35) Kahaly MU, Waghmare UV. Contrast in the electronic and magnetic properties of doped carbon and boron nitride nanotubes: A first-principles study. *Journal of Physical Chemistry C*, 112, 10, 3464-3472, 2008.
- 36) Das SK, Juergen Horbach, Kurt Binder. Kinetics of phase separation in thin films: Lattice versus continuum models for solid binary mixtures. *Physical Review E*, 79, 021602, 2009.
- 37) Kurt Binder, Das SK, Juergen Horbach. Surface-directed spinodal decomposition: lattice model versus ginzburg-landau theory. *Modern Physics Letters B*, 23, 549, 2009
- 38) Nagar A, Jain K. Exact phase diagram of quasispecies model with mutation rate modifier. *Phys. Rev. Lett.*, 102, 038101, 2009.
- 39) Pushpa R, Ghosh P, Narasimhan S, Gironcoli S de. Effective Coordination as a Predictor of Adsorption Energies: a Model Study of NO on Rh(100) and Rh/MgO(100) Surfaces. *Phys. Rev. B*, 79, 165406, 2009.
- 40) Marathe M, Imam M, Narasimhan S. Elastic and chemical contributions to the stability of magnetic surface alloys on Ru(0001). *Phys. Rev. B*, 79, 085413, 2009.
- 41) Imam M, Marathe M, Narasimhan S. NiPt<sub>1-x</sub>/Rh(111): A Stable Surface Alloy with Enhanced Magnetic Moments. *Solid State Commun.*, 149, 559, 2009.
- 42) Sudipta Dutta, Pati SK. Electrical Rectification: A Tale of Two Isomers. *Resonance* (Feature Article), 14, 80, 2009.
- 43) Prakash Parida, Lakshmi S, Pati SK. Negative differential resistance in nanoscale transport in the Coulomb blockade regime. *J. Phys. Cond. Matt.*, 21, 095301, 2009.
- 44) Sudipta Dutta, Manna AK, Pati SK. Intrinsic Half-Metallicity in modified Graphene Nanoribbons. *Phys. Rev. Lett.* 102, 096601, 2009.
- 45) Anasuya Kundu, Pati SK. Quantum Phase Transitions in a Dimerized Bose-Hubbard Model: A DMRG Study. *Europhys. Lett.*, 85, 43001, 2009.
- 46) Sairam SM, Prakash Parida, Pati SK. Organometallic Vanadium-Borazine Systems: Efficient One-Dimensional Half-Metallic Spin Filters. *J. Mater. Chem.* 19, 1761, 2009.
- 47) Anukul Jana, Sen SS, Roesky HW, Schulzke C, Sudipta Dutta, Pati SK. Unprecedented End-On Nitrogen Insertion of a Diazo Compound into a Germanium(II) Hydrogen Bond and Comparable Reactions with Azide and Diethyl Azodicarboxylate. *Angew. Chem. Int. Ed.* 48, 4226, 2009.
- 48) Karmakar S, Dasgupta C, Sastry S. Growing length and time scales in glass forming liquids. *PNAS*, 106, 3675, 2009.





- 49) Mangalam RVK, Nirat Ray, Waghmare UV, Sundaresan A, Rao CNR. Multiferroic Properties of Nanocrystalline BaTiO<sub>3</sub>. *Sol. State. Comm.*, 149, 1-5, 2009.
- 50) Aditi Datta, Waghmare UV, Ramamurty U. First-principles Study of Stacking Faults and Twinning in Nano-Ni. *Scripta Materialia*, 60, 124-127, 2009
- 51) Sairam SM, Pati SK. Conformational Tuning of Magnetic Interactions in Metal-DNA. *Angew. Chem. Int. Ed.* 2009 (In Press).
- 52) Mohakud S, Pati SK. Large Carrier Mobility in Octathio-Circulene Crystals: A Theoretical Study. *J. Mater. Chem.*, 2009 (In Press).
- 53) Mondal TK, Sudipta Dutta, Pati SK. Electronic Absorption Spectra and Nonlinear Optical Properties of CO<sub>2</sub> molecular aggregates: A Quantum Chemical Study. *J. Chem. Sci.*, 2009 (In Press).
- 54) Prakash K, Madhu C, Golam Mostafa, Maji TK, Sundaresan A, Pati SK, Rao CNR. "A planar  $\text{Cu}^{2+}$  (S = 1/2) kagome network pillared by 1,2-bis(4-pyridyl) ethane with interesting magnetic properties. *Dalton Transaction*, 2009 (In Press).
- 55) Tinku Baidya, Gargi Dutta, Hegde MS, Waghmare UV. Noble metal ionic catalysts: correlation of increase in CO oxidation activity with increasing effective charge on Pd ion in Pd ion substituted Ce<sub>1-x</sub>MxO<sub>2</sub>- (M = Ti, Zr and Hf). *Dalton Trans.*, 2009, (In Press)
- 56) Manna AK, Pati SK. Tuning the electronic structure of graphene by molecular charge transfer: A theoretical study. *Chem. Asian J.*, 2009 (to appear)
- 57) Sairam SM, Ashutosh Gupta, Pati SK. Fluctuations at the Base Pair Level Effecting Charge Transfer in DNA. *J. Phys. Chem. A*, 2009 (to appear)
- 58) Prakash Parida, Anasuya Kundu, Pati, SK. The Electronic and Magnetic Properties of a Few Transition-Metal Clusters. *J. Cluster Sci.*, 2009 (to appear).
- 59) Rakesh V, Pati SK, Rao CNR. Effect of Electronic Coupling Between CdSe Nanocrystals on the Photoluminescence Spectra. *J. Nanosci. Nanotech.* 2009 (to appear).
- 60) Reji Thomas, Sairam SM, Lakshmi S, Pati SK, Kulkarni GU. Conjugation in 1,4-diphenylbutadiyne and 1,2-diphenylacetylene: A Combined Experimental and Theoretical study. *J. Mol. Struct.: THEOCHEM*, 2009 (to appear).
- 61) Sinha KB, Schurmann M, Sahu L. Unitary Processes with Independent increments and Hilbert Tensor algebras", *Publications of the Research Institute of Math.Sciences*, Kyoto University, Japan, 2009. (to appear)
- 62) Sinha KB, Sahu L. Characterisation of Unitary processes with independent stationary increments. *Annals of Institute Henri Poincare- B (Paris)*, 2009. (accepted)
- 63) Dhritiman Gupta, Vidhyadhiraja NS, Narayan KS. Transport of photogenerated charge carriers in polymer semiconductors. *Proceedings of the IEEE*, 2009. (accepted)

#### Articles/Chapters in Books and Papers Presented at Confernces

- 1) Das SK, Ali Kerrache, Juergen Horbach, Kurt Binder. Phase behavior and microscopic transport processes in binary metallic alloys: Computer simulation studies, *Phase Transformations in Multicomponent Melts* (Wiley, Weinheim), ed. D.M. Herlach, 141, 2008.
- 2) Sairam SM, . Pati SK. DNA Scaffold for Spintronics Applications: A Theoretical Study. *Proc. of the 53rd DAE Solid State Physics Symposium*, 39, 2008.
- 3) Sinha KB. A chapter on "Probability and Stochastic Processes "in the book entitled "Indian Contributions in the world of Physics": Then and Now ", Ed. A.N.Mitra, Centre for Studies in Civilisations, Project of History of Indian Science, Philosophy and Culture, New Delhi , 2008.
- 4) Sinha KB, Goswami D. Quantum Stochastic Dilation of symmetric covariant Completely positive semigroups with unbounded generators. *Infinite Dimensional Stochastic Analysis* (in honour of Prof. H-H Kuo ) Eds. A.Sengupta and P.Sundar, Vol 22, *Quantum Probability and White Noise Analysis*, *World Scientific, Singapore*, 2008.

(vii) Chemical Biology Unit

- 1) Bhat S, Maitra U. Facially amphiphilic thiol capped gold and silver nanoparticles. *J. Chem. Sci*, 120, 507-513, 2008.
- 2) Ghosh S, Usharani D, Paul A, De S, Jemmis ED, Bhattacharya S. Design, Synthesis, and DNA Binding Properties of Photoisomerizable Azobenzene-Distamycin Conjugates: An Experimental and Computational Study. *Bioconjugate Chem.*, 19, 2332-2345, 2008.
- 3) Chatterjee S, Vasudev PG, Raghothama S, Shamala N, Balaram P. Solid State and Solution Conformations of a Hybrid alpha gamma alpha alpha gamma alpha Hexapeptide. Characterization of a Backbone Expanded Analog of the alpha-Polypeptide 3(10)-Helix. *Biopolymers*, 90, 759-771, 2008.
- 4) Mehta G, Likhite NS. A total synthesis of ( $\pm$ )-frondosins A and B. *Tetrahedron lett.* 49, 7113-7116, 2008.
- 5) Bajaj K, Dewan PC, Chakrabarti P, Goswami D, Barua B, Baliga C, Varadarajan R. Structural Correlates of the Temperature Sensitive Phenotype Derived from Saturation Mutagenesis Studies of CcdB. *Biochemistry*, 47, 12964-12973, 2008.
- 6) Ghosh S, Usharani D, De S, Jemmis ED, Bhattacharya S. Photophysical and Duplex-DNA-Binding Properties of Distamycin Dimers Based on 4,4'- and 2,2'-Dialkoxyazobenzenes as the Core. *Chem. Asian J.* 3, 1949-1961, 2008.
- 7) Raghava S, Barua B, Singh PK, Das M, Madan L, Bhattacharyya S, Bajaj K, Gopal B, Varadarajan R, Gupta MN. Refolding and simultaneous purification by three-phase partitioning of recombinant proteins from inclusion bodies. *Protein Sci.* 17, 1987-1997, 2008.
- 8) Terech P, Maitra U. Structural and Rheological Properties of Aqueous Viscoelastic Solutions and Gels of Tripodal Cholamide-Based Self-Assembled Supramolecules. *J. Phys. Chem. B.* , 112, 13483-13492, 2008.
- 9) Bhattacharya S, Bajaj A. Fluorescence and thermotropic studies of the interactions of PEI-cholesterol based PEI-chol lipopolymers with dipalmitoyl phosphatidylcholine membranes. *Biochim. Biophys. Acta, Biomembr.*, 1778, 2225-2233, 2008.
- 10) Chatterjee S, Vasudev PG, Ananda K, Raghothama S, Shamala N, Balaram P. Multiple conformational states in crystals and in solution in alpha gamma hybrid peptides. Fragility of the C-12 helix in short sequences. *J. Org. Chem.*, 73, 6595-6606, 2008.
- 11) Bhattacharya S, Chaudhuri P. Medical implications of benzimidazole derivatives as drugs designed for targeting DNA and DNA associated processes. *Curr. Med. Chem.*, 15, 1762-1777, 2008.
- 12) Mehta G, Roy S, Davis RA. On the stereostructures of (+)-eupenoxide and (-)-3',4'-dihydrophomoxide: a caveat on the spectral comparisons of oxygenated cyclohexenoids. *Tetrahedron lett.*, 49, 5162-5164, 2008.
- 13) Bajaj A, Kondaiah P, Bhattacharya S. Synthesis and gene transfection efficacies of PEI-cholesterol-based lipopolymers. *Bioconjugate Chem.*, 19, 1640-1651, 2008.
- 14) Vasudev PG, Chatterjee S, Ananda K, Shamala N, Balaram P. Hybrid alpha gamma polypeptides: Structural characterization of a C-12/C-10 helix with alternating hydrogen-bond polarity. *Angew. Chem. Int. Ed.* 47, 6430-6432, 2008.
- 15) Basit H, Pal A, Sen S, Bhattacharya S. Two-component hydrogels comprising fatty acids and amines: Structure, properties, and application as a template for the synthesis of metal nanoparticles. *Chem. Eur. J.*, 14, 6534-6545, 2008.
- 16) Aravinda S, Shamala N, Balaram P. Aib residues in peptaibiotics and synthetic sequences: Analysis of nonhelical conformations. *Chem. Biodiversity*, 5, 1238-1262, 2008.
- 17) Chatterjee B, Saha I, Raghothama S, Aravinda S, Rai R, Shamala N, Balaram P. Designed peptides with homochiral and heterochiral diproline templates as conformational constraints. *Chem. Eur. J.*, 14, 6192-6204, 2008.
- 18) Gowd KH, Dewan KK, Iengar P, Krishnan KS, Balaram P. Probing peptide libraries from *Conus achatinus* using mass spectrometry and cDNA sequencing: identification of delta and omega-conotoxins. *J. Mass Spectrom.*, 43, 791-805, 2008.
- 19) Saha I, Chatterjee B, Shamala N, Balaram P. Crystal structures of peptide enantiomers and race mates: Probing conformational diversity in heterochiral Pro-Pro sequences. *Biopolymers*, 90, 537-543, 2008.



- 20) Vasudev PG, Rai R, Shamala N, Balaram P. Conformations of beta-amino acid residues in peptides: X-ray diffraction studies of peptides containing the achiral residue 1-aminocyclohexaneacetic acid, beta(3,3)Ac(6)c. *Biopolymers*, 90, 581-582, 2008.
- 21) Raghava S, Aquil S, Bhattacharyya S, Varadarajan R, Gupta MN. Strategy for purifying maltose binding protein fusion proteins by affinity precipitation.. *J. Chromatogr. A* 1194, 90-95, 2008.
- 22) Bajaj A, Paul B, Kondaiah P, Bhattacharya S. Structure-activity investigation on the gene transfection properties of cardiolipin mimicking gemini lipid analogues, *Bioconjugate Chem.*, 19, 1283-1300, 2008.
- 23) Bajaj A, Mishra SK, Kondaiah P, Bhattacharya S. Effect of the headgroup variation on the gene transfer properties of cholesterol based cationic lipids possessing ether linkage. *Biochim. Biophys. Acta, Biomembr.*, 1778, 1222-1236, 2008.
- 24) Hegde RP, Aravinda S, Rai R, Kaul R, Vijayalakshmi S, Rao RB, Shamala N, Balaram P. Conformation of di-n-propylglycine residues (Dpg) in peptides: crystal structures of a type I 'beta-turn forming tetrapeptide and an alpha-helical tetradecapeptide. *J. Pept. Sci.*, 14, 648-659, 2008.
- 25) Pal A, Chhikara BS, Govindaraj A, Bhattacharya S, Rao CNR. Synthesis and properties of novel nanocomposites made of single-walled carbon nanotubes and low molecular mass organogels and their thermo-responsive behavior triggered by near IR radiation.. *J. Mater. Chem.*, 18, 2593-2600, 2008.
- 26) Mehta G, Sen S, Pallavi K. Understanding the self-assembling process in crystalline cyclooctitols: an insight into the conformational flexibility of medium-sized rings. *Cryst. Engg. Comm.*, 10, 534-540, 2008.
- 27) Saikumari YK, Balaram P. An internally quenched fluorescent substrate for collagenase. *Biopolymers*, 90, 131-137, 2008.
- 28) Vasudev PG, Rai R, Shamala N, Balaram P. Conformations of beta-amino acid residues in peptides: X-ray diffraction studies of peptides containing the achiral residue 1-aminocyclohexaneacetic acid, beta(3,3)Ac(6)c. *Biopolymers*, 90, 138-150, 2008.
- 29) Thakur SS, Balaram P. Fragmentation of peptide disulfides under conditions of negative ion mass spectrometry: Studies of oxidized glutathione and contryphan. *J. Am. Soc. Mass Spectrom.*, 19, 358-366, 2008.
- 30) Nonappa, Maitra U. Unlocking the potential of bile acids in synthesis, supra-molecular/materials chemistry and nanoscience. *Org. Biomol. Chem.*, 6, 657-669, 2008.
- 31) Vasudev PG, Shamala N, Balaram P. Nucleation, growth, and form in crystals of peptide helices. *J. Phys. Chem. B*, 112, 1308-1314, 2008.
- 32) Mandal AK, Bisht S, Bhat VS, Krishnaswamy PR, Balaram P. Electrospray mass spectrometric characterization of hemoglobin Q (Hb Q-India) and a double mutant hemoglobin S/D in clinical samples. *Clin. Biochem.*, 41, 75-81, 2008.

**(viii) Condensed Matter Theory Unit**

- 1) Ray SS, Mitra D, Pandit R. The Universality of Dynamic Multiscaling in omogeneous, Isotropic Navier-Stokes and Passive-Scalar Turbulence. *New Journal of Physics*, 10, 033003, 2008.
- 2) Frisch U, Kurien S, Pandit R, Pauls W, Ray SS, Wirth A, Zhu J-Z. Hyperviscosity, Galerkin truncation and bottlenecks in turbulence. *Phys. Rev. Lett.* 101, 144501, 2008
- 3) Baule A, Vijay Kumar K, Ramaswamy S. Exact solution of a Brownian inchworm model for self-propulsion, *J. Stat. Mech*, 11008, 2008.
- 4) Vijay Kumar K, Ramaswamy S, Rao M. Active elastic dimers: self-propulsion and current reversal on a featureless track. *Phys. Rev. E (Rapid Comm.)* 77, 020102 R, 2008.
- 5) Demontis P, Suffritti GB, Yashonath S. Comment on "High-Accuracy Estimation of 'Slow' Molecular Diffusion Rates in Zeolite Nanopores, Based on Free Energy Calculations at an Ultrahigh Temperature". *Journal of Physical Chemistry C*, 112(43), 17030-17031, 2008.
- 6) Sharma M, Yashonath S. Correlation between conductivity or diffusivity and activation energy in amorphous solids. *Journal of Chemical Physics*, 129 (14) 144103, 2008.
- 7) Sanyal P, Gupta SS, Nandan Pakhira, Krishnamurthy HR, Sarma DD, Ramakrishnan TV. Theory of the unusual doping and temperature dependence of photoemission spectra in manganites. *Europhysics Letters*, 82, 47010, 2008.

- 8) Batrouni GG, Krishnamurthy HR, Mahmud KW, Rousseau VG, Scalettar RT. Canonical trajectories and critical coupling of the Bose-Hubbard Hamiltonian in a harmonic trap. *Phys. Rev. A* 78, 023627, 2008.
- 9) Saha SK, Waghmare UV, Krishnamurthy HR, Sood AK. Phonons in few-layer graphene and interplanar interaction: A first-principles study. *Phys. Rev. B*, 78, 165421, 2008.
- 10) Mukherjee B, Maiti PK, Dasgupta C, Sood AK. Strongly anisotropic orientational relaxation of water molecules in narrow carbon nanotubes and nanorings. *ACS Nano* 2, 1189, 2008.
- 11) Ray SS, Mitra D, Pandit R. The Universality of Dynamic Multiscaling in Homogeneous, Isotropic Navier-Stokes and Passive-Scalar Turbulence. *New Journal of Physics*, 10, 033003, 2008.
- 12) Frisch U, Kurien S, Pandit R, Pauls W, Ray SS, Wirth A, Zhu J-Z. Hyperviscosity, Galerkin truncation and bottlenecks in turbulence. *Phys. Rev. Lett.*, 101, 144501, 2008.
- 13) Demontis P, Sufritti GB, Yashonath S. Comment on "High-Accuracy Estimation of 'Slow' Molecular Diffusion Rates in Zeolite Nanopores, Based on Free Energy Calculations at an Ultrahigh Temperature". *Journal of Physical Chemistry C*, 112 (43): 17030-17031, 2008.
- 14) Shajahan TK, Nayak AR, Pandit R. Spiral-Wave Turbulence and its Control in the Presence of Inhomogeneities in Four Mathematical Models of Cardiac Tissue. *PLoS ONE*, 4(3): e4738, 2009.
- 15) Krishna C, Yashonath S. Dependence of self-diffusivity on size of impurity atoms in a face-centred cubic solid: existence of an anomalous maximum. *Molecular Simulation*, 35 (1-2), 151-161, 2009.
- 16) Karmakar S, Dasgupta C, Sastry S. Growing length and time scales in glass forming liquids. *Proc. Natl. Acad. Sci (USA)*, 106, 3675, 2009.
- 17) Dasgupta C, Valls OT. Hydrodynamics of superfluids confined in blocked rings and wedges. *Phys. Rev. E*, 79, 016303, 2009.

#### Articles/Chapters in Books and Papers Presented at Conferences

- 1) Hena Das, Waghmare UV, Saha-Dasgupta T, Sarma DD. Electronic structure, phonons, and dielectric anomaly in ferromagnetic insulating double perovskite La<sub>2</sub>NiMnO<sub>6</sub>. *Physical Review Letters*, 100 (18): Art. No. 186402, May 2008.
- 2) Baule A, Vijay Kumar K, Ramaswamy S. Exact solution of a Brownian inchworm model for self-propulsion. *Journal of Statistical Mechanics-Theory and Experiment*: Art. No. P11008, Nov. 2008.
- 3) Middey S, Mahadevan P, Sarma DD. Invalidity of a localized spin mechanism for SrRuO<sub>3</sub> and CaRuO<sub>3</sub>. *Magnetic Materials*, 1003: 148-150, 2008. (AIP Conference Proceedings, International Conference on Magnetic Materials (ICMM 2007))
- 4) Nandy AK, Mahadevan P, Sarma DD. Chemical pressure effects on T<sub>c</sub> in double perovskite oxides A<sub>2</sub>FeMoO<sub>6</sub> (A= Ba, Sr). *Magnetic Materials*, 1003: 166-168, 2008. (AIP Conference Proceedings, International Conference on Magnetic Materials (ICMM 2007))
- 5) Jana S, Mahadevan P, Sarma DD. Electronic structure of Ca<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub>. *Magnetic Materials*, 1003: 175-177, 2008. (AIP Conference Proceedings, International Conference on Magnetic Materials (ICMM 2007))
- 6) Raj S, Chakraborty A, Choudhury D, Sato T, Takahashi T, Mahadevan P, Fujii J, Vobornik I, Sarma DD. Three-dimensional band structure of highly metallic Na<sub>0.8</sub>WO<sub>3</sub> by angle-resolved photoemission spectroscopy. *Physical Review B*, 79 (3): Art. No. 035119, Jan 2009.
- 7) Sharma M, Yashonath S. How does contrasting dependence of impurity-atom diffusivity on the density of host disordered medium arise? *Indian Journal of Physics and Proceedings of The Indian Association For The Cultivation Of Science*, 83 (1), 31-47, 2009.
- 8) Shajahan TK, Sinha S, Pandit R. The Mathematical Modelling of Inhomogeneities in Ventricular Tissue in Complex Dynamics in Physiological Systems: From Heart to Brain (Eds.S.K. Dana, P.K. Roy and J. Kurths), Springer, pp 51-67. 2009.



## 2. Research publications of Hon. Faculty/Endowed Professors

- 1) Majumder PP. Genomic inferences on peopling of south Asia. *Current Opinion in Genetics & Development*. 18, 280-284, 2008
- 2) Vimalaswaran KS, Radha V, Ramya K, Babu HNS, Savitha N, Roopa V, Dhar M, Deepa R, Ghosh S, Majumder PP, Rao MRS, Mohan V. A novel association of a polymorphism in the first intron of adiponectin gene with type 2 diabetes, obesity and hypoadipo-nectinemia in Asian Indians. *Human Genetics*, 123, 599-605, 2008.
- 3) Bairagya BB, Bhattacharya P, Bhattacharya SK, Dey B, Dey U, Ghosh T, Maiti S, Majumder PP, Mishra K, Mukherjee S, Narayanasamy K, Poddar S, Sarkar Roy N, Sengupta P, Sharma S, Sur D, Sutradhar D, Wagener DK. Genetic variation and haplotype structures of innate immunity genes in eastern India. *Infection, Genetics and Evolution*. 8, 360-366, 2008.
- 4) Majumder PP and other authors from six CSIR institutes. Indian Genome Variation Consortium Genetic landscape of the people of India: a canvas for disease gene exploration. *Journal of Genetics*, 87, 3-20, 2008.
- 5) Sarkar Roy N, Farheen S, Roy N, Sengupta S, Majumder PP. Portability of Tag SNPs Across Isolated Population Groups: An Example from India. *Annals of Human Genetics*, 72, 82-89, 2008.
- 6) Majumder PP. Peopling of India: Insights from Genetics. In: Encyclopedia of Life Sciences (ELS). John Wiley & Sons, Ltd: Chichester. 2008.
- 7) Vasu K, Saravanan M, Bujnicki JM, Nagaraja V. Structural integrity of the Beta Beta Alpha-Metal finger motif is required for DNA binding and stable protein-DNA complex formation in R.KpnI. *Biochim. Biophys. Acta.*, 1784, 269-275, 2008
- 8) Sengupta S, Nagaraja V. Studies with glutamate racemase, a DNA gyrase inhibitory protein from *Mycobacterium smegmatis*. *FEMS Microbiol. Lett.*, 279, 40-47, 2008
- 9) Sengupta S, Nagaraja V. Yac G from E.coli is a specific endogeneous inhibitor of DNA gyrase. *Nucl. Acids Res*. 36, 4310-4316, 2008
- 10) Mitra A, Angamuthu K Nagaraja V. Genome-wide analysis of the intrinsic terminators of transcription across the genus *Mycobacterium*. *Tuberculosis (Edinb)*. 88, 566-575, 2008.
- 11) Sengupta S, Ghosh S, Nagaraja V. Moonlighting function of Glutamate Racemase from *Mycobacterium tuberculosis*: Racemization and DNA gyrase inhibition are two independent activities of the enzyme. *Microbiology* 154, 2796-2803, 2008.
- 12) Saravanan M, Vasu K, Nagaraja V. Evolution of sequence specificity in a restriction endonuclease by a point mutation. *Proc. Natl. Acad. Sci, USA*. 105, 10344-10347, 2008.
- 13) Lamba S, Chandrasekhar K, Gadagkar R. Signalling hunger through aggression - the regulation of foraging in a primitively eusocial wasp. *Naturwissenschaften*, 95, 677-680, 2008.
- 14) Bhadra A, Gadagkar R. We know that the wasps 'know': cryptic successors to the queen in *Ropalidia marginata*. *Biol. Lett.*, 4, 634-637, 2008.
- 15) Gadagkar R. Why I do not discourage my students from "wasting" their time with the "theatre"? *MOITREE, The Bangla Theatre Festival in Bengaluru*, 3-4, 2008.
- 16) Gadagkar R. What's happening at the Centre for Contemporary Studies and Why? *Voices, No.6, Indian Institute of Science, Bangalore*. 2008.
- 17) Gadagkar R. Open-access more harm than good in developing world. *Nature*, 453, .450, 2008.
- 18) Mehrotra R, Soni V, Jain S. Diversity sustains an evolving network. *Journal of the Royal Society Interface*, doi:10.1098/rsif.2008.0412 (2008).
- 19) Vyas N, Goswami D, Manonmani A, Sharma P, Ranganath HA, VijayRaghavan K, Shashidhara LS, Sowdhamini R, Mayor S. Nanoscale organization of Hh is essential for long range signaling. *Cell* 133, 1214-1227, 2008.

- 20) Gupta RK, Tripathi R, Naidu BJ, Srinivas UK, Shashidhara LS. Cell cycle regulation by the pro-apoptotic gene Scotin. *Cell Cycle*, 7, 2401-2408, 2008.
- 21) Ramesh Rao P, Makhijani K, Shashidhara LS. Human APC sequesters b-catenin even in the absence of GSK-3b in a Drosophila model. *Oncogene*, 27, 2488-2493, 2008.
- 22) Swapna G. Saravnan M, Nagaraja V. Conformational Changes Triggered by Mg<sup>2+</sup> Mediate Transactivator Function. *Biochemistry*, 48, 2347-2354, 2009.
- 23) Bhadra A., Jordan F, Gadagkar R. A comparative social network analysis of wasp colonies and classrooms: linking network structure to functioning. *Ecological Complexity*, 2008. (in press)
- 24) Gadagkar R. What can we learn from insect societies? In: *Nature and Culture* (Eds.) Roddam Narasimha and Sangeetha Menon, National Institute of Advanced Studies, Bangalore, 2008. (in press).
- 25) Mukherjee S, Sarkar-Roy N, Wagener D, Majumder PP. Signatures of natural selection are not uniform across genes of innate immune system, but purifying selection is the dominant signature. *Proceedings of the National Academy of Sciences, USA*, 2009. (in press)
- 26) Sumithra Sankararaman, Ramaswamy S. Instabilities and waves in thin films of living fluids, *Phys. Rev. Lett.*, 2009. (in press)
- 27) Pramod P, George Thomas K, George MV. Organic nanomaterials: Morphological control for charge stabilization and charge transport. *Chemistry-an Asian Journal*, 4, Issue 6, 2009. (accepted for publication)

#### Articles/Chapters in Books and Papers Presented at Conferences

- 1) Gadagkar R. Cooperation. In: *Behavioural Ecology*. Vol.1 of *Encyclopedia of Ecology*, (Eds.) S.E. Jorgensen and Fath, B.D., Elsevier Ltd., Oxford, pp. 776-777, 2008.  
Gadagkar R. Why are animals nice to each other? In: *The Seventy Great Mysteries of the Natural World*, (Ed.) M.J. Benton, Thames & Hudson Ltd., London, pp. 225-228, 2008.

#### Books/Proceedings authored/ edited by Faculty

- Rao CNR. Trends in Chemistry of Materials, selected research papers of CNR Rao, World Scientific, 2008.
- Chandrashekar MK, Sharma VK. Tidal rhythms. In: *Ultradian Rhythms*. Llyod, D. and E. Rossi (eds.). Springer-Verlag, Berlin, 2008.
- Valdiya KS. Facing the Hazards: Earthquakes and Landslides. Gyanodaya Prakashan, Nainital, 87, 2008.
- Subir K Das, Ali Kerrache, Juergen Horbach, Kurt Binder. Phase behavior and microscopic transport processes in binary metallic alloys: Computer simulation studies, Phase Transformations in Multicomponent Melts, in *Phase Transformations in Multicomponent melts*, (ed) Herlach DM, Wiley, Weinheim, 141, 2008.

#### Books/Proceedings authored/ edited by Hon. Faculty

- Nagaraja V (Ed) Antimicrobial resistance-The Modern Epidemic, Macmillan Publishers India Ltd., 2008.
- Shajahan TK, Sinha S, Pandit R. The Mathematical Modelling of Inhomogeneities in Ventricular Tissue in *Complex Dynamics in Physiological Systems: From Heart to Brain* (Eds. Dana SK, Roy PK, Kurths J), Springer, pp. 51-67, 2009



## AWARDS/DISTINCTIONS

The following faculty and honorary faculty members of the Centre have received various honors and awards both at the national and international level in recognition of their significant contributions to the progress of science and technology.

Awards & Honours

**Prof C N R Rao**

Nikkei Asia Prize For Science, Technology and Innovation from Japan (2008).

Order of Friendship, by the President of Russia (2009).

First Laureate of the 21<sup>st</sup> Khwarizmi International Science Award by the Iranian Research Organization for Science & Technology (2008).

The First International Prize for Materials Science by MRSI (India) (2009)

**Prof Anuranjan Anand**

National Bioscience Award for Career development -2008

**Prof S Balasubramanian**

Bronze medal of the Chemical Research Society of India, 2009

**Prof Namita Surolia**

Ranbaxy award for Basic Science and DBT's Tata Innovation Fellowship both in 2007.

**Prof K S Narayan**

DAE outstanding research investigator award of the Department of Atomic Energy, Mumbai, 2008-09.

**Prof Srikanth Sastry**

CV Raman Young Scientist, KSCST

S S Bhatnagar Prize, 2008

**Prof Tapas Kumar Kundu**

National Academy of Science, India- Reliance Industries Platinum Jubilee Award, 2008, for the outstanding contribution in the area of regulation of human gene expression (transcription) and its link to disease and therapeutics.

**Prof Umesh Waghmare**

DAE outstanding research investigator award of the Department of Atomic Energy, Mumbai, 2008-09.

**Dr RA Mashelkar**

Honorary Doctorate from University of Goa (2009)

IIFA Ben Gurion Award (2009) for contributions in Science & Technology

**Prof V Nagaraja**

IISc Alumni Award for Excellence in Research, 2009

**Prof Raghavendra Gadagkar**

H.K. Firodia Award 2008 for Excellence in Science & Technology, 2008.

**Prof Rahul Pandit**

Professor Rustom Choksi Award of the Indian Institute of Science for excellence in research.

**Prof M M Sharma**

INSA Medal for promotion and service to Science

SIES Sri Chandrasekarendra Saraswati National Eminence Award: Science & Technology

**Dr L S Sashidhara**

SS Bhatnagar Award in Biological Sciences in the year 2008

**Prof R Varadarajan**

G D Birla Award (2008)

## FELLOWSHIPS

### **Prof M. K. Chandrashekar**

Ramanna Fellow of DST.

### **Prof Hemalatha Balaram**

Elected Fellow of Indian Academy of Sciences, 2008

### **Prof Srikanth Sastry**

Fellow, National Academy of Science, Allahabad

Fellow, Indian Academy of Sciences, Bangalore

### **Prof Tapas Kumar Kundu**

Elected Fellow of Indian Academy of Sciences, 2008

### **Dr T N C Vidya**

Ramanujan Fellow of DST.

### **Dr V Sheeba**

Ramanujan Fellow of DST.

### **Dr RA Mashelkar**

Foreign Fellow, Australian Academy of Technological Sciences and Engineering (ATSE) (April 2008)

### **Prof V Nagaraja**

Fellowship of National Academy of Sciences, Allahabad (NASI)

J. C. Bose Fellowship Award of Dept. of Science and Technology

### **Dr Sampathkumaran**

JC Bose Fellowship from July 2008

### **Prof Santanu Bhattacharya**

J.C. Bose Fellowship of DST (2008)

### **Prof Uday Maitra**

J.C. Bose Fellowship of DST (2008)

## EDITORIAL BOARDS

### **Prof M. K. Chandrashekar**

Member, Council of Editors, *Resonance*

### **Prof Amitabh Joshi**

Chief Editor, *Journal of Genetics*.

Member, Council of Editors, *Resonance*.

Member, Board of Editors, *International Journal of Evolutionary Biology*.

### **Prof Maneesha S Inamdar**

Member, Journal of *Stem Cell Reviews and Reports*

### **Prof K S Narayan**

Guest Editor for Special Issue in Organic Electronics - *Proceedings of the IEEE (to appear in 2009)* along with J. Lewis, J. Burroughes, and Y. Ohmori Regional Editor: Synthetic Metals

### **Prof Swapan K Pati**

Member, International Advisory Board for Journal of Materials Chemistry,  
Journal of Physical Chemistry

### **Prof Vijay Kumar Sharma**

Member, Editorial Board, *Journal of Circadian Rhythms*.

Member, Editorial Board, *Journal of Genetics*.

Editor-in-chief of the News Letter of the Indian Society for Chronobiology.





**Dr Sanjay Jain**

Member, Editorial Board of the Journal "Artificial Life" (MIT Press).

**Prof Shobo Bhattacharya**

Member, Editorial Board, Reviews of Progress in Physics (UK)

**MEMBERSHIPS/APPOINTMENTS****Prof C N R Rao**

Distinguished Visiting Professor, University of California, Berkeley (2008 - )  
International Adviser of the National Institute of Materials Science (NIMS) of Japan.

**Prof Amitabh Joshi**

Member, DST Project Advisory Committee for Animal Sciences.  
Member, Curriculum Committee, Indian Institute of Science Education and Research, Mohali.  
Member, Biology Advisory Body, Poornaprajna Institute of Scientific Research, Bangalore.  
Member, CSIR-HRDG Animal Sciences and Biotechnology Research Committee.  
Member Board of Studies (5 Yr Integrated MSc) in Life Sciences, Bangalore University.

**Prof G U Kulkarni**

Co-convener, Indo-US workshop on Nanomaterials for Energy, JNCASR, Aug. 2008  
Co-convener, Molecules & Materials, JNCASR, Dec. 2008  
Co-convener, Purdue-JNC workshop on Interfaces, Purdue, March, 2009

**Prof Maneesha S Inamdar**

Member, National International Contact, Scientific Advisory Board, hES cell Registry, Europe  
Member, Ethics Working Group, International Stem Cell Banking Initiative of ISCF all in 2008

**Prof K S Narayan**

Co-Chair for the session on Charge transport in excitonic solar cells MRS Spring Meeting,  
San Francisco 2010

**Prof Vijay Kumar Sharma**

Member, Planning Committee DST-SERC School on Clocks, Rhythms and Behaviour.  
Vice-President, Indian Society for Chronobiology.

**Dr RA Mashelkar**

Sir Louis Matheson Distinguished Visiting Professor, Monash University, Australia  
Visiting Professor at the Harvard/MIT/School (HST), Boston (2007)

**Prof Raghavendra Gadagkar**

Chairman, Animal Sciences & Biotechnology Research Committee, Council of Scientific & Industrial  
Research, New Delhi, 2008-2011.

Member, Sectional Committee – VII, Indian National Science Academy, New Delhi, 2009.

Chief Editor, Indian Journal of History of Science, 2009-

Member, International Scientific Advisory Council, Indian Institute of Scientific Education & Research,  
Government of India, Pune, 2008.

Chairman, Research Council for History of Science, Indian National Science Academy, New Delhi, 2009-

Member, Indian National Commission for History of Science, Indian National Science Academy, New  
Delhi, 2009-

**Dr Sampathkumaran**

Elected Member, Asia-Pacific Academy of Materials

**Prof Shobo Bhattacharya**

Member, Editorial Board, Reviews of Progress in Physics (UK)  
Member, Technology Advisory Council, British Petroleum

**Prof Sriram Ramaswamy**

Member, Advisory Board of *Soft Matter*, a Journal of the Royal Society of Chemistry, since May 2008.  
Vice-chair, Commission C3 (Statistical Physics) of the IUPAP and Member, Steering Committee for Statphys 24, to be held in Cairns, Australia, July 2010.

**LECTURESHIPS**

**Prof C N R Rao**

Kelly Lecture, Cambridge University (2009)

**Prof Vijay Kumar Sharma**

Keynote Speaker at the National Symposium of Indian Society for Chronobiology, 2008.

**Prof A Sundaresan**

Materials Research Society of India Medal Lecture 2009

**Prof P P Majumder**

Delivered the *Professor S.P. Ray-Chaudhuri Memorial Lecture* titled "Darwin, Haldane and the Footprints of War", S.P. Ray-Chaudhuri Foundation, Banaras Hindu University, 2 March 2009.

**Prof Raghavendra Gadagkar**

Diamond Jubilee Colloquium – Raman Research Institute, Bangalore, 4 April 2008.

Plenary Lecture delivered at the 38th World Congress of the International Institute of Sociology, Central European University, Budapest, Hungary, 28 June 2008.

Plenary Lecture delivered at the 23<sup>rd</sup> International Congress of Entomology 2008, Durban, South Africa, 10 July 2008.

Centenary Lecture delivered at the University of Pretoria, South Africa, 15 July 2008.

Plenary Lecture delivered at Mokpo University, Korea, 20 August 2008.

Invited lecture at the World Knowledge Dialogue Foundation Symposium, Crans-Montana, Switzerland, September 2008.

Public Lecture, Wissenschaftskolleg zu Berlin, Germany, 23 November 2008

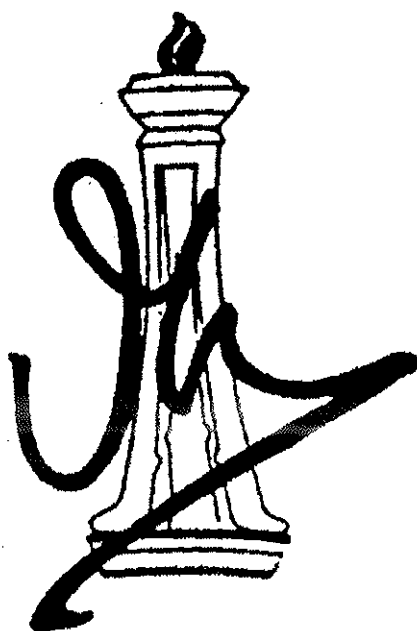
Darwin Bicentenary Lecture, Kerala Shastra Sahitya Parishad, Calicut, Kerala, 13 February 2009.

Frontiers of Science Lecture, University of Calicut, Calicut, Kerala, 14 February 2009.

☆☆☆



# FINANCIAL STATEMENTS



**Name** : JAWAHARLAL NEHRU CENTRE FOR  
ADVANCED SCIENTIFIC RESEARCH

**Address** : JAKKUR POST, BANGALORE – 560 064

**Year Ended** : 31<sup>st</sup> MARCH 2009

**Assessment Year** : 2009-10

## Auditor's Report to the Members of the Governing Body of Jawaharlal Nehru Centre for Advanced Scientific Research

We have audited the attached Balance Sheet of **Jawaharlal Nehru Centre For Advanced Scientific Research** as at March 31, 2009 and also the Income & Expenditure Account for the year ended on that date and the Receipts and Payment account for the year ended on that date annexed thereto. These financial statements are the responsibility of the management of Jawaharlal Nehru Centre for Advanced Scientific Research. 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 plan and perform the audit to obtain reasonable assurance about whether the financial statements are free of material misstatement. An audit includes examining, on a test basis, evidence supporting the amounts and disclosures in the financial statements. 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 our audit provides reasonable basis for our opinion.

### We report that:

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 far 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:
  - (i) 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]
  - (ii) 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.
5. In our opinion and to the best of our information and according to the explanations given to us and subject to notes on accounts and our qualifications in para 4 above, the said accounts give a true and fair view in conformity with the accounting principles generally accepted in India:
  - (a) in the case of Balance Sheet, of the state of affairs of the Jawaharlal Nehru Centre for Advanced Scientific Research as at March 31, 2009; and
  - (b) in the case of Income and Expenditure Account, of the excess of Income over Expenditure for the year ended on that date.

For M/s G R Venkatanarayana  
Chartered Accountants  
(G R Venkatanarayana)  
Partner  
Membership No. 18067

Place : Bangalore

Dated: 05.09.2009



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH  
BALANCE SHEET AS AT 31<sup>ST</sup> MARCH 2009**

Description	Schedule	Current year		Previous year	
		2008-09		2007-08	
		Rs.	Ps.	Rs.	Ps.
<b>LIABILITIES</b>					
Corpus/Capital Fund	1	1,173,065,129.54		912,811,821.54	
Reserves & Surpluses	2	1,489,467.77		62,612,039.99	
Earmarked and Endowment Funds	3	140,946,710.15		103,169,159.05	
Secured loans and Borrowings	4		0.00		0.00
Unsecured loans and Borrowings	5		0.00		0.00
Deferred Credit Liabilities	6		0.00		0.00
Current Liabilities and Provisions	7	7,905,034.14		22,397,147.14	
Other funds-Cluster Studies		39,541.00		39,541.00	
Scheme Balances		106,846,299.16		83,341,564.57	
Total		<b>1,430,292,181.76</b>		<b>1,184,371,273.29</b>	
<b>ASSETS</b>					
Fixed Assets ( gross )	8	1,173,065,129.54		912,811,821.54	
Investments-Endowment Funds	9	136,505,750.00		66,625,000.00	
Investment - Others	10		0.00		0.00
Current Assets, Loans, Advances etc.	11	120,721,302.22		204,934,451.75	
Total		<b>1,430,292,181.76</b>		<b>1,184,371,273.29</b>	
Significant accounting policies(Enclosed)	24				
<b>Contingent Liabilities &amp; Notes on Accounts</b>	25				

Schedule 1 to 25 form integral part of Accounts

For Jawaharlal Nehru Centre for Advanced Scientific Research

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

for **M/S GR Venkatanarayana**  
Chartered Accountants  
Sd/-  
(**GR Venkatanarayana**)  
Partner  
Membership No. 018067

Sd/-  
**RS Gururaj**  
Accounts Officer

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

Place : Bangalore  
Date : 05.09.2009

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH  
INCOME & EXPENDITURE ACCOUNT FOR THE YEAR ENDED 31<sup>ST</sup> MARCH 2009**

Description	Schedule	Current year		Previous year	
		2008-09		2007-08	
		Rs.	Ps.	Rs.	Ps.
<b>Income</b>					
Income from services	12	840499.00		962,200.68	
Grants/Subsidies received	13	395,016,136.00		280,037,595.00	
		395,856,635.00		280,999,795.68	
Less: Extent of fixed assests procured		260,253,308.00		128,997,573.00	
		<b>135,603,327.00</b>		<b>152,002,222.68</b>	
Income from Fees/Subscriptions etc	14	921,483.00		949,827.00	
Income from investments	15		0.00		0.00
Royalty Income,Publication,Licence fee etc	16	568,579.91		380,775.51	
Interest earned	17	29,165,340.18		7,089,418.49	
Other income	18	19,749,245.48		16,319,415.00	
Increase/decrease in stocks	19		0.00		0.00
<b>Total</b>		<b>186,007,975.57</b>		<b>176,741,658.68</b>	
<b>Expenditure</b>					
Establishment expenses	20	92,579,259.00		64,847,130.00	
Other administrative expenses	21	124,505,090.46		86,171,691.52	
Expenditure on Grants,Subsidies etc	22		0.00		0.00
Interest & bank charges	23	46,198.33		8,772.88	
<b>Total</b>		<b>217,130,547.79</b>		<b>151,027,594.40</b>	
Excess of expenditure over income		-31,122,572.22		25,714,064.28	
Balance brought forward		62,612,039.99		44,897,975.71	
		<b>31,489,467.77</b>		<b>70,612,039.99</b>	
Transferred to Corpus Fund Account		30,000,000.00		8,000,000.00	
Balance carried to Balance sheet		<b>1,489,467.77</b>		<b>62,612,039.99</b>	
<b>Significant accounting policies (Enclosed)</b>	24				
<b>Contingent Liabilities &amp; Notes on Accounts</b>	25				

Schedule 1 to 25 form an integral part of Accounts

For Jawaharlal Nehru Centre for Advanced Scientific Research

This is the Income and Expenditure account referred to in our report of even date.

for M/S GRVenkatanarayana  
Chartered Accountants  
Sd/-  
(GRVenkatanarayana)  
Partner  
Membership No. 018067

Sd/-  
RS Gururaj  
Accounts Officer

Sd/-  
Prof MRS Rao  
President

Place : Bangalore  
Date : 05.09.2009



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH  
RECEIPTS AND PAYMENTS ACCOUNT FOR THE YEAR ENDED 31.03.2009**

Opening Balances & Receipts	2008-09 Rs. Ps.	2007-08 Rs. Ps.	Payments & Closing Balances	2008-09 Rs. Ps.	2007-08 Rs. Ps.
<b>I. Opening Balances:</b>			<b>I. Expenses:</b>		
a. Cash in hand & Imprest at centre	273,565.00	274,063.00	a. Establishment Expenses	92,579,259.00	64,847,130.00
b. Bank balances:			b. Administrative Expenses	124,505,090.46	86,059,786.52
<i>In savings bank Accounts:</i>			c. Expenditure of endowments	936,280.00	929,819.00
At Canara bank	5,268,086.18	1,719,659.21			
At Union Bank of India	756,295.00	4,967.00	II. Payment made against funds for various projects:	0.00	0.00
<i>In Deposit accounts:</i>					
At IDBI bank	600,000.00	3,100,000.00	III. Investments and Deposits made:		
At HDFC trust	12,125,000.00	12,125,000.00	a. Out of earmarked /Endowment funds	0.00	0.00
At ICICI Bank	20,000,000.00	5,000,000.00	b. Out of own funds	0.00	0.00
At Union Bank of India	98,981,750.00	48,000,000.00			
At Canara Bank	137,731,131.18	69,949,626.21	IV. Expenditure on Fixed assets and Capital Work-in-progress:		
<b>II. Grants Received:</b>			a. Purchase of fixed assets	260,253,308.00	115,040,366.00
From DST travel grant	247,970.00	358,178.00	b. Outstanding Creditors paid	15,927,567.59	0.00
From DST-Grant in aid	385,800,000.00	270,000,000.00			
From DST for Building	0.00	6,000,000.00	V. Refund of surplus money/Loans	0.00	0.00
From DST for Meeting/Seminars	8,968,166.00	3,679,417.00	VI. Finance charges(Bank charges)	46,198.33	8,772.88
From Reliance Industries	5,000,000.00	0.00			
From Prof. CNR Rao & Smt. Indumati Rao	1,000,000.00	2,500,000.00			
On behalf of Endowments	249,700.00	2,058,450.00			
<b>III. Income on Investments from:</b>	401,265,836.00	284,596,045.00			
A. Interest on FD's:					
a. From Earmarked/Endowment Funds	7,903,947.00	4,724,408.00			
b. From Own funds	28,884,292.00	6,960,246.00			
<b>IV. Interest received:</b>	36,788,239.00	11,684,654.00			
a. On Bank S.B A/c	281,048.18	129,172.49			
<b>Balance Carried Over</b>	576,339,819.36	366,633,560.70	<b>Balance Carried Over</b>	494,247,703.38	266,885,874.40

Contd...)



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH  
RECEIPTS AND PAYMENTS ACCOUNT FOR THE YEAR ENDED 31.03.2009**

Opening Balances & Receipts	2008-09 Rs. Ps.	2007-08 Rs. Ps.	Payments & Closing Balances	2008-09 Rs. Ps.	2007-08 Rs. Ps.
Balance Brought Forward	576,339,819.36	366,633,560.70	Balance Brought Forward	494,247,703.38	266,885,874.40
<b>V. Other Income:</b>			<b>VII. Other payments:</b>		
a. Royalty	434,214.91	1,171,074.51	Caution money deposit returned	0.00	20,000.00
b. Licence Fee	134,365.00	151,407.00	Staff advances	72,100.00	0.00
c. Collections from Visitors, Guest room etc.	2,438,742.00	2,192,469.00	Statutory liability paid	0.00	170,064.00
d. From fee, subscription etc.	921,483.00	949,827.00	Other advances paid	630,542.00	70,426.00
e. CSIR fellowships, SRFP reimbursements	10,916,484.00	11,345,958.00	Contingent Advances paid	0.00	59,894.00
f. Donations	0.00	0.00		702,642.00	320,384.00
g. From services	840,499.00	962,200.68			
h. From others	394,019.48	280,988.00	<b>VIII. Closing Balances:</b>		
	16,079,807.39	17,053,924.19	a. Cash in hand & Imprest at Centre	561,864.00	273,565.00
<b>VI. Amount borrowed</b>	0.00	0.00	b. Bank balances:		
<b>VII. Other receipts:</b>			<i>In savings bank accounts:</i>		
Amount transferred from schemes	0.00	15,898,236.00	Canara Bank	8,308,064.06	5,268,086.18
Dues received from schemes	0.00	2,000,000.00	Union Bank of India	1,631,688.00	756,295.00
EMD / CMD Received	1,435,454.69	3,530,612.00	<i>In deposit accounts:</i>		
Cont adv/ Advances Returned back-staff	28,320.00	36,900.00	At canara bank	76,480,750.00	98,981,750.00
TDS Received	174,310.00	0.00	At IDBI bank	0.00	600,000.00
SRFP caution money	0.00	6,000.00	At Union bank of India	0.00	20,000,000.00
Unascertained receipts(NIMS-Sumitomo)	0.00	51,721.69	At HDFC Trust	12,125,000.00	12,125,000.00
<b>TOTAL</b>	1,638,084.69	21,523,469.69		98,545,502.06	137,731,131.18
	594,057,711.44	405,210,954.58	<b>TOTAL</b>	594,057,711.44	405,210,954.58

For Jawaharlal Nehru Centre for Advanced  
Scientific Research

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

for M/s G.R.VENKATANARAYANA  
Chartered Accountants

Sd/-  
(G.R.VENKATANARAYANA)  
Partner

Membership No. 18067  
Place : Bangalore Date :05.09.2009

Sd/-  
R.S.Gururaj  
Accounts Officer

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



## Schedule No. 24

### Accounting Policies for the Year 2008-09

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. The interest on investment is accounted on accrual basis.
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. No provision for income tax has been made as the Institution is exempt U/s 35 (1) (ii) of the Income Tax Act, 1961.

For M/s G R Venkatanarayana  
Chartered Accountants

Sd/-  
**RS Gururaj**  
Accounts Officer

Sd/-  
**(G R Venkatanarayana)**  
Partner  
Membership No.18067

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

Place: Bangalore  
Date : 05.09.2009

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH**

**Schedule forming part of the accounts**

Description	2008-09		2007-08	
	Rs.	Ps.	Rs.	Ps.
<b>Schedule 1- Capital Fund</b>				
Balance as at the beginning of the year	912,811,821.54		783,814,248.54	
	<b>912,811,821.54</b>		<b>783,814,248.54</b>	
Less : Depreciation up to the end of previous year	198,294,845.30		193,295,837.00	
	<b>714,516,976.24</b>		<b>590,518,411.54</b>	
Add : Addition to Fixed Assets during current year	260,253,308.00		128,997,573.00	
	<b>974,770,284.24</b>		<b>719,515,984.54</b>	
Less : Depreciation for the current year	48,285,403.00		37,080,398.00	
	<b>926,484,881.24</b>		<b>682,435,586.54</b>	
Add : Depreciation Reserve per contra	246,580,248.30		230,376,235.00	
<b>TOTAL</b>	<b>1,173,065,129.54</b>		<b>912,811,821.54</b>	
<b>Schedule 2- Reserves And Surpluses:</b>				
<b>General Reserve:</b>				
Surplus in Income and Expenditure account	1,489,467.77		62,612,039.99	
<b>Schedule 3- Earmarked / Endowment Funds:</b>				
<b>A : Infrastructure Corpus Fund</b>				
Opening Balance	61,198,549.65		33,614,232.65	
Additions during the year	30,000,000.00		8,000,000.00	
Funds-Income from Investments made	5,898,502.00		19,584,317.00	
<b>Total : Infrastructure Corpus fund</b>	<b>97,097,051.65</b>		<b>61,198,549.65</b>	
<b>B : Other funds</b>				
Opening Balance of the Funds	41,970,609.40		38,431,942.50	
<b>Add : Additions :</b>				
Funds/Donations/Grants/Royalties	249,700.00		2,058,450.00	
Funds-Income from Investments made	2,565,629.00		2,410,036.00	
	<b>44,785,938.40</b>		<b>42,900,428.50</b>	
Less : Funds-utilisation/Expenditure incurred	936,280.00		929,819.10	
<b>Total : Other Funds</b>	<b>43,849,658.40</b>		<b>41,970,609.40</b>	
<b>Grand Total - Infrastructure Corpus and Other Funds</b>	<b>140,946,710.05</b>		<b>103,169,159.05</b>	
<b>Schedule 4-Secured Loans And Borrowings:</b>		0.00		0.00
<b>Schedule 5-Unsecured Loans And Borrowings:</b>		0.00		0.00
<b>Schedule 6-Deferred Credit Liabilities:</b>		0.00		0.00
<b>Schedule 7- Current liabilities and provisions:</b>				
Sundry Creditors EMD	5,365,063.00		4,214,433.00	
Sundry Creditors CMD	354,009.69		69,185.00	
Sundry Creditors for others	2,150,961.45		18,077,843.14	
Statutory Liabilities	35,000.00		35,686.00	
<b>TOTAL</b>		<b>7,905,034.14</b>		<b>22,397,147.14</b>

Sd/-  
R S Gururaj  
Accounts Officer



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH**  
**Schedule forming part of the accounts**

Description	2008-09		2007-08	
	Rs.	Ps.	Rs.	Ps.
<b>Schedule 8- Fixed Assets:</b>				
Land - Free Hold	17,715,351.00		17,715,351.00	
Buildings :				
General	79,658,165.26		79,658,165.26	
Hostel Building	15,570,835.00		15,570,835.00	
New Lab Building - AMRL	25,930,339.00		25,930,339.00	
Animal House	5,614,415.00		5,614,415.00	
Staff Housing	4,156,168.00		4,156,168.00	
ETU Building	2,048,814.00		2,048,814.00	
Engineering & Mechanical Unit Block	7,426,272.00		7,234,709.00	
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	
Extention to Pauling Building - Biology Block	4,680,084.00		4,680,084.00	
Dining Hall & Kitchen Block	10,155,893.00		8,582,843.00	
Radio Active Lab	203,233.00		203,233.00	
International Centre for Material Science	40,550,264.00		24,577,230.00	
Lecture Hall & Academic Block	9,636,712.00		8,556,759.00	
Hostel Phase II	19,552,377.00		19,552,377.00	
STP Building	291,699.00		291,699.00	
Extention to Animal House	1,172,929.00		0.00	
Hostel Phase III	18,765,243.00		13,426,253.00	
International house	18,231,179.00		12,768,383.00	
CNR Rao Hall of Science	8,661,132.00		1,143,087.00	
Extention to HIV lab	1,016,085.00		703,054.00	
Security Office Block	90,373.00		90,373.00	
Animal House - Additional Block	3,964,783.00		0.00	
	<b>296,303,529.26</b>		<b>253,715,355.26</b>	
Infrastructure Facilities:				
Roads, Streetlights, Drainages, partitions etc	58,370,100.32		44,850,873.32	
Tubewells and water supply	248,912.00		248,912.00	
	<b>58,619,012.32</b>		<b>45,099,785.32</b>	
Plant/Machinery/Equipment:				
Scientific Equipments/Plant/Machinery	473,704,305.45		347,804,738.45	
ICMS-Laboratory equipments & facilities	23,653,181.00		0.00	
Equipments - Chemistry & Physics of Materials	74,041,456.00		74,041,456.00	
	<b>571,398,942.45</b>		<b>421,846,194.45</b>	
<b>Others :</b>				
Vehicles	1,356,527.00		1,356,527.00	
Furniture and fixtures	42,507,663.87		31,154,628.87	
Office equipment	5,491,101.63		5,491,101.63	
Computer/peripherals	41,714,390.00		33,364,684.00	
Electrical installations	33,226,058.00		15,830,859.00	
Library Books	18,116,192.21		15,960,352.21	
Library Journals	86,616,361.80		71,276,982.80	
<b>TOTAL</b>	<b>1,173,065,129.54</b>		<b>912,811,821.54</b>	
Less - Depreciation up to the end of previous year	198,294,845.30		193,295,837.00	
Depreciation for the current year	48,285,403.00		37,080,398.00	
Written down value of the assets as at the year end	926,484,881.24		682,435,586.54	
Add - Depreciation reserve per contra	246,580,248.30		230,376,235.00	
<b>TOTAL</b>	<b>1,173,065,129.54</b>		<b>912,811,821.54</b>	

Sd/-

**RS Gururaj**  
Accounts Officer

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH**  
**Schedule forming part of the accounts**

Description	2008-09		2007-08	
	Rs.	Ps.	Rs.	Ps.
<b>Schedule 9- Investments - Earmarked/Endowment Funds:</b>				
<b>Long Term Deposits</b>				
Fixed Deposits and Bonds with IDBI Bank		0.00		600,000.00
Fixed Deposits with HDFC Trust		12,125,000.00		12,125,000.00
Govt of India 8% Savings Bonds 2003 [SHCIL & SBI]		47,900,000.00		47,900,000.00
Fixed Deposits with Canara bank		76,480,750.00		6,000,000.00
<b>TOTAL</b>		<b>136,505,750.00</b>		<b>66,625,000.00</b>
<b>Schedule 10 - Investments - Others:</b>				
Short Term Deposits		0.00		0.00
<b>TOTAL</b>		<b>0.00</b>		<b>0.00</b>
<b>Schedule 11-Current Assets, Loans, Advances etc.,:</b>				
Cash & Bank Balances				
Cash in hand - Schemes Account		42,300.00		82,319.00
Cash at Bank -Schemes - Canara Bank		10,586,539.33		14,422,023.74
Cash at Bank -Schemes - State Bank of India		238,291.83		6,621,531.83
Fixed deposit with Canara Bank ( Schemes )		95,979,168.00		62,215,690.00
Cash in hand at Centre		121,529.00		57,174.00
Cash at Bank - Canara Bank		8,308,064.06		5,268,086.18
Cash at Bank - Union Bank		1,631,688.00		756,295.00
Fixed deposit with Canara Bank ( Grants )		0.00		92,981,750.00
Fixed deposit with Union Bank of India		20,000,000.00		
Imprest balance		36,652.00		36,652.00
Imprest with Faculty		403,683.00		179,739.00
Advances to staff		190,067.00		117,967.00
Contingent Advances		95,000.00		123,320.00
Other advances		1,213,926.00		655,926.00
TDS receivable		744,523.00		918,833.00
Amount receivable from Income Tax Department		461,473.00		461,473.00
Interest receivable ( Endowment Account )		560,184.00		0.00
Linus and CPF accounts		108,214.00		35,672.00
<b>TOTAL</b>		<b>120,721,302.22</b>		<b>204,934,451.75</b>
<b>Schedule 12-Income from sales / services:</b>				
Consultancy fee		416,749.00		60000.68
DNA sequencing fee		423750.00		902200.00
<b>TOTAL</b>		<b>840499.00</b>		<b>962200.68</b>

Sd/-  
**RS Gururaj**  
Accounts Officer



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH**

**Schedule forming part of the accounts**

Description	2008-09		2007-08	
	Rs.	Ps.	Rs.	Ps.
<b>Schedule 13 - Grants/subsidies :</b>				
Grants - DST	385,800,000.00		270,000,000.00	
Grants - Discussion meetings/Seminars	8,968,166.00		3,679,417.00	
Grants - Travel grants	247,970.00		358,178.00	
Grants - DST towards CCMS Building	0.00		6,000,000.00	
<b>TOTAL</b>	<b>395,016,136.00</b>		<b>280,037,595.00</b>	
<b>Schedule 14 - Income from Fee/Subscriptions etc :</b>				
Income from fee, subscriptions,medical contribution etc.,	921,483.00		949,827.00	
<b>TOTAL</b>	<b>921,483.00</b>		<b>949,827.00</b>	
<b>Schedule 15 - Income from investments;</b>				
	0.00		0.00	
<b>Schedule 16-Royalty Income,Publication,Licence fee etc :</b>				
From Royalty	434,214.91		229,368.51	
Licence fee	134,365.00		151,407.00	
<b>TOTAL</b>	<b>568,579.91</b>		<b>380,775.51</b>	
<b>Schedule 17 - Interest earned:</b>				
From Term deposits	28,884,292.00		6,960,246.00	
From SB accounts with nationalised banks	134,569.18		129,172.49	
From interest from others	146,479.00		0.00	
<b>TOTAL</b>	<b>29,165,340.18</b>		<b>7,089,418.49</b>	
<b>Schedule 18 - Other income:</b>				
Donations - Reliance Industries towards Hall Of Science	5,000,000.00		0.00	
Donations - Prof.CNR Rao & Smt.Indumati Rao	1,000,000.00		2,500,000.00	
From Visitors house, Guest rooms, Students residence etc,	2,438,742.00		2,192,469.00	
CSIR Fellowships, SRFP reimbursement etc.,	10,916,484.00		11,345,958.00	
From others( tender fee & other fee collected)	394,019.48		280,988.00	
<b>TOTAL</b>	<b>19,749,245.48</b>		<b>16,319,415.00</b>	
<b>Schedule 19 - Increase / Decrease in stock:</b>				
	<b>0.00</b>		<b>0.00</b>	

Sd/-  
**R S Gururaj**  
 Accounts Officer

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH**

**Schedule forming part of the accounts**

Description	2008-09		2007-08	
	Rs.	Ps.	Rs.	Ps.
<b>Schedule 20 Establishment Expenses:</b>				
Salaries & Scholarship to students	74,904,569.00		50,288,818.00	
Wages	10,795,653.00		10,289,252.00	
Allowances ( Medical reimbursements etc.,)	2,898,623.00		1,512,162.00	
Bonus	255,442.00		143,086.00	
Contribution to CPF	2,603,973.00		1,227,162.00	
Contribution to new pension scheme	629,036.00		350,925.00	
Contribution to retirement benefit scheme	21,610.00		585,564.00	
Leave encashment benefits	0.00		369,107.00	
LTC	470,353.00		81,054.00	
<b>TOTAL</b>	<b>92,579,259.00</b>		<b>64,847,130.00</b>	
<b>Schedule 21- Other Administrative expenses</b>				
Electricity & Power	19,929,882.00		14,933,589.00	
Water charges	953,811.00		3,027,127.00	
Insurance	409,089.00		383,612.00	
Repairs & maintenance	16,495,995.00		9,079,550.00	
Rents,rates & taxes	1,609,621.00		958,832.00	
Vehicles running & maintenance	4,084,997.00		3,168,563.00	
Postage, telephone & communication	3,321,730.00		3,278,015.00	
Printing & stationery	3,103,473.00		1,965,855.52	
Travelling and conveyance	5,353,982.46		3,729,737.00	
Expenses on Seminars/workshops/discussion meetings	17,735,861.00		7,205,339.00	
Subscriptions	399,348.00		394,760.00	
Fees towards training etc.,	115,000.00		218,880.00	
Professional charges	6,435,829.00		5,949,779.00	
Laboratory Consumables	29,276,894.00		25,768,810.00	
Frieght Inwards	2,782,128.00		1,791,535.00	
Other consumables	971,813.00		951,106.00	
Advertisement & Publicity	2,363,334.00		1,213,886.00	
Other miscellaneous expenses	1,097,779.00		721,640.00	
Statutory Audit fee	35,000.00		25,000.00	
POBE programme	229,220.00		220,413.00	
Student Research Fellowship Programme	1,031,744.00		1,185,663.00	
Fellowships - Department of Bio-Technology	76,230.00		0.00	
ICMS - Workshops, Schools etc.,	964,342.00		0.00	
ICMS - Visitor Programmes ( National & International)	486,253.00		0.00	
ICMS - Recurring expenses	4,811,776.00		0.00	
ICMS - Scientists & Supporting Staff	429,959.00		0.00	
<b>TOTAL</b>	<b>124,505,090.46</b>		<b>86,171,691.52</b>	
<b>Schedule 22-Expenditure on grants, subsidies etc:</b>	0.00		0.00	
<b>Schedule 23- Interest and Bank charges:</b>	46,198.33		8,772.88	
<b>TOTAL</b>	<b>46,198.33</b>		<b>8,772.88</b>	
1. Claims against the entity not acknowledged as debts	Nil		NIL	
2. Letter of credit outstanding	Nil		NIL	
<b>B. Notes on Accounts :</b>				
1. Estimated amount of contracts remaining to be executed on capital account and not provided for.				
a. In respect of Equipments	0.00		48,733,425.00	
b. In respect of Buildings ( Civil & Electrical )	0.00		22,591,770.00	
	<b>0.00</b>		<b>71,325,195.00</b>	

Sd/-

**R.S.Gururaj**  
Accounts Officer



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH  
CPF & NPS FUND STATEMENT OF AFFAIRS FOR THE YEAR ENDED 31.03.2009**

Particulars	Rs.	Ps.	Particulars	Rs.	Ps.
<b>CONTRIBUTORY PROVIDENT FUND</b>			<b>INVESTMENT OF FUNDS:</b>		
<b>SUBSCRIPTION:</b>			Investments in:		
Opening Balance	3,804,472.00	17,129,511.55	Government of India 8 % Bonds ( SHCIL)	12,500,000.00	
Add: Subscriptions received during the year	875,352.00		State Government Securities (25 lakhs)	2,640,416.67	
Loan repayments	1,461,249.00	6,141,073.00	Fixed Deposits at Canara Bank	20,000,000.00	
Interest on subscriptions		23,270,584.55	Fixed Deposit at HDFC	2,000,000.00	37,140,416.67
Less: Loans granted during the year	1,305,386.00		<b>Closing Cash and Bank Balance :</b>		
Less: Withdrawals on retirement/death	66,794.55	1,372,180.55	Cash at Bank :		
<b>Closing Balance</b>	<b>21,898,404.00</b>		SB A/C No.17513		1,496,085.10
			Canara Bank, IISc branch		
<b>CONTRIBUTION</b>			<b>Amounts recoverable :</b>		
Opening balance	2,520,131.00	12,076,829.00	TDS receivable for the year 2005-06	8,008.00	
Add : Contribution during the year	960,295.00	3,480,426.00	TDS receivable for the year 2006-07	10,140.00	
Interest on total contributions		15,557,255.00	TDS receivable for the year 2007-08	103,000.00	121,148.00
Less: Withdrawals on retirement/death		69,772.00			
<b>Closing Balance</b>		<b>15,487,483.00</b>			
<b>NEW PENSION SCHEME</b>					
<b>SUBSCRIPTION</b>			Due to be remitted to bank on account		179.00
Opening Balance	586,297.00	997,037.00	of short payment during 2007 08		
Add : Subscriptions received during the year	100,642.00	686,939.00	<b>Expenses incurred :</b>		
Interest on subscriptions		1,683,976.00	Bank Charges 2004-05	749.00	
<b>Closing Balance</b>			Bank Charges 2005-06	643.55	1,392.55
			<b>Accrued interest on Deposits :</b>		
<b>CONTRIBUTION</b>			On Fixed deposits with Canara Bank		1,874,001.00
Opening balance	585,875.00	646,108.00			
Add : Contribution during the year	50,950.00	636,825.00			
Interest on total contributions		1,282,933.00			
Closing Balance		280,426.32			
Surplus for the year 2008-09					
<b>Total</b>		<b>40,633,222.32</b>	<b>Total</b>		<b>40,633,222.32</b>

for Jawaharlal Nehru Centre for Advanced Scientific Research

for M/s G R Venkatanarayana  
Chartered Accountants

Sd/-  
(G R Venkatanarayana)  
Partner  
Membership No. 18067

Sd/-  
R S Gururaj  
Accounts Officer

Sd/-  
Prof M R S Rao  
President, JNCASR









## Jawaharlal Nehru Centre for Advanced Scientific Research

Jakkur, Bangalore – 560 064.

Editorial Support: Dr. Princy Jaison Pereira K. Ramakrishnan.

Phone: + 91 80 2208 2750

Fax: + 91 80 2208 2766

E-mail: [admin@jncasr.ac.in](mailto:admin@jncasr.ac.in)

Website: [www.jncasr.ac.in](http://www.jncasr.ac.in)

ISSN:0973-9319