

ISSN.0973-9319

ANNUAL REPORT

2016-17



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	
Foreword	1
Introduction	3
Objectives	4
Progress	5
Highlights of research and other activities	7
Activities Chart	17
Organisation Chart	18
The Organisation	
Council of Management	19
Finance Committee	20
Academic Advisory Committee	20
Faculties	21
Administration	21
Units, Centres, Computer Laboratory, Library and Endowed Research Professors	23-73
Academic Programmes	
Academic Activities	74
Discussion Meetings/Workshops	76
Endowment Lectures	76
Symposia/Workshops/Conferences/Winter School	77
Fluid Dynamics Colloquia	77
Seminars and Unit Lecture series	78
Lectures delivered at Annual Faculty Meeting	82
Other Programmes	82
Fellowship and Extension Programmes	
Visiting Fellowship Programme	84
Summer Research Fellowship Programme	85
Project Oriented Chemistry Education	86
Project Oriented Biology Education	86
Intellectual Property	87
Research Programmes	
Research Areas	91
Research Facilities	93
Sponsored Research Projects	
Ongoing Sponsored Projects	94
New Sponsored Projects	100
Publications	
Research Publications of Units	104
Research Publications of Honorary Faculty / Endowed Professors	130
Awards / Distinctions	133
Financial Statements	139

THE CENTRE

FOREWORD

I am delighted to present the twenty-eighth Annual Report of the Centre for the year 2016-17. To begin with, it is a matter of great pride that JNCASR has been accredited for NAAC with 3.76 out of the total score of 4 points. The Centre also ranked 4th among Universities and 11th under Overall category in National Institutional Ranking Framework (NIRF) Ranking 2017.

During the reporting period, under various academic programme, 52 students joined JNCASR in August 2016, and 11 students joined during January 2017. This makes the current student strength of the Centre to 305. Thirty-five were awarded Ph.D. degrees, three with M.S. (Engg.), and in M. S. of Integrated Ph.D. – seven students were awarded M.S. in Biological Sciences, five students with M.S. in Chemical Sciences and three students with M.S. in Materials Science. In addition, three students were awarded the Postgraduate Diploma in Materials Science (PGDMS).

We continue to excel in our efforts by initiating newer activities in addition to our core programmes for science popularisation such as Festival of Science and the event organised for school children to mark 100-years of the discovery of the chemical bond. These events were successful in inculcating the joy of learning science and provided an orientation towards research to school children. Our efforts under Fellowships and Extension Programmes have been significant in popularizing science and encouraging scientists from developing countries.

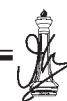
Prof. C.N.R. Rao was felicitated with Honorary Doctor of Science from Yenepoya University, Karnataka, Kaziranga University, Jorhat, Assam and Jamia Hamdard University, New Delhi. It is also heartening to note that, as per the recent survey conducted by Wiley-VCH (Angewandte family), Prof. C.N.R. Rao was voted as the most probable scientist for the Nobel Prize in Chemistry for 2016. As part of “Breathe” Team – Dr. Sebastian C. Peter, Prof. Umesh V. Waghmare and Mr. Rakshith Raghavan (JNC Alumnus), have entered the semifinals of \$20m Green Prize. Many of other faculty colleagues have received awards and honours during the year 2016-17 (a detailed list is given under Awards/Distinctions in pg. no. 130). Under the abled-guidance of our faculty members, the students have also marked their presence in national and international conferences and received several accolades, to name a few, Sheikh Saqr Student Fellowships and Gandhian Young Technological (GYTI) Award 2016 under Technological-Edge category (BIRAC-GYTI). The discovery reported by researchers from IISc and JNCASR on “*Bacteria powered Micro Heat Engine*” is another major contribution of our faculty member, Dr. Rajesh Ganapathy. Two Faculty Fellows have joined JNC recently, Dr. Diwakar S. Venkatesan joined in EMU during May 2016 and Dr. Premkumar Senguttuvan as Faculty Fellow jointly with ICMS and NCU in November 2016.

Researchers in JNCASR have continued to excel in science through their discoveries and inventions. Increasing number of publications in reputed high-impact factor international journals is one of the indicators of our scientific performance. The quality of our research is also evident from the fact that during the financial year

2016-17, 23 patent applications were filed (PCT-5, Canada-2, Europe-3, Hong Kong-1, India-5, Japan-1, Singapore-1, S. Africa-1, S. Korea-1, USA-3), and 13 patent grants were obtained (Australia-1, Europe-3, India-2 and USA-7). Taken together, the Centre till date has filed 241 National and International Patent Applications (PCT-49, Australia-5, Brazil-3, Canada-5, China-6, Europe-22, Germany-2, Hong Kong-2, India-78, Israel-1, Japan-8, Korea-2, Singapore-1, S.Africa-3, S.Korea-3, USA-50 and Vietnam-1) and obtained 63 patent grants (Australia-2, China-4, Europe-9, India-10, Japan-4, Korea-1, S.Africa-2, S.Korea-1 and USA-30), in addition to registering Copyright-1, Industrial Design-1 and Trade Mark-1.

A delegation of the Parliamentary Standing Committee on S&T, led by Smt. Renuka Choudhury visited JNCASR on August 29, 2016 and had interactions with the faculty and staff. They also had interactions with the students/research scholars who presented posters on Centre's research activities. The Centre has been registered with National Apex Committee for Stem Cell Research & Therapy under Ministry of Health & Family Welfare for a period of three years from 2016, strengthening our association with government agencies for stem cell research.

Prof. V. Nagaraja
President, JNCASR



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 is steadily increasing year by year. The Centre, completed twenty-eight years of establishment, is creating news regularly in the scientific world with its breakthrough discoveries. The Centre has research collaborations with several national and international institutions. In recognition of the achievements of the Centre, the Ministry of Human Resource Development (GOI) has accorded the status of Deemed University, to enable the Centre to train quality manpower. The faculty members of the Centre have received national and international recognitions. Several faculty members of the Centre are Fellows of National and International science and engineering academies.

Prof. C.N.R. Rao, the founder of the Centre, held the office of President from 1989 to 1999. He is presently the Honorary President of the Centre. Prof. V. Krishnan, who succeeded him, served as its President from 2000 to 2003. Prof. M.R.S. Rao served his term as President since 2003 to 2013. Prof. K.S. Narayan served as In-charge President from 2013 to 2015. Prof. V. Nagaraja is serving as President since October 2015.

OBJECTIVES

The objectives of the Centre are:

- Establish and conduct world-class research in science and engineering;
- Foster interdisciplinary and collaborative research;
- Establish state-of-the-art laboratories, computational and infrastructural facilities for conduct of scientific research;
- Generate human capital through high-quality Ph.Ds in science and engineering;
- Increase awareness about science and research among school and college students through science outreach and extension activities;
- Take research from laboratory to society.



PROGRESS

We have accounted several memorable and exciting moments including some major discoveries and innovations during the reporting year. Significant progress has been reported by the research units of the Centre namely, Chemistry and Physics of Materials Unit, Educational Technology Unit, Evolutionary and Integrative Biology Unit, Engineering Mechanics Unit, Geodynamics Unit, Molecular Biology and Genetics Unit, New Chemistry Unit, Neuroscience Unit, Theoretical Sciences Unit and International Centre for Materials Science. The Nanoscience Centre also houses the state of the art facilities for advanced research in materials science.

The Centre is equipped with a good quality library, an excellent computer support facility, lecture halls, Chemistry 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 part of the Centre's infrastructure located at Indian Institute of Science (IISc) campus.

There was a regular intake of students during 2016-2017 admissions, wherein 52 students joined JNCASR in August 2016, and 11 students joined during January 2017. This makes the current student strength of the Centre to 305. Thirty-five students were awarded Ph.D. degrees, three with M.S. (Engg.), and in M. S. of Integrated Ph.D. – seven students were awarded M.S. in Biological Sciences, five students with M.S. in Chemical Sciences and three students with M.S. in Materials Science. In addition, three students were awarded the Postgraduate Diploma in Materials Science (PGDMS). The research and training at the Centre have led to the award of total 243 Ph.D. degrees, 61 M.S. (Engg.), 3 M.S. (research), 118 M.S. (of Int. Ph.D.), 1 M.Sc. (by research) degrees and 8 PGDSE and 15 PGDMS 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. In recognition of its contributions to research and training, the Centre and its faculty members have received various national and international honors and accolades during the year.

Among faculty members, Prof. C.N.R. Rao received Hon. Doctorates from Assam Kaziranga University, Jorhat, Jamia Hamdard University, New Delhi and Yenepoya University, Mangalore. He also received Gitam Foundation Annual Award and Bhaskaracharya Award by Poojya Shree Channaveerswamiji Sarangamath, Sindgi, Vijayapur. Prof. Roddam Narasimha was felicitated by the Indian Mathematics Consortium (TIMC), for great impact on research, teaching and service to the Indian Mathematical community, on its first Conference at BHU organized in collaboration with the American Mathematical Society on December 15, 2016. Prof. V. Nagaraja received G. N. Ramachandran Gold Medal for Excellence in Biological S&T for the year 2016. Prof. K. S. Narayan received the National Prize for Research on Energy Materials and Devices given by the C. N. R. Rao Education Foundation, supported by the AVRA Laboratories Pvt. Ltd., Hyderabad. Prof. K. S. Valdiya was awarded "Pramathanath Bose Memorial Medal" of Asiatic Society for his outstanding contribution in the field of Practical & Theoretical Geology. Prof. Hemalatha Balaram was chosen for Dr. Raja Ramanna State Award 2015-16 from the Department of Information Technology, Biotechnology and Science and Technology, Government of Karnataka. Prof. Tapas Kumar Kundu was felicitated with G.P. Chatterjee Memorial Award for 2015-2016, awarded by the Indian Science Congress Association, Ministry of Science and Technology, Govt. of India. Prof. S. M. Shivaprasad received Distinguished Lectureship Award from the Materials Research Society of India, at its AGM held at IIT-Bombay. He was also conferred with Honorary Doctorate (D. Sc.) by the Vijayanagara SriKrishnadevaraya University, Bellary, Karnataka. Prof. Umesh Waghmare was chosen for Distinguished Alumnus Award 2017, IIT Bombay. Prof. Chandrabhas Narayana received MRSI-ICSC Super Conductivity and Materials Science Senior Award 2017. Dr. T. Govindaraju received Indian Peptide Society-Young Scientist Award 2016-2017; MRSI Medal 2016-2017, Materials Research Society of India; AVRA Young

Scientist Award (2015), AVRA Laboratories; CRSI Bronze Medal (2016) of Chemical Research Society of India. Dr. Subi J. George received 'Author Profile' in *Angewandte Chemie* journal for publishing his 10th article in this journal in 10 years. Dr. Sebastian C. Peter was selected as Emerging Investigator by the Journal of Materials Chemistry A, Royal Society of Chemistry (RSC), Materials Research Express, IOP Science and Institute of Physics in Material Science. Dr. Ranjani Viswanatha received DST young career award in Nano Science and Technology for the year 2017 and SERB Womens' Excellence Award. Dr. Sarit Agasti received the Innovative Young Biotechnologist Award (IYBA) from DBT. Dr. Jayanta Halder was awarded CSIR-CDRI Awards 2017 for Excellence in Drug Research in chemical sciences. Dr. Kanishka Biswas was selected as Emerging Investigator by the Journal of Materials Chemistry C, Royal Society of Chemistry (RSC) in 2017. He was awarded Materials Research Society (MRSI) Medal (2017), Young Scientist Medal, Indian National Science Academy (INSA), India (2016) for probing and developing new thermoelectrics for energy harvesting; Alkyl Amines and Chemicals Ltd. and ICT Young Scientist Award, (2016); "IUMRS–MRS Singapore Young Researcher Merit Award", jointly instituted by the International Union of Materials Research Societies (IUMRS) and the Materials Research Society (MRS) of Singapore.

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

The Faculty members of the Centre have published around 299 scientific papers in reputed international journals, conference proceedings and books during the year 2016-17. Most of the publications are from journals with a high impact factor. The average impact factor of the total 283 journal articles published for the year 2016 is 4.96.

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

The interactions with academic institutions and universities globally have continued and the Centre is expanding its formal ties in respect of collaborative research, exchange of graduate students and consultancy projects.

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

Summer Research Fellowships, Project Oriented Chemistry Education Programme, Project Oriented Biology Education Programme, Visiting Fellowships Programmes and several other academic exchange programmes have attracted wide attention and have been highly successful. Fifteen scientists from research institutions across the country were selected for the Centre's Visiting Fellowships 2016-17. The selected scientists were hosted by the faculty of CPMU, EIBU, MBGU, NCU, NSU, and TSU. For SRFP 2016, 63 students availed the scholarship and received research training in various areas of Physics, Chemistry, Biology or Engineering at research institutes in Bangalore, and elsewhere in the country. The advertisement of SRFP 2017 was announced on the JNCASR website and emailed to around 150 college principals in the country. A total of 1396 applications were received and 94 offers have been sent. For Project Oriented Biology Education (POBE), out of 171 applications received, 10 students have been selected and under Project Oriented Chemical Education (POCE), out of 274 applications received, 11 students were selected. Eight students each from POCE and POBE 2014-16 completed the programme successfully. Under Student Buddy Programme, 94 students of class XI/XII from Jawahar Navodaya Vidyalaya and Kendriya Vidyalaya have benefitted during the year 2016.

During the financial year 2016-17, eighteen Discussion Meetings, seven international conferences, workshops, and symposia were supported, either wholly or partially by the Centre. Around sixty-five seminars were held in addition to five Endowment Lectures, four Fluid Dynamic Colloquia, three Unit lecture series and one special lecture delivered by eminent scientists.



HIGHLIGHTS OF RESEARCH AND OTHER ACTIVITIES

Chemistry and Physics of Materials Unit (CPMU)

The Light Scattering lab was involved in developing methodology to understand potential drug molecules binding to therapeutically important proteins using MD simulations in Schrodinger software and verifying the same using Raman spectroscopy. A customized diagnostic Raman spectrometer was developed with scanning ability to make a prototype for viral RNA/DNA detection from body fluids. Interesting MOFs are being synthesized and studied under pressure and temperature to understand the microscopic picture using X-ray and Raman studies.

Computational studies showed that CO₂ uptake in a metal organic framework is not only dependent on the nature of the adsorption site but also on the availability of a kinetic pathway to access the same and the latter can be modulated by ligand dynamics. A correlation between density and accessible surface area of amorphous microporous polymers (CO₂ adsorbents) which will be quite useful to experimentalists has been obtained using molecular modelling methods.

In the area of imaging organic solar cells, imaging methods to examine the heterogeneity in photoconducting polymer blends from 10 nm to several micron length scales has been explored. The notable thing is that the capability has been developed to zoom in on a stationary sample from confocal microscopy length scales to Atomic Force Microscope scales. This utilizes a combination of tips: including glass aperture tips for near field access and convention AFM tips.

In fabrication of organic devices, the design and characterizing of new organic electronic materials has led to collaborations that were established with leading chemists in this field and provide feedback in the quest for developing high mobility polymers and small molecules, acceptor molecules for bulk heterojunction based solar cells, high and low-k dielectrics.

In the area of bioelectronics, recent research breakthrough was in interfacing organic-electronic with visual systems, specifically “Organic optoelectronic structures as artificial visual elements for a blind retina”. Interfacing biological systems with electronic components augments the possibility of repairing and restoring various physiological processes. In recent studies, the efficacy of polymer semiconductors as artificial receptors for interfacing with the visual systems was highlighted.

Research in the Soft Matter Lab, under a collaborative project, a microscopic heat engine was designed and implemented that is powered by bacterial activity. On the glass transition front, new analysis techniques were devised that allows researchers to distinguish between competing mechanisms of glass formation. On the colloidal self-assembly front, special surfaces have been developed that not only aid in deciding the symmetry of the growing crystallites but also helps in directing particles to specific sites prior to nucleation.

The research group in Epitaxy Lab demonstrated nano structuring of GaN thin film that significantly enhances the band-edge emission, due to structural and geometrical effects. In polarization induced two-dimensional confinement of carriers in wedge shaped polar semiconductors, a novel route to achieve two-dimensional (2D) carrier confinement in a wedge-shaped wall structure made of a polar semiconductor has been demonstrated theoretically. A kinetically controlled two-step growth process for the formation of an array of dislocation free high mobility InN nanorods (NRs) on GaN nanowall network (NWN) by Molecular Beam Epitaxy was demonstrated. In the early stages of plasma induced nitridation of Si (111) surface and study of interfacial band alignment, researchers of this Lab also reported a systematic study of the nitridation of the Si (111) surface by nitrogen plasma exposure.

Research Group in Superconductivity and Magnetism Lab discovered a new family of polar magnetic oxides, $RFeWO_6$ ($R = Dy, Eu, Tb$ and Y) which crystallize in an ordered aeschynite - type structure with a polar space group ($Pna2_1$), below the antiferromagnetic ordering of Fe^{3+} spins at $T = 15 - 18$ K. A detailed neutron diffraction analysis in $DyFeWO_6$ reveals a commensurate non-collinear antiferromagnetic ordering of Fe^{3+} spins (~ 18 K), which induce Dy-spins to order at the same temperature.

In Nanomaterials and Catalysis Lab, efficient membranes based on 2D materials have been fabricated for separation of industrially important gases such as H_2 from a mixture of H_2 and CO_2 . An alternative method to prepare high surface area, ordered, porous carbon has been discovered, which has been implemented for high capacity supercapacitors. A noble metal free catalyst has been developed by this group for direct synthesis of hydrogen peroxide from H_2 and O_2 .

In one of the reports created by the group working in Molecular Materials Lab, an in-depth investigation was made to find out multiple phase transitions in a flexible entangled framework based on different external stimuli such as temperature, pressure, and guest molecules. The research group has synthesized pyrene and anthracenemonocarboxylatechromophores based two metal-organic complexes which show Förster resonance energy transfer (FRET) process due to unique structural arrangement of linkers. In other work, the light-harvesting properties of two pyrenes based fluorescent dynamic conjugated microporous organic polymers have been explored.

In Polymer Lab, the limited structure tenability of poly(lactide) has led to the search for other biocompatible polymers. In this context, the possibility of living polymerization of β -hydroxy acid was explored. Cyclic monomers that can polymerized with nucleophilic catalyst have been synthesized and the nucleophilic ring opening polymerization of these materials is currently being attempted. A cyanide free synthesis of amino acids was developed using a carbonate as a source of carboxyl group.

The Molecular Design Lab, Nanoscopic Lab and Biomolecular Lab have worked towards developing new techniques along with generating compatible molecular probes so that the diffraction limit ($\sim 200-300$ nm) of light microscopy could be overcome and molecules inside cells are localized in nanometer precision. In addition, the research group was integrated an important feature with this imaging technique, i.e., the ability to simultaneously image and quantitate 100s of target molecules from a single cell. The research group is in process of developing a novel method for super-resolution imaging that combines click chemistry based specific and autonomous target labeling approach with single molecule localization technique. This technique was named **SISAC** (**S**uper-resolution **I**maging using **S**tochastic and **A**utonomous **C**licking). The research group has generated a functionalized gold nanoparticle based system that showed the ability to undergo supramolecular recognition mediated assembly and disassembly process. An important feature of this system is that in the assembled state it can incorporate various drug molecules.

Education Technology Unit (ETU)

The C.N.R. Rao Hall of Science and Education Technology Unit have been successfully conducting the highly popular Lecture Programmes/Workshops for students and teachers. These Lecture programs and workshops are conducted in different subjects like Physics, Chemistry, and Biology. The Unit started a 'STUDENT MENTORING PROGRAM' in May 2016 which gives an opportunity to students to witness how research is conducted and how laboratories work through providing academic support to prepare for their forthcoming and other competitive exams and solve their difficulties in science and math subjects.

The work of designing, formatting and editing the print-ready copy of a book 'A Life in Science' authored by Prof. C.N.R. Rao was undertaken.



The Summer 2016 Science Outreach Programme conducted in association with Himalayan Gram Vikas Samiti, Gangolihat conducted at Dashaithal, Gangolihat, Pithoragarh, Uttarakhand during May 11-13, 2016 by Prof. K. S. Valdiya. 150 students and teachers from various schools participated in the programme.

The Unit conducted nine lecture programs for students and teachers during 2016-2017, in addition, a 10-day orientation programme (Chetana program) for SSLC toppers and a three-day special lecture program for Chandan School students (Gadag) were also conducted.

The awardees of 2015 prizes for Outstanding Science Teachers were Shri. Purandaranarayana Bhat K. and Shri. Sanjay Kumar Srivastava.

In association with an NGO Parikrma, the 'Parikrma Festival of Science' was organized on February 14-16, 2017 and the theme was 'Soil and Agriculture'. Over 220 students from 42 schools and 80 teachers and volunteers participated.

National Science Day on February 28, 2017 was celebrated with students and teachers from Jawahar Navodaya Vidyalaya, Bangalore Urban and Bangalore Rural, Doddaballapur and from School Chandan, Laxmeshwar, Gadag. Over 150 students and teachers participated in the event comprising of popular science lectures and quiz.

Engineering Mechanics Unit (EMU)

It has been demonstrated that a vortex gas model for a spatially evolving 2D turbulent free shear flow yields a universal growth rate that is in surprisingly close agreement with data from high Reynolds number experiments. This agreement is considered significant as the model is extremely simple and very easy to code for a parallel computer.

Work on the large gains achieved by the use of GPUs in combination with CPUs (Maruthi et al. 2017) won the Best Paper Award at a recent Symposium at IISc on Computational Science. This will help better simulation and design of aircraft gas turbine blades.

Through a project, a test facility was designed and established at HPCL green Campus, Bangalore to evaluate the performance of Drag Reducing Polymers. Facility can quantify and compare performance of different polymers and estimate aging/polymer breakdown while in a pumping loop.

The first results of the DNS simulation of a transient diabatic plume, which offers a low-order model for cumulus cloud flows, have been obtained. Preliminary assessments of the results were promising.

Evolutionary and Integrative Biology Unit (EIBU)

Long-term selection experiments on rapid development and adaptation to larval crowding continued during the year. New results include the evidence for different ecological conditions promoting the evolution of hard-wired versus phenotypically plastic feeding rate responses under crowding.

Work on the social structure of female and male Asian elephants was continued in Nagarahole and Bandipur National Parks. Extensive analysis comparing social structure in this population with that of a population of a different genus of elephant, the African savannah elephant in Samburu suggested that there were underlying similarities in the social structure of the two genera.

Using individual-based simulations, the effect of social structure on bias in mark-recapture population size estimation was studied. A framework to examine how group size distributions could arise based on different rules of resource use and dominance between social groups was set up.

Ongoing studies to examine the connections between the circadian pacemaker and the sleep homeostat using the fruit fly *Drosophila melanogaster* demonstrate a time-of-day dependent homeostatic efficiency for recovery sleep, post sleep deprivation.

Studies demonstrate that expression of pathogenic human Huntingtin (HTT) in *Drosophila* circadian neuronal subset ventral lateral neurons (LNv) results in loss of the neuropeptide pigment dispersing factor (PDF) only from soma of small LNv (sLNv) and an associated arrhythmicity in circadian locomotor activity in constant darkness (DD).

Preliminary results suggest the role of neurotransmitter serotonin in behavioural entrainment to thermal cycles.

Putative regions have been identified in the fly-brain that may be involved in modulating a specific temperature dependent rhythmic behaviour that appears to be adaptive - suppression of mid-day activity under thermal cycles.

Studies using long term selection for early and late phase of emergence leads to divergent evolution of molecular circadian clocks and individuals with advanced and delayed phase-of-entrainment (chronotypes) are associated with a similar advanced and delayed phase of entrained molecular oscillation of core clock genes, and propose that such differences in entrained molecular oscillations might drive an advanced or delayed expression of output components and other downstream factors thereby driving different phases-of-entrainment.

Evolution of life-history traits differences in independently evolving replicate populations of *D. melanogaster* exhibiting *early* and *late* emergence chronotypes suggested that the genetic architecture underlying emergence gate/emergence at specific times of the day (emergence chronotypes) is correlated with several life-history traits.

International Centre for Materials Science (ICMS)

Studies carried out on synthesis, characterization and properties of anions substituted metal oxides and chalcogenides where in oxygen is replaced by nitrogen and fluorine or sulfur by phosphorus chlorine research on 2D materials specially phosphorene.

A novel route to achieve two-dimensional (2D) carrier confinement in a wedge-shaped wall structure made of a polar semiconductor has been demonstrated theoretically.

It was found that nanostructuring of GaN thin film significantly enhances the band-edge emission, due to structural and geometrical effects. A kinetically controlled two-step growth process for the formation of an array of dislocation free high mobility InN nanorods (NRs) on GaN nanowall network (NWN) was also achieved by the researchers in ICMS. The surface and interface chemical composition and surface morphology are investigated by using RHEED, X-ray photoelectron spectroscopy, and atomic force microscopy (AFM). At the initial stage of nitridation two superstructures —“8×8” and “8/3×8/3”—form, and further nitridation leads to 1×1 stoichiometric silicon nitride.

Cyclic monomers that can polymerized with nucleophilic catalyst have been synthesized and the nucleophilic ring opening polymerization of these materials is currently being attempted.

The development of dendritic materials for the efficient quantification of low viral loads in HIV infected individuals has been attempted. Attachment of Raman markers to dendrimers is expected to enable the enhanced viral RNA using SERS technique.



A cyanide free synthesis of amino acids was developed using a carbonate as a source of carboxyl group. Transformation of the carbonate to a carboxyl group was accomplished via the use of a nucleophile. It was shown that this nucleophilic activation of carbonates is dependent on cation- π interactions.

Diffusion of dopants or impurities in host nanocrystals out of the host has been used proactively to obtain uniformly doped QDs. It has been shown that uniform doping, specifically for magnetic impurities is crucial with up to two orders of magnitude increase in room temperature ferromagnetism.

The mechanism of Mn emission has been developed and uncovered an important long-standing puzzle regarding the Mn emission. Air stable Sn doped perovskite materials with excellent optical properties have also been synthesized.

A microscopic heat engine has been designed and implemented that is powered by bacterial activity. A new analysis techniques was developed that allows the researchers to distinguish between competing mechanisms of glass formation. Special surfaces were developed that not only aid in deciding the symmetry of the growing crystallites but also helps in directing particles to specific sites prior to nucleation.

Work has been undertaken in developing novel NASICON compounds as potential sodium ion cathodes.

Molecular Biology and Genetics Unit (MBGU)

The characterization of autophagy pathways in yeast and mammalian cells has revealed novel signaling pathways that govern autophagy flux. In addition to these pathways, the Group has uncovered mechanisms that negatively regulate autophagosome lysosome fusion.

Research collaboration was established and MoU signed between JNCASR and the University of Strasbourg, based on the discovery made by the research group of an activator of histone acetyltransferase p300 conjugated with CSP, to elucidate its effect in the Huntington Disease Model.

Novel metabolic regulators have been identified that maintain the stem cell state in human pluripotent stem cells and regulate differentiation. Researchers of the Unit have shown that oxidative phosphorylation status is key to determining cell fate.

In the area of HIV research, some important leads show that the same viral protein Tat can activate as well as suppress transcription from viral promoter. For the first time, the work done by the research group provides a scientific explanation for the presence of a unique NF- κ B binding motif in subtype C, a major HIV-1 genetic family responsible for half of the global HIV-1 infections. The results offer compelling evidence that subtype C viral promoter is not only stronger but also is endowed with a qualitative-gain-of-function advantage.

In the area of molecular genetics of hereditary, prelingual, sensorineural hearing impairment, researchers have completed an analysis of a large multi-generation family in which severe-to-profound hearing loss is found associated with a variety of skin-related anomalies. Genome-wide analysis of the family showed that the locus maps to chromosome region 13p tel-q12.1 and that novel mutation, p.N54K in Cx30, co-segregates with the phenotype. Unlike wild-type Cx30, p.N54K Cx30 is predominantly localized in the cytoplasm and does not permit transfer of neurobiotin, suggesting improper cellular localization and abolishment of gap-junction activity.

In protein engineering and molecular parasitology, the group has undertaken 3-dimensional structure solution using X-ray crystallography of numerous enzymes that are under investigation in the laboratory including the structures of MjGATase and MjATPPase-ligand complex solved using molecular replacement and apo-MjFH using Se-SAD. The group has also solved the structures of PflSN1 and complexes through a collaborative effort with Dr. Aghajari (France) using a combination of cryoEM and Se-SAD.

In the studies related to mechanisms underlying pathogenesis of human cerebral malaria, the role of Autophagy on growth and development of malaria parasite *Plasmodium falciparum* was explored. It was found that the gene expression profiles of some of the representative Autophagy genes involved at various steps of the pathway are significantly upregulated during intra-erythrocyte stages of parasite proliferation.

In the area of Chromatin Biology and Genomics, researchers have identified various post-translational modifications on TH2B across the tetraploid and haploid stages of spermatogenesis. By computational analysis, it was also shown that the amino acid differences in the N-terminal tail and the post-translational modifications acquired by some of the residues could cause the destabilization of the nucleosomes.

Neuroscience Unit (NSU)

Sleep arousal circuits and the interactions between circadian clock circuit and the sleep homeostat using the fruitfly *Drosophila melanogaster* have been studied. A role for a mechanosensor *nanchung* expressing cells in inducing daytime sleep in male flies was uncovered.

A comparative study was done to analyse the rhythmic behaviour, putative circadian pacemaker neurons, circadian clock properties and sleep characteristics in a diurnal and a crepuscular species of *Drosophila*.

A study of the interactions between circadian oscillators modulating feeding and activity rhythms in fruit flies *Drosophila melanogaster* was also undertaken.

Efforts were made to understanding the following functions of *Syngap1* in brain development. The Research Group tried to answer how does *Syngap1* heterozygous mutation affects the function of GABA by modulating the switch of Cl⁻ transporters during development. The preliminary results show that this mutation advances the switch of Cl⁻ transporters during development, thereby regulating the function of GABA during development.

It was found that neuronal maturation in FMRP KO is opposite to *Syngap1* Heterozygous mutations i.e., delayed maturation in FMRP. This will help researchers in the Lab to design therapeutic drugs targeting protein that regulate FMRP and reverse the behavioral and functional deficits observed in *Syngap1*.

The preliminary data suggests that the astrocyte expression was reduced in *Syngap1* heterozygous mice, which can affect how the neurons (excitatory and inhibitory) neurons mature and function.

To understand whether the phenotypes observed in *Syngap1* Het mutations can be rescued by targeting perineuronal nets that forms at the time of neuronal maturation (3 weeks in mice), preliminary results shows that the number of perineuronal nets are reduced in *Syngap1* Hets.

Research on characterization of autophagy pathways in yeast and mammalian cells has revealed novel signaling pathways that govern autophagy flux. In addition to these pathways, mechanisms have been uncovered that negatively regulate autophagosome lysosome fusion.

Host of modern materials offer a unique combination of optoelectronic and mechanical properties as recently demonstrated for sensing and stimulating neuronal activity and evoking response in retinal ganglion cells. This possibility of triggering neuronal signals in a blind retina has opened a route for utilizing these (intelligent) substrates as a prosthetic element.

The utility of ultra-high impedance, dry-contact capacitively coupled electric potential sensors has been examined. Standard cell lines on a variety of substrates were utilized to demonstrate the efficacy of this sensor placed in close proximity without physical contact. Conventional imaging methods and multi-electrode array recordings are used in tandem to validate and ascertain this new method developed at JNCASR.



The study related to lncRNAs involved one such lncRNA known as Mrhl (mouse recombination hotspot locus). Mrhl is 2.4 kb in length, intronic, single-exonic, polyadenylated and has tissue specific expression in the adult mouse. It is also syntenically conserved in humans. The role of Mrhl in regulating meiotic commitment during germ cell differentiation has been established by researchers in this Unit. By analyzing ENCODE datasets, it was found that Mrhl exhibits differential expression in the mouse embryonic and adult brain and it was shown that it is spatio-temporally expressed in the developing mouse embryonic brain. Mechanistic studies reveal Pax6 as the major transcription factor that might be involved in regulating Mrhl RNA during neuronal differentiation. Furthermore, ChIP studies for histone modifications shows that Mrhl might be regulated epigenomically during mouse brain development. Current studies are being focused on decoding the mechanisms associated with regulation of neuronal differentiation/commitment by lncRNA Mrhl.

Research on EFHC1 which has been identified as a causative gene for Juvenile Myoclonic Epilepsy (JME) by researchers of the Unit, report contribution of EFHC1 in JME patients from India. The complete structure of the EFHC1 transcript has been examined from 480 JME patients and 700 control chromosomes by direct sequencing. Functional correlates of mutations were studied using immuno-localization experiments in cultured mammalian cells and in silico protein homology modeling studies. Thirteen mutations, of which 11 were previously not known, were identified in 28 JME patients.

The studies revealed the identification of three mutations of genes causing Hot water epilepsy (HWE) i.e., p. Asp174Asn, p.Val251Ile and p.Ile304Met in the SLC1A1 protein, a glutamate transporter. It was also found that all three mutations affect glutamate uptake in cultured cells in a temperature-dependent manner.

New Chemistry Unit (NCU)

Prof. C. N.R. Rao's research group has worked in areas related to artificial photosynthesis involving photocatalytic oxidation of water by nanoparticles of Mn and Co oxides and the other on photocatalytic H₂ generation by hybrid nanostructures by using the Z-scheme; and Synthesis, characterization and properties of anions substituted metal oxides and chalcogenides where in oxygen is replaced by nitrogen and fluorine or sulfur by phosphorus chlorine research on 2D materials specially phosphorene.

Dr. T. Govindaraju's research group had focused on the development of diagnostics and therapeutics for currently incurable neurodegenerative diseases such as Alzheimer's (AD) and Parkinson diseases (PD). Several solutions were explored to address issues related these diseases by elegantly combining the multidisciplinary chemical biology approaches. Hybrid peptoids, a small molecule-based molecular tools was developed in his laboratory, which can clear the toxic plaques through the natural cellular process.

Dr. Jayanta Halder's research group has worked in the area of multi-drug resistant Gram-positive bacteria like vancomycin resistant Enterococci (VRE) and Staphylococci (VISA and VRSA); as well as pan-drug resistant New Delhi metallo- β -lactamase-1 (NDM-1) producing Gram-negative bacteria which have become a threat to the global public health. The research group has developed novel vancomycin analogues which not only overcome acquired resistance against VRE, VISA and VRSA but also took care of the inherent vancomycin resistance towards Gram-negative bacteria due to incorporation of novel membrane disrupting mechanism and pyrophosphate binding moiety in vancomycin. Recently, the Group also engineered new generation of polymeric biomaterials from synthetic and natural polymers to make any surface antimicrobial. These inactivate various pathogenic bacteria completely on contact and can be used to prevent the spread of infectious diseases. The Group also developed antibacterial hydrogels that could prevent bacterial infections at wound site without displaying any toxicity towards mice used as the model animal for the experiment.

Dr. Kanishka Biswas's research group is directed towards research in solid state chemistry; understanding (crystal and electronic) structure-property relationship and electronic and phonon transport properties of metal chalcogenides and metal halides. In last one year, the Group discovered several new classes of inorganic metal chalcogenides and developed new concepts to decrease the thermal conductivity (lone pair induced rattling, bonding asymmetry and phonon scattering due to intergrowth 2D nanostructures) which resulted in high thermoelectric performance. The low cost and earth abundant inorganic solids discovered in his laboratory can convert waste heat to electricity with 12-15 %. The Group has designed new concept to tailor the electronic structure of topological crystalline insulators (SnTe and $Pb_{1-x}Sn_xTe$) and GeTe based materials, which resulted in significant improvement of its thermoelectric performance.

Dr. Subi Jacob George's research Group has been worked towards spatio-temporal control over the self-assembly and functions of supramolecular systems for material applications such as development of novel functional organic and hybrid materials.

Dr. Ranjani Viswanatha's research group worked on doping of magnetic ions into CdS nanocrystals and its corresponding magnetism. Work has been initiated in the area of spintronics which is a new upcoming area of research for various applications. The Group worked on the mechanism of Mn emission and uncovered an important long-standing puzzle regarding the Mn emission. Air stable Sn doped perovskite materials with excellent optical properties was also synthesized.

Dr. Sebastian C. Peter's research group developed several stable and efficient non-Pt based compounds as electrode materials alternative to the state-of-the-art materials Pt or PtRu on carbon in fuel cell industry. The Group filed two patent applications and is in the process of scaling up the materials towards the commercialization in collaboration with various industries and national facilities. The Group also developed several low-cost materials for the efficient conversion of waste CO₂ into useful chemicals and fuels. The waste CO₂ produced at the coal power generation and cement factories are targeting in this research.

Dr. Sarit S. Agasti's research Group has been oriented towards engineering small molecules and programmable molecular materials to address challenges in bioimaging and to create novel approaches for diagnostic sensing and therapeutic delivery. The Group is in a process of developing a novel method for super-resolution imaging that combines click chemistry based specific and autonomous target labeling approach with single molecule localization technique.

Dr. Premkumar Senguttuvan's research group has worked to develop novel electrode and electrolyte materials for Li- and beyond Li-ion Batteries. The group also worked to develop novel NASICON compounds as potential sodium ion cathodes.

Prof. H. Ila's research group work towards design and development of new general, highly efficient synthetic methods for biologically important five and six membered heterocyclic compounds using novel organosulphur building blocks/synthons derived from broad range of active methylene compounds. The various methodologies involve transition metal (especially palladium and copper) catalyzed C-C, C-N and C-S bond formation reactions, regio- and chemoselective C-C and C-heteroatom bond formations with various carbon and heteronucleophile on these synthons, heteroaromatic annulations with bifunctional heteronucleophiles and cycloadditions with activated isocyano methylene compounds on these substrates.

Dr. Sridhar Rajaram's research group has started exploring the possibility of living polymerization of β -hydroxy acid. The research group also focused on the development of dendritic materials for the efficient quantification of low viral loads in HIV infected individuals. Attachment of Raman markers to dendrimers is expected to enable the enhanced viral RNA using SERS technique. The group also developed a cyanide free synthesis of amino acids using a carbonate as a source of carboxyl group. Transformation of the carbonate to a carboxyl group was accomplished via the use of a nucleophile.



Theoretical Sciences Unit (TSU)

In collaboration with experiments groups, the electronic and phonon-based mechanisms were identified for increasing thermoelectric performance of a material through enhancement of Seebeck coefficient and reduction of thermal conductivity. The efficacy of the newly developed SCAN metaGGA functional of density functional theory in prediction of transition temperatures of ferroelectric perovskite oxides was also demonstrated.

The Mott metal-insulator transition is known to be a first order phase transition. The Group found, for the first time, a lattice model that exhibits a whole surface of continuous quantum critical Mott transitions.

Researchers in TSU have addressed a major theoretical challenge that hinders detailed investigations of real strongly correlated materials that is access to a well benchmarked, computationally feasible, and real-frequency based method. A multi-orbital iterated perturbation theory method has been developed. Furthermore, a completely open source implementation of this method, called MO-IPT along with detailed instructions, sample data and examples has been released,

The first quantitative study was carried out in the area of slow quench dynamics when a nonequilibrium system with isolated critical point is quenched in the critical region. This work has been included in the 'EPL highlights of 2016'.

Progress has been made in identifying descriptors for several classes of problems and materials, including noble and transition metal catalysts, supramolecular host-guest assemblies and binary surface alloys. These are all quantities that can be computed rapidly, and can help one quickly identify a group of systems that are likely candidates for possessing the desired properties, and merit further investigation using abinitio techniques.

Three-layer Phosphorene, which shows anisotropic mobility values has been studied in detail. With appropriate substitution, it was found that the g-C₃N₄ Quantum Dots show photocatalytic behavior in Visible Light. It was also shown that an improved catalytic activity of 25% Mn substituted Co₃O₄ Material for Water Oxidation Reaction (Oxygen Evolution Reaction).

New understanding has been achieved on Active Matter. Influence of active particles on the phase behavior of demixing systems has been studied and obtained insight on how to map such nonequilibrium problems to equilibrium ones. Coarsening in phase separating binary fluid confined in nanochannels have been studied via Molecular Dynamics Simulations and the work has practical relevance in the technology related to extraction of oil and natural gas from porous rocks.

Problems have been addressed related to the co-evolutionary patterns of amino acids in viruses which help them evade immune surveillance while remaining functional, bacterial strategies for nutrient acquisition and the relevance of chemotaxis mechanism for bacterial population multiplication, and quantitative structure activity relationships for a new class of drug candidates that disrupt the membranes and have smaller chances of developing resistance.

Through extensive computer simulations and numerical calculations, researchers have shown that the self-organization necessary for shear jamming occurs even for frictionless particles, and that jamming occurs at a precisely defined state at which the mean contact number reaches a value of $D + 1$ (D being the spatial dimension) and a percolation transition of stressed regions takes place, establishing new connections with analyses of rigidity in covalent glasses.

Academic Activities

During 2016-2017 admissions, 52 students joined JNCASR in August 2016, and 11 students joined during January 2017. Thirty-five students were awarded Ph.D. degrees, three with M.S. (Engg.), and in M. S. of Integrated Ph.D. – seven students were awarded M.S. in Biological Sciences, five students with M.S. in Chemical Sciences

and three students with M.S. in Materials Science. In addition, three students were awarded the Postgraduate Diploma in Materials Science (PGDMS).

Fellowship & Extension Programmes

Fifteen scientists from research institutions across the country were selected for the Centre's Visiting Fellowships 2016-17. The selected scientists were hosted by the faculty of CPMU, EIBU, MBGU, NCU, NSU, and TSU. For SRFP 2016, 63 students availed the scholarship and received research training in various areas of Physics, Chemistry, Biology or Engineering at research institutes in Bangalore, and elsewhere in the country. The advertisement of SRFP 2017 was announced on the JNCASR website and emailed to around 150 college principals in the country. A total of 1396 applications were received and 94 offers have been sent. Eight students each from Project Oriented Chemistry Education and Project Oriented Biology Education 2014-16 completed the programme successfully. Under Student Buddy Programme, 94 students of class XI/XII from Jawahar Navodaya Vidyalaya and Kendriya Vidyalaya have benefitted during the year 2016.

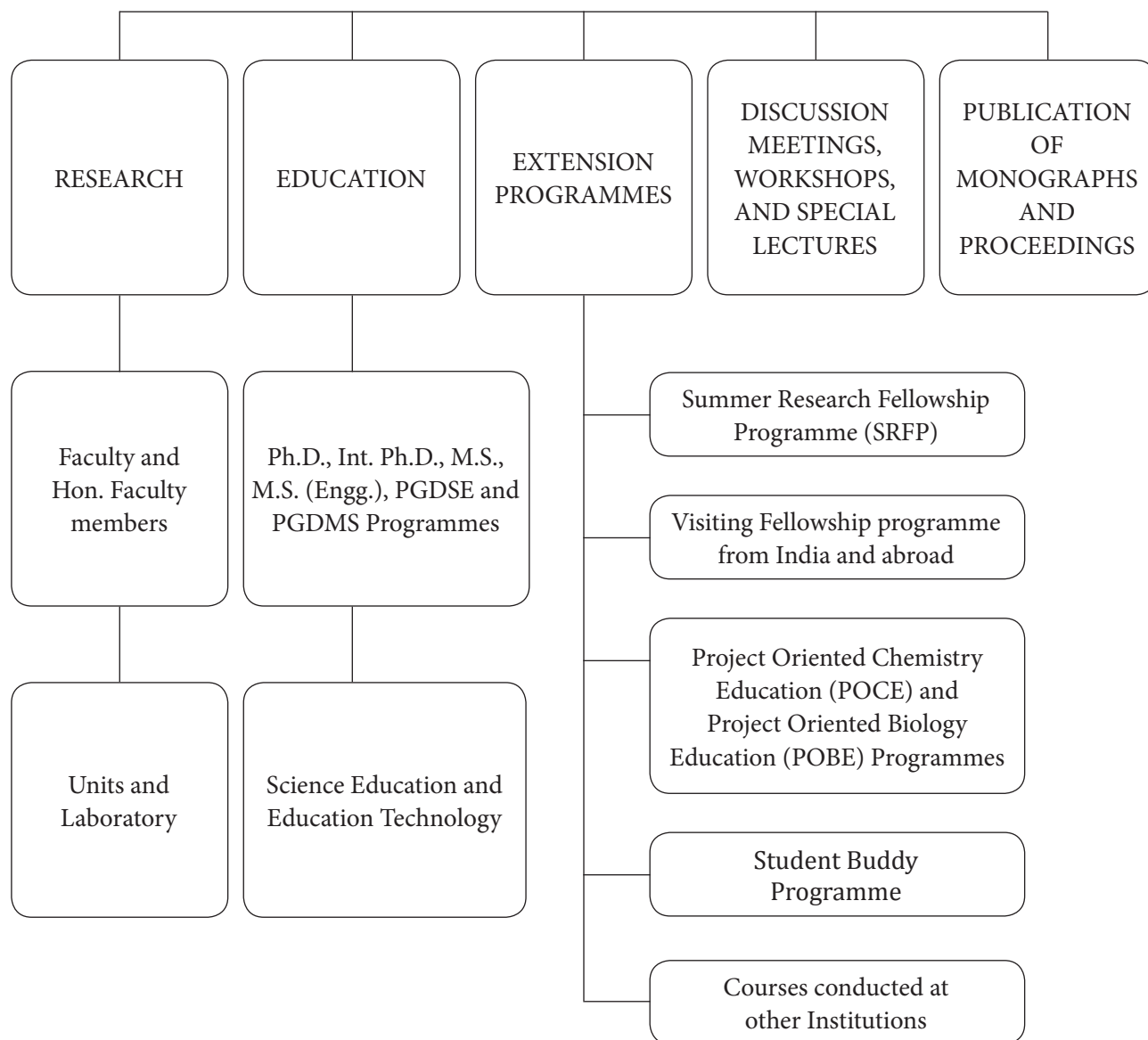
Reservation, Official Language and Implementation of the judgments/orders of the CAT

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



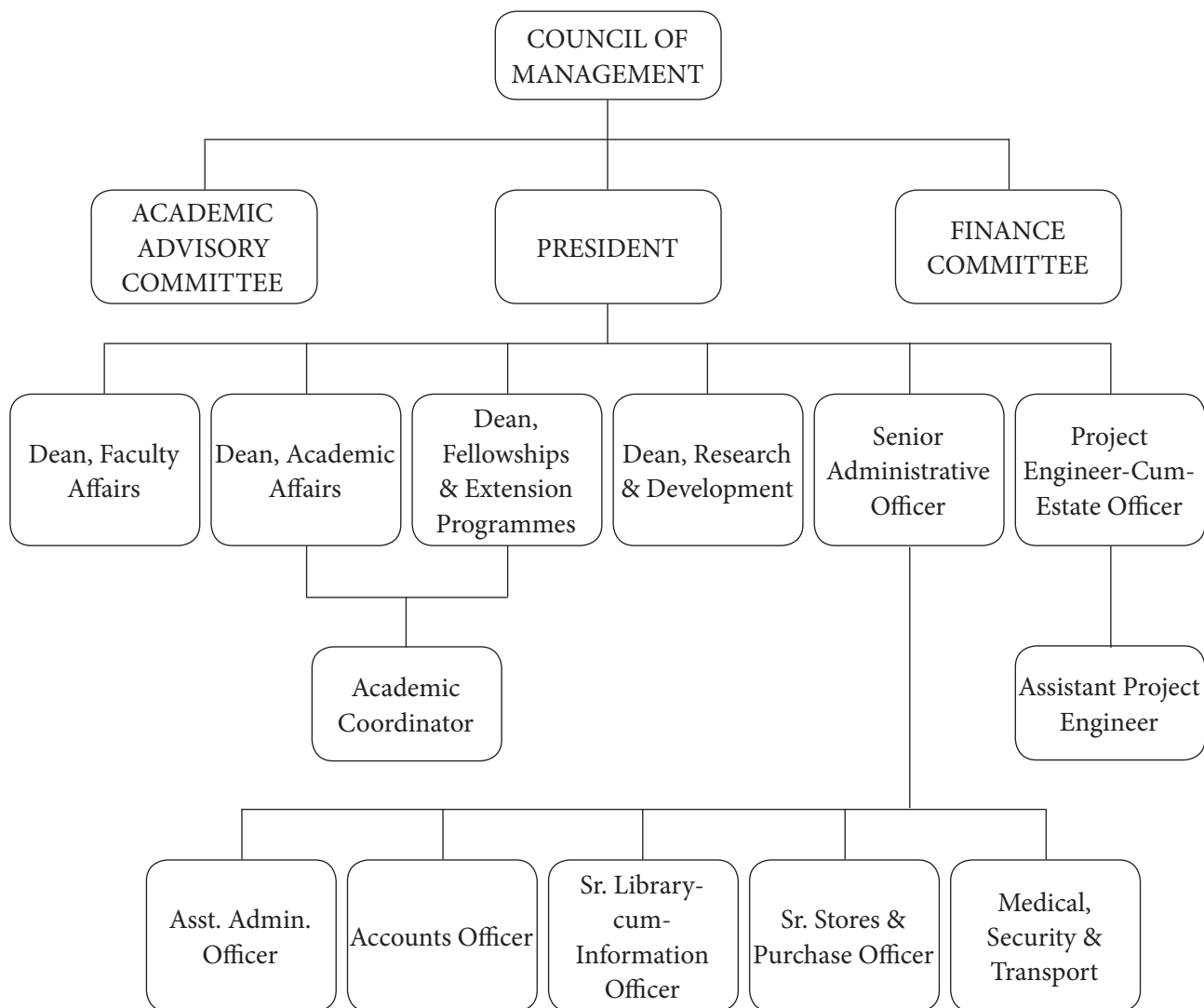
ACTIVITIES CHART

JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH



ORGANISATION CHART

JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH



THE ORGANISATION

COUNCIL OF MANAGEMENT

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

The following are the members of the Council:

Dr. P. Rama Rao Hyderabad	Chairman
Prof. V. Nagaraja President, JNCASR	Member
Prof. C.N.R. Rao Hon. President, JNCASR	Member (JNC nominee)
Prof. Ashutosh Sharma Secretary, DST	Member
Shri J.B. Mohapatra JS & FA, DST	Member
Dr. Baldev Raj Director, NIAS	Member (DST nominee)
Prof. S.K. Joshi NPL, New Delhi	Member (UGC nominee)
Prof. Anurag Kumar Director, IISc	Member
Prof. Chandan Dasgupta IISc	Member (IISc nominee)
Mr. A.N. Jayachandra Sr. Administrative Officer, JNCASR	Secretary

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:

Prof. V. Nagaraja President	Chairman (Ex-officio)
Prof. C.N.R. Rao National Research Professor	Member
Shri J. B. Mohapatra Joint Secretary and Financial Advisor, DST	Member
Mr. Sampad Patra Accounts Officer	Member (Ex-officio)
Prof. Chandan Dasgupta Dean, Undergraduate Studies, IISc	Member
Mr. A.N. Jayachandra Sr. Administrative Officer, JNCASR	Member (Ex-officio)

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:

Prof. V. Nagaraja President, JNCASR	Chairman (Ex-officio)
Prof. Hemalatha Balaram Dean, Faculty Affairs, JNCASR	Member (Ex-officio)
Prof. Shobhana Narasimhan (till December 2016) Dean, Academic Affairs, JNCASR	Member (Ex-officio)
Prof. Umesh V Waghmare (January 2017 onwards) Dean, Academic Affairs, JNCASR	Member (Ex-officio)
Prof. Maneesha S Inamdar Dean, Fellowships and Extension Programmes, JNCASR	Member (Ex-officio)



Prof. K.S. Narayan Dean, R&D, JNCASR	Member (Ex-officio)
Prof. U. Ramamurty Mat. Engg., IISc	Member
Prof. George K Thomas IISER, Thiruvananthapuram	Member
Prof. D.D. Sarma SSCU, IISc	Member
Prof. Devang V. Khakhar Director, IIT, Mumbai	Member (UGC Nominee)
Mr. A. N. Jayachandra Sr. Administrative Officer, JNCASR	Secretary (Ex-officio)

FACULTIES

All the faculty members are involved in various academic activities of the Centre and assist the Academic Advisory Committee in discharging its functions. The last Annual Faculty Meeting was held in November 2016 which included lectures by the faculty on the advances made in various research areas.

ADMINISTRATION

President V Nagaraja	Ph D, F A Sc, F N A Sc
Dean, Faculty Affairs Hemalatha Balaram	Ph D
Dean, Academic Affairs Umesh V. Waghmare	Ph D
Dean, Fellowships and Extension Programmes Maneesha S Inamdar	Ph D
Dean, Research and Development K. S. Narayan	Ph D, F N A Sc, F A Sc
Warden & Student Counsellor Tapas Kumar Maji	Ph D
Associate Warden Ranjani Viswanatha	Ph D
Sr. Administrative Officer A. N. Jayachandra	B Com, ICWA (Inter)
Assistant Administrative Officer C. S. Chitra	B Com
Academic Coordinator Princy Jaison Pereira	Ph D

Accounts Officer	
Sampad Patra	B Com, PGDCA, MBA (Finance)
Sr. Stores & Purchase Officer	
K. Bhaskara Rao	M Sc, M Phil
Sr. Library-cum-Information Officer	
Nabonita Guha	MLIS
Sr. Secretary to President	
A. Srinivasan	B A
Jr. Accounts Officer	
B. Venkatesulu	B Sc
Project Engineer	
S. Chikkappa	B E
Project Engineer Gr. II	
Nadiger Nagaraj	DCE
Assistant Project Engineer (Elec.)	
Sujeeth Kumar S.	DEE
Junior Project Engineer (Civil)	
Veerasha N. R.	DCE
Consulting Medical Officer	
G. R. Naghabhushan	MBBS, FCCP, FCGP, P G Dip in M&CHL
Consulting Lady Medical Officers	
Kavitha Sridhar	MBBS
Archana, M. L. V.	MBBS
HV Chandralekha	MBBS
Physiotherapist	
Y. Yogesh	BPT
Honorary Medical Officers	
Sharada	MBBS
C. Satish Rao	MBBS
P. K. Raghupathy	MBBS
R. Nirmala	MBBS
Honorary Security Officer	
M. R. Chandrasekhar	B Sc, LLB



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

CHEMISTRY AND PHYSICS OF MATERIALS UNIT (CPMU)

Research Activities and Achievements

Prof. Chandrabhas Narayana (Light Scattering Lab)

High pressure studies on Electronic Topological Materials using X-ray, Raman and resistivity studies were carried out on systems like AgBiSe₂, and was a demonstration that these indirect methods can be the best method to study electronic topological transitions. The lab was also involved in developing methodology to understand potential drug molecules binding to therapeutically important proteins using MD simulations in Schrodinger software and verifying the same using Raman spectroscopy, for example, binding of nitrodipine or amlodipine to HSA or BSA proteins. The lab was also involved in a customized diagnostic Raman spectrometer with scanning ability to make a prototype for viral RNA/DNA detection from body fluids. The lab has undertaken studies in adsorption effects of liquids and gases in Metal Organic Frameworks (MOFs). Interesting MOFs are being synthesized and studied under pressure and temperature to understand the microscopic picture using x-ray and Raman studies.

Prof. S. Balasubramanian (Molecular Stimulation Lab)

Computational studies showed that CO₂ uptake in a metal organic framework is not only dependent on the nature of the adsorption site but also on the availability of a kinetic pathway to access the same and the latter can be modulated by ligand dynamics. A correlation between density and accessible surface area of amorphous microporous polymers (CO₂ adsorbents) which will be quite useful to experimentalists has been obtained using molecular modelling methods. Product release mechanisms in many enzymes and in particular, in phosphoribosyltransferases in human and in the malarial parasite has been delineated using advanced MD simulation methods. Protic organic ionic plastic crystals have been studied using ab initio MD methods for their proton and ion transport properties. A related compound that should exhibit enhanced electrical conductivity than what is currently known has been predicted using molecular modelling. Room temperature ionic liquids have been investigated for their ability to adsorb the acidic gas, sulfur dioxide. Molecular level insights into their adsorption has been provided.

Prof. K. S. Narayan (Molecular Electronics Lab)

Imaging organic Solar Cells: Tailor-made, custom-designed experimental methods to probe characteristic responses, time scales and length scales is pursued routinely. For example: imaging methods to examine the heterogeneity in photoconducting polymer blends from 10 nm to several micron length scales has been explored. The notable thing is that the capability has been developed to zoom in on a stationary sample from confocal microscopy length scales to Atomic Force Microscope scales. This utilizes a combination of tips: including glass aperture tips for near field access and convention AFM tips. Therefore, if the sample has contrast features arising from optical/dielectric/topological etc. at these length scales, the researchers have investigated and analyzed and shown if there are any correlations existing with bulk properties.

Noise Measurements in Organic Electronics: Noise measurements are also extensively used to probe the fluctuations in electrical transport which are inherent in these disordered systems. The novelty of this approach is that it was possible to carry out noise measurements under constant photoexcitations. The fluctuations in the current with steady state of pumping carriers in the system directly reveals the trap kinetics, and importantly

it reveals the condition of a photovoltaic module. Switching studies were carried out to examine the speed and the limitations of Field Effect Transistors (FET) over a frequency range extending up to 100 MHz. It was found that as organic FETs have response beyond 1 MHz, it is possible to operate these FETs and make basic circuits in the MHz regime.

Fabrication of Organic devices: Design and characterizing new organic electronic materials was also taken up for research. Collaborations were established with leading chemists in this field and provide feedback in the quest for developing high mobility polymers and small molecules, acceptor molecules for bulk heterojunction based solar cells, high and low-k dielectrics. Considerable effort was given in optimizing processing conditions for a desired property. Processing tools include spin-coating and printing methods, annealing under electric field conditions, soft-lithography approaches, vapor deposition, etc.

Bio Electronics: Soft-electronic polymers in biomedical arena exhibit utility in tissue engineering and for vision prosthetic elements. Many aspects were examined of this important research topic, For example, recent research breakthrough in interfacing organic-electronic with visual systems, specifically “Organic optoelectronic structures as artificial visual elements for a blind retina”.

Interfacing biological systems with electronic components augments the possibility of repairing and restoring various physiological processes. In recent studies, the efficacy of polymer semiconductors as artificial receptors for interfacing with the visual systems was highlighted. Extensive interaction is underway with biophysicists, electrical engineers, neurophysiologists, and ophthalmologists to translate some of these demos to more in-depth in-vitro and in-vivo studies and hope to bring a polymer-retina as an option for visual-retinal disorders.

Dr. Rajesh Ganapathy (Soft Matter Lab)

Research in the Soft Matter Lab at ICMS focused on three key research themes namely (1) stochastic thermodynamics, (2) glass transition and (3) colloidal self-assembly. As a part of a collaborative effort, a microscopic heat engine was designed and implemented that is powered by bacterial activity. On the glass transition front, new analysis techniques were devised that allows to distinguish between competing mechanisms of glass formation. On the colloidal self-assembly front, special surfaces have been developed that not only aid in deciding the symmetry of the growing crystallites but also helps in directing particles to specific sites prior to nucleation.

Prof. S. M. Shivaprasad (Epitaxy Lab)

Polarization induced two-dimensional confinement of carriers in wedge shaped polar semiconductors: A novel route to achieve two-dimensional (2D) carrier confinement in a wedge-shaped wall structure made of a polar semiconductor has been demonstrated theoretically. Tapering of the wall along the direction of the spontaneous polarization leads to the development of charges of equal polarity on the two inclined facades of the wall. Polarization induced negative (positive) charges on the facades can push the electrons (holes) inward for a n-type (p-type) material which results in the formation of a 2D electron (hole) gas at the central plane and ionized donors (acceptors) at the outer edges of the wall. The theory shows that this unique mode of 2D carrier confinement can indeed lead to a significant enhancement of carrier mobility. It has been found that the reduced dimensionality is not the only cause for the enhancement of mobility in this case. Ionized impurity scattering, which is one of the major contributor to carrier scattering, is significantly suppressed as the carriers are naturally separated from the ionized centers. A recent experimental finding of very high electron mobility in wedge shaped GaN nanowall networks has been analyzed in the light of this theoretical reckoning.

Nano structuring GaN thin film for enhanced light emission and extraction: The research group demonstrate that nano structuring of GaN thin film significantly enhances the band-edge emission, due to structural and geometrical effects. Films of increasing roughness are formed by kinetic control in a PA-MBE system and their morphological, structural and optical properties are compared by complementary characterization probes. The



nanowall configuration with largest pore size (≈ 215 nm) shows a two orders of magnitude enhancement of integrated PL intensity in comparison to a GaN epilayer. Finite difference time domain (FDTD) simulation was performed to explain the role of total internal reflection and scattering on light extraction. The extended defects terminate proximal to interface, leading to most regions of the nanowalls were defect free, enhancing light generation. The observation of broad HRXRD rocking curves is attributed to amosaicity that originates due to mutual misorientation of the nanowalls. Thus, the low dislocation density in the nanowalls and their suitable geometry promotes high light emission and extraction, respectively, offering this nanostructure as a potential material for high brightness LED fabrication.

Electron mobility of self-assembled and dislocation free InN nanorods grown on GaN nano wall network template: A kinetically controlled two-step growth process for the formation of an array of dislocation free high mobility InN nanorods (NRs) on GaN nanowall network (NWN) by Molecular Beam Epitaxy was demonstrated. The epitaxial GaN NWN is formed on c-sapphire under nitrogen rich conditions, and then changing the source from Ga to In at appropriate substrate temperature yields the nucleation of a self assembled spontaneous m-plane side faceted-InN NR. By HRTEM, the NRs were shown to be dislocation-free and have a low band gap value of 0.65 eV. Hall measurements are carried out on a single InN NR along with J-V measurements that yield mobility values as high as ≈ 4453 cm²/V s and the carrier concentration of $\approx 1.1 \times 10^{17}$ cm⁻³, which are unprecedented in the literature for comparable InN NR diameters.

Early stages of plasma induced nitridation of Si (111) surface and study of interfacial band alignment: Researchers of this Lab also reported a systematic study of the nitridation of the Si (111) surface by nitrogen plasma exposure. The surface and interface chemical composition and surface morphology were investigated by using RHEED, X-ray photoelectron spectroscopy, and atomic force microscopy (AFM). At the initial stage of nitridation two superstructures—"8×8" and "8/3×8/3"—form, and further nitridation leads to 1×1 stoichiometric silicon nitride. The interface is seen to have the Si¹⁺ and Si³⁺ states of silicon bonding with nitrogen, which suggests an atomically abrupt and defect-free interface. The initial single crystalline silicon nitride layers are seen to become amorphous at higher thicknesses. The AFM image shows that the nitride nucleates at interfacial dislocations that are connected by sub-stoichiometric 2D-nitride layers, which agglomerate to form thick over-layers. The electrical properties of the interface yield a valence band offset that saturates at 1.9 eV and conduction band offset at 2.3 eV due to the evolution of the sub-stoichiometric interface and band bending.

Prof. A Sundaresan (Superconductivity and Magnetism Lab)

Research Group led by Prof. A. Sundaresan discovered a new family of polar magnetic oxides, $R\text{FeWO}_6$ ($R = \text{Dy, Eu, Tb and Y}$) which crystallize in an ordered aeschynite - type structure with a polar space group ($Pna2_1$) below the antiferromagnetic ordering of Fe³⁺ spins at $T = 15 - 18$ K. A detailed neutron diffraction analysis in DyFeWO_6 reveals a commensurate non-collinear antiferromagnetic ordering of Fe³⁺ spins (~ 18 K), which induce Dy-spins to order at the same temperature. The electric polarization in all these compounds are affected by applied magnetic field demonstrating a strong magnetoelectric effect. Further, the coupling between different magnetic R-ion and Fe-ion moments influence the polarization to a different extent. While the measured polarization in polycrystalline DyFeWO_6 at 3.5 K is about 3 $\mu\text{C}/\text{m}^2$, the calculated value of resultant ionic polarization of the form $(p_x, 0, p_z)$ is 75000 $\mu\text{C}/\text{m}^2$ where p_x comes from magnetic ordering and p_z is associated with the polar structure. The finding achieved by the research group related to magnetoelectric properties in these materials opens new avenue to explore further new compounds with other transition metals in the ordered aeschynite-type structure.

Prof. M. Eswaramoorthy (Nanomaterials and Catalysis Lab)

Nanomaterials and Catalysis Lab has been involved in various research projects involving different applications of porous materials and nanomaterials. Main highlights are as follows: Efficient membranes based on 2D

materials have been fabricated for separation of industrially important gases such as H₂ from a mixture of H₂ and CO₂. An alternative method to prepare high surface area, ordered, porous carbon has been discovered, which has been implemented for high capacity supercapacitors. A noble metal free catalyst has been developed by this group for direct synthesis of hydrogen peroxide from H₂ and O₂. This group, in collaboration with scientists from ICAR have been involved in developing porous materials for slow release of insect pheromone to trap agriculturally harmful insects.

Dr. Tapas Kumar Maji (Molecular Materials Lab)

Gas Storage and separation: Over the years, a fascinating property of metal–organic frameworks (MOFs), popularly known as “dynamics” or “flexibility”, has become increasingly important because of its applicability especially in gas storage and separation. In general, flexible MOFs showing structural transformations in the presence of external stimuli, and having relatively stable intermediate phases, are useful for the selective trapping/capture of different guest molecules, either kinetically or thermodynamically. The research group led by Dr. Tapas Kumar Maji focused on synthesis of different types of flexible frameworks, and to study their structural dynamics, especially CO₂ uptake, small chain hydrocarbon (CH₄, C₂H₄, C₂H₆, C₃H₈) storage and separation. For example, in one of the reports created by the group, an in-depth investigation was made to find out multiple phase transitions in a flexible entangled framework based on different external stimuli such as temperature, pressure, and guest molecules. The various phases have been characterized by single-crystal structures and explained explicitly. In one of the group’s work, the dynamics of a redox-active flexible framework was explored for gas storage and separation. The research group also delineate the growth and stabilization of ultra-small (2–3 nm) MOF nanoparticles on a 2D layered amino clay template and utilize these composites for CO₂ storage and separation. Post-synthetic modification of pore surface by [2+2]cycloaddition reaction between host-guest has been reported that resulted high CO₂/N₂ selectivity compared to the unmodified framework.

Energy transfer/light harvesting: The design and synthesis of luminescent metal-organic complexes, polymers, or supramolecular frameworks are gaining interest as they find applications in molecular sensing, tunable emission for various light emitting devices, and light harvesting. Pyrene and anthracenemonocarboxylate chromophores based two metal-organic complexes have been synthesized which show Förster resonance energy transfer (FRET) process due to unique structural arrangement of linkers. In other work, the light-harvesting properties of two pyrenes based fluorescent dynamic conjugated microporous organic polymers have been explored. Interestingly, these polymers rapidly encapsulate various fluorescent chromophoric guests at room temperature and further investigated for energy transfer process.

Magnetism: Stimuli-responsive molecular switches are of tremendous importance from both fundamental and application point of view. Guest responsive magnetic bi stability involving phase transitions, change in T_c and guest-dependent spin-crossover have been explored in magnetic coordination compounds, as they can be ideal switches owing to their tunability and flexibility. Hetero-metallic clusters and 2D coordination polymers for magnetic studies were also undertaken.

Mechanochromism, liquid crystallinity and self-cleaning behaviour in MOF: The research group also worked on design, synthesis, of a new multifunctional π-conjugated oligo-(p-phenyleneethynylenes) (OPEs) based frameworks. The inherent π-conjugation of OPE based linkers imparts luminescence to the system and structural flexibility brings in mechanochromism property. By suitable functionalization of side chain self-cleaning property was also realized in nano scaleope-based metal-organic framework.

Hydrogel/Organogel and their properties: In recent times, significant attention has been paid to the development of functional coordination polymer gels (CPGs) from rationally designed low molecular weight gelators (LMWGs) and metal ions. The research group has recently focused on the coordination of polymer gels and studied their photophysical and catalytic properties. Removal of heavy metal ions from aqueous solution was also studied.



Dr. Sridhar Rajaram (Polymer Lab)

Biodegradable polymers are a class of materials that have found applications in drug delivery and in biocompatible stents. Currently, the material of choice was the polymer of lactic acid which is an α -hydroxy acid. The limited structure tenability of poly(lactide) has led to the search for other biocompatible polymers. In this context, the possibility of living polymerization of β -hydroxy acid was explored. Cyclic monomers that can polymerized with nucleophilic catalyst have been synthesized and the nucleophilic ring opening polymerization of these materials is currently being attempted.

In another project, focus was on the development of dendritic materials for the efficient quantification of low viral loads in HIV infected individuals. Attachment of Raman markers to dendrimers is expected to enable the enhanced viral RNA using SERS technique.

Recently, a cyanide free synthesis of amino acids was developed using a carbonate as a source of carboxyl group. Transformation of the carbonate to a carboxyl group was accomplished via the use of a nucleophile. The research group shown that this nucleophilic activation of carbonates is dependent on cation- π interactions. Currently, new reactions using this approach is under development.

Dr. Sarit S. Agasti (Molecular Design Lab and Nanoscopic Lab and Biomolecular Lab)

The primary research focus of this lab was oriented towards engineering small molecules and programmable molecular materials to address challenges in bioimaging and create novel approaches for diagnostic sensing and therapeutic delivery. In the field of bioimaging, it has been a challenging task to visualize biomolecules at nanoscopic resolution (~ 10 - 20 nm) as well as to track them while they function inside the cells. Over the last one year the lab has worked towards developing new techniques along with generating compatible molecular probes so that the diffraction limit (~ 200 - 300 nm) of light microscopy could be overcome and molecules inside cells are localize in nanometer precession. In addition, the research group was integrated an important feature with this imaging technique, i.e., the ability to simultaneously image and quantitate 100s of target molecules from a single cell. The goal of this group was to ultimately utilize these potentially transformative features, nanaoscopic, quantitative and ultra-multiplexed imaging, to address various biological questions. For example, going forward efforts would to understand the system level changes in synaptic protein compositions and their distribution during aging of neuronal system. Progress achieved towards this goal is highlighted below.

The research group is in process of developing a novel method for super-resolution imaging that combines click chemistry based specific and autonomous target labeling approach with single molecule localization technique. This technique was named **SISAC** (**S**uper-resolution **I**maging using **S**tochastic and **A**utonomous **C**licking). The method is comprising of two key chemical components: (1) Docking unit: a small bioorthogonal click tag that is attached to the target molecule, and (2) Imager unit: a fluorogenic 'Click-On' dye that stochastically assembles with the docking unit via a highly selective click cycloaddition reaction to produce single fluorescence emitter from the target molecule. The idea is to construct the final super-resolution image from high-accuracy single molecule localization of the fluorescent emitters that are autonomously switched ON (by click reaction with target molecule) and turned OFF (by photobleaching) within the sample. Bioorthogonal click tag and fluorogenic 'Click-On' dye being the pivotal components of this super-resolution imaging method, a significant effort was dedicated towards developing these components. Now, the research group has successfully synthesized 1,2,4,5-tetrazine based bioorthogonal click tags. Studies showed that these molecules could undergo spontaneous strain promoted cycloaddition reactions with strained alkenes in biological environment. A series of fluorogenic 'Click-On' dyes has also been synthesized by taking advantages of efficient tetrazine quenching via through-bond energy transfer (TBET) and Förster resonance energy transfer (FRET) mechanism. *In vitro* bench marking of the SISAC imaging method using synthetic DNA-origami nanostructure and translation to live cell setting is underway.

In another approach, work has been undertaken towards generating programmable DNA based molecular probes for super-resolution imaging. The idea is to utilize the transient and specific binding of fluorescently labeled short oligonucleotides (9-10 NT) with the complementary docking strands to obtain programmable and stochastic switching between fluorescence ON and OFF states for single molecule localization based super-resolution imaging. Utilizing this approach, currently the research group can obtain 8 colors super-resolution images from fixed cells. Next, this capability would be extended to 100 targets imaging by synergistically combining DNA barcoding of cellular proteins with DNA-based super-resolution imaging. Concurrently, the group is working towards translating this imaging method in more complex biological system (*e.g.* in neuronal system). Preparation of a manuscript to report a part of this study is also underway.

The second part of research activities of this Laboratory has been directed towards developing stimuli responsive Drug Delivery Systems (DDSs) that minimizes side effects and enhance the efficacy of conventional pharmaceutical agents. The research group is exploring two concepts for this purpose: 1) Supramolecular interaction mediated actuation of therapeutic delivery system, and 2) Light actuated materials for spatiotemporally controlled drug release. An important feature that is intended in the design of these delivery systems is the capability to have an integrated sensing platform to allow understanding of therapeutic outcome. Highlight of research progress towards this goal is given below.

Supramolecular chemistry provides a versatile tool for assembling molecular components into functional structures and actuation of these assemblies for myriad applications. The reversibility of association between complementary molecular components enables numerous mechanisms for modular assembly and disassembly. Harnessing this concept, the research group has generated a functionalized gold nanoparticle based system that showed the ability to undergo supramolecular recognition mediated assembly and disassembly process. An important feature of this system is that in the assemble state it can incorporate various drug molecules. These drug molecules can then be released in the cells upon nanoparticle disassembly processes, mediated by the supramolecular trigger. In addition, given the generation of 'hot spots' during assembled state, this system is also currently under investigation for reversible SERS sensors application. Preparation of a manuscript to report this study is underway.

Delivery of drug in a spatiotemporally controlled fashion can serve to minimize side effects and increase its chemotherapeutics efficiency. In this respect, light, being a highly orthogonal external stimulus represents a distinctive way of controlling site- and time-specific delivery of pharmaceuticals. A light responsive charge switchable gold nanoparticle has recently been synthesized. Next, efforts are on to test if these nanoparticles are efficiently taken up by the cancer cell upon light trigger. This will enable delivery of drug molecules in a spatiotemporally controlled fashion.

Nanoparticle-stabilized capsules (NPSCs) represent a kind of microcapsule structural motifs whose shell consists of nanoparticles assembled at the interface of immiscible solvent droplets. Recently, the research group has succeed to develop two new strategies to fabricate NPSCs: 1) Bioorthogonal tetrazine cycloaddition mediated assembly at oil–water interface, and 2) Host-guest recognition mediated assembly of colloidal microcapsules using Cucurbituril 7 (CB[7]) host. Studies showed that these NPSCs have unique ability of simultaneous encapsulation of unmodified small molecules as well as macromolecular cargo (*e.g.* proteins) for co-delivery purpose. Preparation of a manuscript to report this study is underway.

New programmes launched during the year:

1. Work has been started in the domain of large area Photocurrent scanning Technique Development and development of organic Perovskite Devices. (**Prof. K S Narayan**)
2. Molecular biology facility: The molecular biology facility has a set of basic equipment for carrying out molecular biology related and DNA nanotechnology based work. This facility includes thermal cyler, horizontal and vertical gel electrophoresis system, and temperature-controlled centrifuge. (**Dr. Sarit S Agasti**)



3. Tissue culture facility: establishment of a tissue culture lab is in progress that will have the facility to allow culture and processing of human and other eukaryotic cells for variety of biological experiments: biosafety cabinet, CO₂ incubators, fluorescence microscope with phase contrast, fluorescence and digital camera, temperature-controlled centrifuge, liquid N₂ storage, -80°C freezer, -20°C freezer, 4°C freeze, vacuum pump, water bath, stir-hotplate. **(Dr. Sarit S Agasti)**
4. Confinement induced laser-like emission from GaNnanowall network. **(Prof. S M Shivaprasad)**
5. Evaluation of GaN nanostructure as Transparent Conductor. **(Prof. S M Shivaprasad)**
6. A new area of research has been initiated on inorganic-organic hybrid materials for multifunctional properties. **(Prof. A Sundaresan)**
7. New research activities have been initiated on the design and synthesis of new electrocatalyst (Co/Co₃O₄ or Fe/Fe₃O₄@carbon) on MOF derived materials. Currently studies are carried out in their catalytic activities towards oxygen reduction reactions (ORR), oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). Proton conductivity in MOFs and metal-organic cube gels for fuel cell applications. **(Prof. Tapas Kumar Maji)**
8. The light scattering group is involved in developing new MOFs, dendrimer structures for Raman markers and high pressure x-ray diffraction studies using Synchrotron sources. **(Prof. Chandrabhas Narayana)**

Following are the members of the Unit:

Chair

Chandrabhas Narayana Ph D, F N A Sc

Professors

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

S Balasubramanian Ph D, F A Sc

K S Narayan Ph D, F N A Sc, F A Sc.

G U Kulkarni Ph D

Chandrabhas Narayana Ph D

S M Shivaprasad Ph D

A Sundaresan Ph D

M Eswaramoorthy Ph D

Associate Professor

Tapas Kumar Maji Ph D

Faculty Fellow

Sarit S Agasti Ph D, jointly with NCU

Technical Officers

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

Technical Support

N R Selvi

Research students

A.Z. Ashar, Abdul Azeez H., Abhijit Chatterjee, Abhijit Sen, Abhiroop Lahiri, Anaranya Ghorai, Anirudha Mirmira, Ankush Kumar, Apoorva Singh, Arpan De, Ashutosh Kumar Singh, Avula Venkata Siva Nikhil, Badri Vishal, Bharath B., Brijesh, C. S. Deepak, Chaitali Sow, Chandan De, Chandan Kumar, Devendra Singh Negi, Dheeraj Kumar Singh, Divya C., Ganesh N., Gopalakrishnan K, Janaky S, Kompella V. K. Srinath, Korlepara Divya Bharathi, Koushik Pal, Lakshay Dheer, Manodeep Mondal, Meenkshi Pahwa, Momin Ahamed, Narendra Kumar, Navneet Singh, Nijita Mathew, Nikita Gupta, Niloyendu Roy, Nimish D., Nivedita Sikdar, Papri Sutar, Parul Verma, Pavitra Nityanand Shanbhag, Pragya Arora, Prashant Kumar, Priyanka Jain, Raaghesh A.V, Raagya Arora, Rajendra Kumar, Rajendra Singh, Rajib Sahu, Ravi Shankar P. N., S. Kiruthika, Sanjay Kumar Nayak, Shantanu Aggarwal, Sharona Thomas Horta, Shashank Chaturvedi, Shivani Grover, Shivaram B. Kubakaddi, Sisir Maity, Sohini Bhattacharyya, Somnath Ghara, Sonu K.P, Soumita Chakraborty, Sreedhara M.B, Srimayee Mukherji, Subhajit Laha, Suchitra, Sudip Das, Sukanya Das, Sunita Dey, Swathi, Syamantak Roy, Tarandeep Singh, Usha Manjunath Bhat, Uttam Gupta, V. Rajaji, Yanda Premakumar



EDUCATION TECHNOLOGY UNIT (ETU)

Activities and Achievements

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

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

The CNR Rao Education Foundation in association with the CNR Rao Hall of Science and ETU, JNCASR started a 'STUDENT MENTORING PROGRAM' in May 2016. The broad objectives of this programme are to give an opportunity to selected students to witness how research is conducted and how laboratories work through providing academic support to prepare for their forthcoming and other competitive exams and solve their difficulties in science and math subjects. It is proposed to achieve this by close interaction between the students and mentors. The mentors for the programme are a team of dedicated faculty members and student volunteers of JNCASR.

In the programme, eight students were selected after their Xth standard examinations to spend a month in summer (May 2 – 27, 2016) staying at the JNCASR campus. The students visited the campus again in October (October 13- 21, 2016) for a week. During their stay at JNCASR, the students learnt concepts broadly based on the CBSE/ICSE syllabus in all the subjects. In addition to the lecture classes, they participated in tutorials where they had interactive sessions with mentors for better understanding. They were given assignments and were evaluated. They conducted experiments in the laboratories, were given study materials and books that could help them in their preparation for exams and in the long term will motivate them to take up science as a career.

On June 14, 2016, JNCASR, ICMS in collaboration with the CNR Rao Education Foundation presented the National Prizes for Research in Energy Materials and Devices (Donated by AVRA Laboratories, Hyderabad) to Prof. K.S. Narayan (JNCASR) and Dr. K. Vijayamohanan Pillai (CSIR- Central Electrochemical Research Institute, Karaikudi). Prof. Sir Richard Friend presented the award and felicitated the awardee. Prof. V. Nagaraja Presided over the function. ETU collaborated with ICMS in organising and conducting the programme.

The CNR Rao Hall of Science and ETU organized a meeting of the Resource Persons on July 4, 2016, to decide the Teachers/students program schedule for the year 2015-2016. The meeting was chaired by Prof. C.N.R. Rao. Prof. Rao mentioned that the CNR Rao Education Foundation is exploring the possibility of conducting science outreach programs in North Karnataka like the one being done in Uttarakhand. At the meeting, following programmes were planned: two lecture programmes each in Physics, Chemistry, and Biology; a chemistry program to be conducted jointly with New Chemistry Unit, one for X class students and one for Classes XI & XII. It was also proposed to have a lecture program exclusively for X class students and a 'Celebration of Science' programme for the National Science Day.

ETU collaborated with Prof. C.N.R. Rao in designing, formatting and editing the print-ready copy of a book 'A Life in Science' authored by Prof. C.N.R. Rao. It was published by Penguin Books India. The book was released on November 4, 2016, at the 82nd Annual Meeting of the Indian Academy of Sciences held at Indian Institute of Science Education and Research, Bhopal. Prof. Ram Ramaswamy, President, Indian Academy of Sciences released the book. A book-release function was organized at the Faculty Hall, IISc on December 23, 2016. Justice Shivaraj Patil released the book and Dr. Kasturirangan presided over the function.

The Parliamentary Standing Committee on S&T, Environment and Forests visited the centre on August 29, 2016. As part of an exhibit where all units of the centre displayed posters of their work, ETU and CNR Rao Hall of Science designed and put up posters outlining the activities of ETU and highlighting the science outreach programs conducted by the CNR Rao Hall of Science and ETU at Madan Mohan Malaviya Amphitheatre and also the programmes conducted by Prof. C.N.R. Rao and Mrs. Indumati Rao at various places across the country. The honorable members led by Smt. Renuka Chowdhury, the Chairperson of the Committee, visited the Chemistry of Materials Exposition and Prof. C.N.R. Rao Archives.

At the NAAC Review Committee meeting held on December 6, 2016, Prof. V. Krishnan presented the objectives and achievements of ETU. Mrs. Indumati Rao spoke about the science outreach programmes organised and conducted at the CNR Rao Hall of Science and at various other places in the country, the SOP-POCE laboratory, and its programmes.

Organisation of Programmes

The Summer 2016 Science Outreach Programme sponsored by the CNR Rao Hall of Science, JNCASR was conducted in association with Himalayan Gram Vikas Samiti, Gangolihat and supported by the CNR Rao Hall of Science. The Science Outreach Programme was conducted at Dashaithal, Gangolihat, Pithoragarh, Uttarakhand during May 11-13, 2016 by Prof. K. S. Valdiya, 150 students and teachers from various schools participated in the programme. On May 11, 2016 Prof. Rao delivered the lecture 'Celebration of Chemistry' at Gangolihat. On May 13, 2016 Prof. Rao gave the lecture titled 'Can India become a global leader in Science Education' at Nainital. Faculty Members from JNCASR participated and delivered lectures in the programme. The Autumn Science Outreach Programme was conducted during November 2016.

On June 6 & 7, 2016, ETU presented a one-hour multimedia presentation from the CD-ROM 'NANOWORLD' and the CD-ROM 'A brief history of chemistry' by Prof. Rao was presented to POCE students. The participants visited the Chemistry of Materials Exposition and the Prof. CNR Rao Archives.

The CNR Rao Hall of Science and Education Technology Unit conducted nine lecture programs for students and teachers during 2016-2017. In addition to the planned programmes, a 10-day orientation programme (Chetana program) for SSLC toppers was conducted. The CNR Rao Hall of Science, CNR Rao Education Foundation in association with School Chandan, Laxmeshwar, Gadag jointly organised and conducted a Science Outreach programme at Laxmeshwar. A three-day special lecture program for Chandan School students (Gadag) was conducted at the MMM Amphitheatre, CNR Rao Hall of Science.

The CNR Rao Hall of Science and ETU commenced the Teachers-students programs/workshops conducted under the auspices of the Science Outreach Program for this year on June 30, 2016. The recipients of the CNR Rao Education Foundation sponsored 2015 prizes for Outstanding Science Teachers were Shri. Purandaranarayana Bhat K. and Shri. Sanjay Kumar Srivastava. The Lecture Program had one lecture in Physics and one in Biology. The titles of the lectures are:

- Making Heat Engine out of Bacteria by Prof. Ajay Kumar Sood (IISc., Bangalore),
- Autophagy to the rescue of neurodegenerative diseases such as Parkinson's by Dr. Ravi Manjithaya (JNCASR., Bangalore).

Around 200 students and teachers attended the program.

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

- June 30, 2016 – Lecture Program (Science Teacher Award Function)
- July 22, 2016 – Program in Physics for students'



-
- August 23, 2016 – ‘Program in Chemistry for students’
 - October 17-27, 2016. - ‘Chetana Program’ (Orientation Program for State SSLC toppers)
 - November 9, 2016 - ‘Program in Biology for students’
 - December 5, 2016 – ‘Program in Chemistry for students’
 - January 20-22, 2017 – Science Outreach Program at Laxmeshwar, Gadag
 - February 27 – March 1, 2017 – Special Lecture Program
 - February 28, 2017 – National Science Day Program

In many of the above programs over 200 students and teachers participated. All the above programs consisted of lectures and some demonstrations followed by an interactive Question and Answer session. All the above programs were organized and conducted by CNR Rao Hall of Science & ETU under the auspices of the Science Outreach Program.

The SOP-POCE lab conducted workshops on doing experiments using the College Chemistry Kit for college students on September 1, 14 & 15, 19 and 20 and on November 8 and 28. In some of these programmes, Mrs. Indumati Rao gave the lecture “A tribute to Michael Faraday” to the students. The students visited the Chemistry of Materials Exposition and Prof. CNR Rao Archives. The students were from different colleges.

The CNR Rao Hall of Science & ETU organized and conducted the programme ‘Chetana’ in collaboration with the Department of Information Technology Biotechnology and Science & Technology, Karnataka Govt. at JNCASR from October 17-27, 2016. The program was specially organized only for Girls who are SSLC toppers with the aim of exposing them to latest trends in science and to encourage them to make a career in science. The 10-day program comprised of lectures in Physics, Chemistry, Biology and also on basics of computers, Career options in science and Opportunities in rural sector. There was a Science Quiz, Multimedia Presentations, Laboratory work using college chemistry kits, Demonstration of experiments and Lab. tours. There was an interactive session with Prof. C.N.R. Rao participated by 31 students, and two coordinators. At the Concluding Session, Mrs. Indumati Rao, Prof. V. Nagaraja, and Dr. Maulishree addressed the students. The students were given complimentary copies of the book ‘Climbing the Limitless Ladder’ and ‘Chemistry Today’ from ETU, JNCASR along with the certificate of participation.

On 16 December 2016 Tibetan undergraduate students pursuing life sciences and chemistry at different colleges across the country visited the CNR Rao Hall of Science, JNCASR. The visit of 25 students along with their coordinators was part of a three-day Tibetan Science Conclave held at Bengaluru. The CNR Rao Hall of Science & ETU arranged for a tour of the laboratories at ICMS, NCU, CPMU. In the afternoon, they visited laboratories at MBGU and the Chemistry of Materials Exposition and Prof. C.N.R. Rao Archives.

On 11 January 2017, 75-80 primary school teachers of Govt. Schools (from Bengaluru) visited the CNR Rao Hall of Science. A lecture program was organised and they visited the Chemistry of Materials Exposition and Prof. CNR Rao Archives.

The CNR Rao Hall of Science, CNR Rao Education Foundation in association with School Chandan, Laxmeshwar, Gadag jointly organised and conducted a Science Outreach program during 20-22 January 2017. 450 students and teachers participated in the three-day program where Prof. CNR Rao addressed the students and teachers followed by Multimedia presentation of excerpts from the CD-ROM ‘Understanding Chemistry’ by Mrs. Indumati Rao. Several Faculty from JNCASR delivered lectures, demonstrated various experiments in physics and chemistry and interacted with the participants during the programme.

CNR Rao Hall of Science & ETU, JNCASR worked with Parikrma (an NGO that educates street and slum children and runs four schools and a college for these children) in conducting the 'Parikrma Festival of Science' on 14-16 February 2017. The theme of the Science Festival this year was 'Soil and Agriculture'. Prof. C.N.R. Rao, Prof. Richard Zare, Mr. Pradeep Dutt inaugurated the festival and addressed the students. Prof. V. Nagaraja, Mrs. Indumati Rao, Ms. Audrey Kitagwa were the other distinguished invitees. Over 220 students from 42 schools and 80 teachers and volunteers participated in the event held at the CNR Rao Hall of Science, JNCASR. The teachers participating in this program visited the 'Chemistry of Materials Exposition' and 'Prof. CNR Rao Archives'. The CNR Rao Hall of Science and ETU gave the students the books Learning Science Part 1 to the students and Mrs. Indumati Rao addressed the students and teachers on February 16 and gave away Learning Science books (Set of 4 Parts) to the teachers.

A 'Special Lecture Program' was organized and conducted for School Chandan, Gadag, Laxmeshwar. Fifty students and three teachers participated in the three-day program organized and conducted by the CNR Rao Hall of Science & ETU during February 27 –March 1, 2017. The students conducted experiments at the POCE laboratory. Mrs. Indumati Rao delivered the lecture 'A tribute to Michael Faraday', followed by a Quiz program. The students participated in the National Science Day program conducted at the CNR Rao Hall of Science on February 28, 2017. On March 1, 2017 Faculty from JNCASR delivered lectures in Chemistry and Physics with Q&A session. Dr. N. S. Vidhyadhiraja demonstrated simple experiments in Physics along with the lecture. This was followed by a visit to the Planetarium.

CNR Rao Hall of Science and ETU, JNCASR organized the National Science Day Program on February 28, 2017. The participants invited to celebrate the National Science day at JNCASR were students and teachers from Jawahar Navodaya Vidyalaya, Bangalore Urban and Bangalore Rural, Doddaballapur and from School Chandan, Laxmeshwar, Gadag. Over 150 students and teachers participated in the event. Prof. Maneesha Inamdar, Dean, Fellowships and Extension Programmes welcomed the gathering. Prof. V. Nagaraja, President, JNCASR addressed the students and teachers. Prof. S. M. Shivaprasad delivered the lecture 'Small Questions and Big Answers'. A 'Science Quiz' was conducted by NCU students. Mrs. Indumati Rao addressed the students and gave away the prizes to the three winning teams. There were experimental demonstrations by NCU students and Faculty. They visited various laboratories and the Chemistry of Materials Exposition and Prof. CNR Rao Archives.

Following are the members of the Unit:

Chair

Prof. V. Krishnan PhD, FASc, FNA, FTWAS

Coordinator (Hon.)

Indumati Rao MA, MS, CE

Technical Officer

Jatinder Kaur M.Sc.

Multimedia Asst.(Hon.)

Sanjay Rao BSc, Cert. Multimedia



ENGINEERING MECHANICS UNIT (EMU)

Research Activities and Achievements

Engineering Mechanics Unit pursues research on a variety of topics in the general areas of fluid mechanics and thermal science. Work done in the Unit encompasses those relevant to technological applications and phenomena encountered in nature.

(a) **SankhyaSutra Labs:** On the technology front, the first startup *SankhyaSutra Labs* set up by the EMU faculty Dr. Santosh Ansumali, is on the way to securing an International client from Japan for simulating transport-processes in semiconductor manufacturing.

(b) **Dynamics of Two-Dimensional Turbulent Shear Flow:** It has been demonstrated that a vortex gas model for a spatially evolving 2D turbulent free shear flow yields a universal growth rate that is in surprisingly close agreement with data from high Reynolds number experiments. This agreement is considered significant as the model is extremely simple and very easy to code for a parallel computer. The results for the growth of the shear layer appeal only to one dynamical principle, namely Kelvin's theorem which ensures that the circulation around each point vortex is conserved, and uses only one mathematical tool, namely the Biot-Savart relation. Work on the linear and non-linear instability of free shear layers has shed much light on the mechanism of layer growth, from the emergence of coherent structures to their evolution and merger, and the role of Kelvin-Helmholtz as well as the Karman-Ruback-Lamb monopole instability of the layer.

(c) **Numerical Simulation of Flow around Gas Turbine Blade:** Work on the large gains achieved by the use of GPUs in combination with CPUs (Maruthi et al. 2017) won the Best Paper Award at a recent Symposium at IISc on Computational Science. This will help better simulation and design of aircraft gas turbine blades.

(d) **Establishing a Test facility for evaluating DRP:** Through a project, a test facility was designed and established at HPCL green Campus, Bangalore to evaluate the performance of Drag Reducing Polymers. Facility can quantify and compare performance of different polymers and estimate aging/polymer breakdown while in a pumping loop.

(e) **Numerical Simulation of Diabatic Plumes:** The first results of the DNS simulation of a transient diabatic plume, which offers a low-order model for cumulus cloud flows, have been obtained. Preliminary assessments of the results are very promising.

New programmes launched during the year

A new faculty member, Dr. Diwakar SV joined the Unit this financial year. His area of expertise is interfacial dynamics, mixing under micro-gravity condition, coupled two layer Rayleigh Benard convection.

New research activities include, Research project entitled, "Energy efficient polyhouse and aeroponic system for mini tuber production of tissue cultured potato" under the National Agricultural Science Fund (NASF) in collaboration with IISc, Bangalore; JNCASR Bangalore; UAS, Bangalore; Indian Agricultural Research Institute, New Delhi and Central Potato Research Institute, Jalandhar.

Research Project titled "Project titled "Experimental characterization of dissimilar mode coupling in two-layer Rayleigh-Bénard-Marangoni Systems", funded by SERB, Government of India.

On the broad topic of Complex fluid and Rheology various aspects of suspensions were explored, including (a) Bacterial suspensions: Fluctuations, correlations and rheology, (b) Stability of viscoelastic shearing flows, (c) Effects of inertia on the motion of non-spherical particles, (d) Swimmer motion in a stratified fluid medium: the biogenic contribution to ocean mixing and (e) The micro-hydrodynamic two-body problem.

In the area of Turbulent flows, simulation of Vortex gas, stability theory of coherent structures in mixing layers; structure and evolution of cloud flows; further GPU+CPU DNS studies on gas turbine blade flows are being pursued.

The following are the members of the Unit:

Chair

K R Sreenivas Ph D

Professors

K R Sreenivas Ph D

Meheboob Alam Ph D

Associate Professors

Ganesh Subramanian Ph D

Santosh Ansumali Ph D

Faculty Fellow

Diwakar S Venkatesan Ph D

Research Students

Aghor Pratik Prashant, Albin Prince John, Arun Kumar Varanasi, Biswadeep Roy, K. Siddharth, Mahan Raj Banerjee, Manjusha Namburi N L D B, Mayank Toprani, Mohammad Atif, Mohammad Raifuddin, Nishant Soni, Piyush Garg, Prashanth Ramesh, Prateek Anand, Praveen Kumar K, Pulkit Kumar Dubey, Rama krishna Rongali, Ronak Gupta, Saikat Saha, Samarth Agrawal, Sankalp Nambiar, Shashank H J, Shaurya Kaushal, Sunil V Bharadwaj, Swastik Hegde, Vybhav G R



EVOLUTIONARY AND INTEGRATIVE BIOLOGY UNIT (EIBU)

During the year 2016-2017 the faculty of EIBU (erstwhile EOBUE) continued to conduct research in the broad areas of animal behavior, phylogeography, chronobiology, evolutionary genetics, neurogenetics, neurodegenerative disorders, and population dynamics. Questions in the areas of (a) Asian elephant socioecology and behaviour, (b) simulation and field studies of population size and sex ratio estimation, and (c) foundational problems in evolutionary biology (d) comparative neurobiology - across sympatric species on neuronal underpinnings for differences in rhythmic behaviours, (e) interactions between circadian clocks and sleep homeostat, (f) progression of neurodegenerative disorders using flies, (g) neuronal circuits underlying thermosensory modulation of rhythmic behaviours, (h) evolution of circadian rhythms in nature, (i) evolution of adaptations to crowding, especially the interplay of food deprivation and waste buildup, (j) fruit fly metapopulation dynamics and stability, (k) life history evolution, (l) neurogenetic basis of circadian egg-laying rhythm in fruit flies, (m) connection between circadian clocks and life history traits, (n) molecular-genetic regulation of morning and evening chronotypes (o) social organization and circadian clocks in three ant species, have been addressed.

The Unit also continues to train personnel through the Ph.D. and M.S. programmes, through participation of the faculty in POBE and SRFP programmes of the JNCASR as well as similar outreach programmes run by the three Indian Science Academies and by DST and KVPY.

Research Progress

Long-term selection experiments on rapid development and adaptation to larval crowding continued during the year. New results include the evidence for different ecological conditions promoting the evolution of hard-wired versus phenotypically plastic feeding rate responses under crowding. The evolution of lower levels of sexual conflict in rapidly developing selected populations has been shown to be due to an interplay of breeding ecology and body size reduction. An agent-based simulation framework for studying the ecology and evolution of crowded *Drosophila* cultures has been developed.

Work on the social structure of female and male Asian elephants was continued in Nagarhole and Bandipur National Parks. Extensive analysis comparing social structure in this population with that of a population of a different genus of elephant, the African savannah elephant in Samburu suggested that there were underlying similarities in the social structure of the two genera, and the differences in social organization could be largely attributed to group size differences because of the differences in habitat.

Analyses of social structure and group size across seasons showed the importance of basing such analyses on female clans rather than at the population level. It was also found that fission-fusion dynamics may allow for increased sociality under conditions of a constraint on group size, rather than serving as a means of increasing or decreasing group size in response to resource availability, as generally thought.

A visual method of estimating plant species cover was found to be a useful proxy for estimating biomass in a tropical forest with multiple vegetation strata, which is useful in assessing forage availability of herbivores in such forests. This is particularly useful when food species form a small proportion of all vegetation available, as is usually the case for elephants in tropical forests.

Using individual-based simulations, the effect of social structure on bias in mark-recapture population size estimation was studied. A framework to examine how group size distributions could arise based on different rules of resource use and dominance between social groups was set up.

Working on foundational topics in evolutionary biology, along with other labs in the country niche construction was explored in great detail. Why niche construction is not as central to evolutionary theory as natural selection was explained.

Ongoing studies to examine the connections between the circadian pacemaker and the sleep homeostat using the fruit fly *Drosophila melanogaster* demonstrate a time-of-day dependent homeostatic efficiency for recovery sleep, post sleep deprivation. A functional role has been shown for a known circadian clock output molecule namely Pigment Dispersing Factor Receptor (PDFR) in mediating sleep levels in a time-of-day dependent manner. Putative downstream targets of PDFR action have been identified in modulating sleep levels as being via a subset of dopaminergic neurons in the central brain of flies. Evidence has been shown for a fitness value for sleep through examining the effect of sleep deprivation on reproductive output of female flies.

Studies demonstrate that expression of pathogenic human Huntingtin (HTT) in *Drosophila* circadian neuronal subset ventral lateral neurons (LN_v) results in loss of the neuropeptide pigment dispersing factor (PDF) only from soma of small LN_v (sLN_v) and an associated arrhythmicity in circadian locomotor activity in constant darkness (DD). Surprisingly, despite loss of PDF and central circadian protein Period (PER) from LN_v, circadian oscillations of PDF persist in axonal termini of sLN_v. Moreover, synchronised molecular clock oscillations are also detected among downstream circadian neurons. Temperature regimes was uncovered under which pathogenic HTT phenotypes are rescued both in terms of locomotor behaviour and neuronal features. A genetic screen for modifiers of pathogenic Huntingtin phenotype, it was shown that molecular chaperone HSP40 provides a stronger rescue of pathogenic HTT phenotypes than HSP70.

Preliminary results from this lab suggest the role of neurotransmitter serotonin in behavioural entrainment to thermal cycles. Serotonin receptors modulate different aspects of clock-controlled rhythmic behaviour under thermal cycles, such as, entrainment, suppression of activity during mid-day and appropriate phasing of activity. Putative regions in the fly-brain was identified that may be involved in modulating a specific temperature dependent rhythmic behaviour that appears to be adaptive - suppression of mid-day activity under thermal cycles. Studies also indicate that under constant warm temperatures and cycling light conditions, the combined action of subsets of circadian pacemaker neurons and *dTRPA1* expression determines the appropriate phasing of rhythmic behaviour.

The underlying circadian clock properties of fruitfly populations that have been reared in constant darkness or constant light for over 300 generations were subjected to a detailed characterization of circadian clock properties using adult emergence, activity-rest and oviposition rhythms circadian behaviors. Interestingly, populations kept in constant darkness appear to have evolved a higher power of activity-rest and emergence rhythms. These results appear to negate the notion that if circadian clocks have evolved only to synchronise with the external environment and will regress in organisms that live under constant conditions and been used to support the intrinsic adaptive advantages conferred by circadian clocks. These populations have also evolved higher circadian photosensitivity possibly due to weaker oscillator coupling. A separate study aimed at assessing the evolution of circadian rhythms in populations of *D. melanogaster* maintained under semi-natural conditions in comparison to their laboratory LD12:12 counterparts. This is a unique system, which most likely does not exist anywhere in the world. Initial results suggest that the semi-natural populations exhibit higher power of rhythm and higher accuracy of entrainment as compared to their LD12:12 counterparts.

Studies using long term selection for early and late phase of emergence leads to divergent evolution of molecular circadian clocks and individuals with advanced and delayed phase-of-entrainment (chronotypes) are associated with a similar advanced and delayed phase of entrained molecular oscillation of core clock genes, and propose that such differences in entrained molecular oscillations might drive an advanced or delayed expression of output components and other downstream factors thereby driving different phases-of-entrainment. Furthermore, in accordance with the previously reported behavioural differences divergent phase-of-entrainment was associated with the coevolution of differential photosensitivity and coupling of constituent oscillators which appear to be driven by photoreceptor *cryptochrome* and output molecule PDF



Evolution of life-history traits differences in independently evolving replicate populations of *D. melanogaster* exhibiting *early* and *late* emergence chronotypes suggested that the genetic architecture underlying emergence gate/emergence at specific times of the day (emergence chronotypes) is correlated with several life-history traits; and these correlations are mediated by both clock dependent and independent mechanisms. The difference in the assayed life-history traits of these populations appear to be correlated with altered sensitivity/differential interaction with the LD cycles.

The following are the members of the Unit:

In-charge Chair

V. Nagaraja Ph. D., F. A. Sc., F. N. A. Sc.

Chair (April-October 2016)

Vijay Kumar Sharma (Late) Ph. D., F. A. Sc., F. N. A. Sc.

Professor

Amitabh Joshi Ph. D., F. A. Sc., F. N. A. Sc., F. N. A.

Vijay Kumar Sharma (Late) Ph. D., F. A. Sc., F. N. A. Sc.

Honorary Professor

Raghavendra Gadagkar Ph.D., F.A.Sc., F.N.A., F.T.W.A.S.

Faculty Fellow

T. N. C. Vidya Ph. D.

Associate Faculty from Neuroscience Unit

Sheeba Vasu Ph. D.

Research Students

Abhilash Lakshman, Anuj Menon, Arijit Ghosh, Avani Mital, Dani Chitrang Kamal, Goirik Gupta, Hansraj Gautam, Keerthipriya. P, Kulkarni Rutvij Kaustubh, Manan Gupta, Manaswini Sarangi, Manishi Srivastava, Nandini R Shetty, Neha Pandey, Pavitra Prakash, Pritha Kundu, Revathe T, Satyabrata Nayak, Sheetal Potdar, Singh Viveka Jagdish, Srikant Venkitachalam, Vishwanath Varma.

GEODYNAMICS UNIT

Broad Areas of Research:

1. Tectonics and earthquake generation processes along the Himalaya.
2. Neotectonics and seismicity of the continental interiors.
3. Seismic processes along the Andaman-Nicobar subduction zone and Indian Ocean.
4. Tsunami hazard assessment along the western and eastern coasts of India
5. Holocene climatic evolution in the Himalaya and the role of winter westerlies.

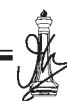
Activities and achievements

The work during the reporting period are mainly directed to gather data to gain understanding of tectonic and earthquake generation processes along the plate boundary regions of the Himalaya and Andaman Islands. The study areas also extended to Ladakh Himalaya. Two new study programs were initiated to understand the tsunami risk on the eastern seaboard of India (funded by *Board of Research in Nuclear Sciences, BRNS*). Another initiative was the study of '*Tsunami risk for the Western Indian Ocean: Steps toward the integration of science into policy and practice*' funded by Natural Environment Research Council, Global Research Fund, United Kingdom. Studies on the climate evolution during the Holocene (last 10000 years) using various geological proxies were also carried out. The program on earthquake generation along the Himalayan arc is funded by Ministry of Earth Sciences and the project on climatic evolution is supported by the Department of Science and Technology. The activities of the Unit members also included organizing science outreach camps in the Himalayan State of Uttarakhand.

As part of the studies on the earthquake generation and recurrence along the Himalaya, the focus of research was the Main Frontal Thrust in the central Himalaya that is to understand the previous occurrences of earthquakes-their timing and magnitudes. For that purpose, excavation was done at the frontal thrust near Chorgalia and Padampur on the foothills of Kumaun Himalaya, a stretch within the central seismic gap. The studies indicate a last massive earthquake (magnitude ≥ 8.5) in central Himalaya about 600 years ago. Considering the long period of quiescence and elapsed time a similar kind of great earthquake is due in the central Himalaya.

Studies on seismo-tectonics, plate boundary deformation and state of stress in the Andaman-Sumatra subduction zone and its vicinity are aimed at generating an understanding of the source processes of oceanic earthquakes, and their tsunamigenic potential. The studies on the long cores drilled from the Port Blair region helped in identifying about 10 previous tsunamis over the last 7000 years and the average recurrence period of 2004-tsunamis is 510 ± 140 years. Work continued at the crustal deformation in the Andaman region that involved collection of GPS data from permanent sites established in the Andamans. The region is now under a post-seismic visco-elastic relaxation phase. Although the subduction interface has become quiet since the great 2004 earthquake (Mw 9.2), the studies indicate that other areas like outer rise of the subducting Indian plate has become more active in terms of generating moderate to large earthquakes.

The climate changes have a significant impact in Himalayas, the higher peaks of these mountain are experiencing heavy snowfall during winters, rapid melting during summers and heavy rainfall and cloud bursting during summer monsoon. The northwest Himalaya receives 70-75% of its annual precipitation due to Indian summer monsoon (ISM) and almost 25-30% is received during winters mostly in the form of snow in higher altitudes by eastward moving extra-tropical cyclone called "western disturbances" or "westerlies". They play an important role to sustain the Himalayan glaciers and to recharge the ground water distribution in the foothills. The past 5,000 yr are characterized by a number of abrupt climatic changes and rapid warming which provides a valuable



opportunity to study this period using proxy data. Researchers of this Unit have cored 8 meters in Wular Lake in Kashmir Himalaya to retrieve the cores to understand the past climatic variations in that region. Additionally, work has been carried out on the mineral chemistry of speleothems (natural carbonates in caves) with bearing on environmental and climate change science and nuclear energy related programs, in collaboration with the scientists in Bhabha Atomic Research Centre.

With the financial support of C N R Rao Hall of Science and C N R Rao Education Foundation (JNCASR), the science outreach program was organized in Uttarakhand in the month of November, 2016. Prof. K. S. Valdiya (Chair, GDU) along with other faculty members of JNC took the lead in the organization of this programme. Students and teachers from various inter-colleges from different districts of Uttarakhand participated in these camps.

Following are the members of this Unit:

Chair & Honorary Professor

K. S. Valdiya Ph D, FASc, FNA, FNASc, FTWAS

Senior Associate

C P Rajendran Ph D

Research Scientist

Jaishri Sanwal Bhatt Ph D

Research Associate

K Anandasabari Ph D

Research Assistant

M. Suresh Kumar

INTERNATIONAL CENTRE FOR MATERIALS SCIENCE (ICMS)

The International Centre for Materials Science (ICMS) has emerged as one of the leading facility in the country for high impact interdisciplinary research. The excellence of faculty and students has created a progressive environment. The various research fellowship programmes and post-graduate diploma programme have been progressing as envisaged. The infrastructure and research facility has grown steadily. The High-Performance Computing facility and the H₂O splitting laboratory are fully operational. The ongoing research programmes are chemistry of materials, surface physics, soft condensed matter and low-dimension materials and other aspects of materials science. In addition to carrying out innovative research, ICMS has also organized seminars, schools and conferences in JNCASR and outside. ICMS has also financially supported conferences and workshops.

Objectives of ICMS:

The International Centre for Materials Science (ICMS), at the Jawaharlal Nehru Centre for Advance Scientific Research, is devoted to carry out high impact interdisciplinary research, promote collaborations, personnel exchange, organize discussions and meetings and promote education in Advanced Materials Science. ICMS was dedicated to the nation by Prime Minister of India Dr. Manmohan Singh on December 03, 2008. The Centre is financially supported by the Department of Science and Technology (DST), Government of India and directed by Prof. C.N.R. Rao, F.R.S.

A Memorandum of Understanding with Ras al Khaimah Centre for Advanced Materials (RAK-CAM) was signed on December 3, 2011 between Prof. A. K. Cheetham, F.R.S., Chairman, Scientific Advisory Board of RAK-CAM and Prof. M.R.S. Rao, President, JNCASR. The support provided by RAK-CAM has been used to establish the Sheikh Saqr Laboratory (SSL) in ICMS and to support various activities, lectures and fellowships.

Objectives of ICMS

- To facilitate in-house research of high quality in selected areas of materials science.
- To promote well-planned programme of collaboration in research and education with important centres and individuals in India and abroad.
- To provide opportunities to students as well as faculty through exchange programmes between ICMS and other centres.
- To conduct discussion meetings, schools and workshops.
- To organize Winter/Summer Schools on Materials Science.
- To provide visiting fellowships to teachers and young research workers from other institutions in India.
- To provide sophisticated instrumental and analytical services of the highest quality to facilitate materials research.

The Centre has established several collaborations and has signed Memorandum of Understandings with leading international research institutions such as Weizmann, SISSA, RMIT – Australia, Waterloo Canada, University of Manchester, under which there are constant exchanges of students and researchers along with frequent technical meetings and workshops. The Centre is a member of several International fora like EICOON, WMRIF and IUSSTF.

ICMS supports Ph.D. and M.S. degree programmes, short-term visits and offers Post-graduate Diploma in Materials Science. It offers Senior and Junior Fellowships under RAK-CAM Programme and also short-term visiting programmes. The students admitted by JNCASR under Ph.D. and M.S. programmes based on their performance in interviews also get an opportunity to use the state of the art facility, attend national/international



conferences, meetings and visit other universities under various collaborative and exchange programmes. Three students graduated under the two semesters (one year) Post Graduate Diploma in Materials Science programme. One student is currently enrolled in this programme.

The following is the list of special annual seminars series:

The International Materials Lecture is an annual lecture series by eminent scientists from all over the world. This series has also been well appreciated and successful. The Ninth International Materials Lecture was delivered by Prof. Clément Sanchez, Collège de France on September 29, 2016.

The **Annual Materials Lecture** initiated in 2011, is another annual lecture series delivered by eminent scientists from all over India. The Sixth Annual Materials Lecture was delivered by Prof. Sir Richard Friend, FRS, Cavendish Laboratory, Cambridge on June 14, 2016

The Sheikh Saqr Materials Lecture: The Sixth annual “Sheik Saqr Materials Lecture” delivered by Professor Martin Jansen, MaxPlanck-Institut für Festkörperforschung on December 5, 2016.

ICMS Seminar by Prof. Chennupati Jagadish, The Australian National University, Canberra on October 26, 2016 and Prof. Anderson, University of Manchester on January 20, 2017.

ICMS also organizes seminars, schools, workshops and conferences in collaboration with colleagues in JNCASR and elsewhere. ICMS has also sponsored various schools and workshops conducted by other organizations.

1. *International Workshop on Advanced Materials (IWAM 2017)*
Organized jointly with Ras-Al Khaimah Centre for Advanced Materials
Venue: Ras-Al Khaimah
Dates: February 19-21, 2017
2. *Winter School on Frontiers in Material Science*
Supported by SSL and University of Cambridge
Venue: JNCASR, Bangalore
Dates: December 5-09, 2016
3. *International Symposium on Solid State Chemistry (SSC 2016)*
Supported by SSL
Venue: JNCASR, Bangalore
Dates: December 1-3, 2016
4. *JNCASR and FCBS-Thiruvananthapuram Workshop*
Venue: Trivandrum
Dates: October 13-15, 2016
5. *12th JNC Conference on Chemistry of Materials, 2016*
Organized by: JNCASR
Dates: September 23-25, 2016
6. *Chemical Frontiers, CF 2016 in Goa*
Date: August 25-28, 2016
Organized by: IIT-Mumbai and JNCASR
Conveners: Prof. R. Murugavel and Dr. Ranjani Viswanatha
7. *International Workshop on Advanced Materials (IWAM 2016)*
Organized jointly with Ras-Al Khaimah Centre for Advanced Materials
Venue: Ras-Al Khaimah
Dates: February 21-23, 2016

8. *ICTP-JNCASR Advanced School on Nano, Structural and Single Molecule Approaches to Biology*

Date: January 11-16, 2016

Organized by: JNCASR

Conveners: Prof. M. Eswaramoorthy and Prof. T. Govindaraju

Sheikh Saqr Laboratory

The International Centre for Materials Science had established a close collaboration with the Ras Al Khaima Centre for Advanced Scientific Research (RAK-CAM) in 2007. The ties were further strengthened by signing of a Memorandum of Understanding in December 2011, to establish the Sheikh Saqr Laboratory at the ICMS of JNCASR, Bangalore. The Sheikh Saqr Laboratory in the New CCMS building was inaugurated by His Highness Sheikh Saud Bin Saqr Al Qasimi in 2013.

SSL infrastructure and research facility has grown steadily since 2013. The SSL and ICMS research facility together has fulfilled the objective as the country's leading research-intensive. The New CCMS building and the SSL laboratories won the NDTV - Design and Architecture Award under the Institutional Architecture Design of the Year for Education-2014.

The Sheikh Saqr Laboratory is headed by Prof. C. N. R. Rao, Director, ICMS. Prof. Anthony K. Cheetham, Chairman of RAK-CAM's Scientific Advisory Board, will hold the title Sheikh Saqr Distinguished Visiting Professor and the Faculty of ICMS and others working in materials science at JNCASR are associated with SSL. This grant also supports Research Associates, Technical Assistants and R&D Assistants.

RAK-CAM - Sheikh Saqr Fellowships

This programme was initiated in January 2008 with the support of grants from RAK-CAM and SSL to motivate the senior and junior scientist in materials science. The grants from RAK-CAM has been used not only to purchase equipment and chemicals, but also to support the research of young people and senior scientists. This fellowship programme has been very successful.

The following fellowships have been awarded to during 2016-17:

Sheikh Saqr RAK CAM Senior Fellow

Prof. Srikanth Sastry

Prof. Chandrabhas Narayana

Sheikh Saqr Career Award Fellows

Dr. Rajesh Ganapathy

Dr. Ranjani Viswanatha

Sheikh Saqr Student Fellows

Mr. K. Gopalakrishnan

Mr. S. R. Lingampalli

Ms. Sunita Dey

Mr. Uttam Gupta



RESEARCH ACTIVITIES

Prof. C. N. R. Rao

Prof. C.N.R. Rao's research group has initiated a few major programmes: one related to artificial photosynthesis involving photocatalytic oxidation of water by nanoparticles of Mn and Co oxides and the other on photocatalytic H₂ generation by hybrid nanostructures by using the Z-scheme. Synthesis, characterization and properties of anions substituted metal oxides and chalcogenides where in oxygen is replaced by nitrogen and fluorine or sulfur by phosphorus chlorine research on 2D materials specially phosphorene.

Prof. S.M. Shivaprasad

Polarization induced two-dimensional confinement of carriers in wedge shaped polar semiconductors:

A novel route to achieve two-dimensional (2D) carrier confinement in a wedge-shaped wall structure made of a polar semiconductor has been demonstrated theoretically. Tapering of the wall along the direction of the spontaneous polarization leads to the development of charges of equal polarity on the two inclined facades of the wall. Polarization induced negative (positive) charges on the facades can push the electrons (holes) inward for a n-type (p-type) material which results in the formation of a 2D electron (hole) gas at the central plane and ionized donors (acceptors) at the outer edges of the wall.

The theory shows that this unique mode of 2D carrier confinement can indeed lead to a significant enhancement of carrier mobility. It has been found that the reduced dimensionality is not the only cause for the enhancement of mobility in this case. Ionized impurity scattering, which is one of the major contributor to carrier scattering, is significantly suppressed as the carriers are naturally separated from the ionized centers. A recent experimental finding of very high electron mobility in wedge shaped GaN nanowall networks has been analyzed in the light of this theoretical reckoning.

Nanostructuring GaN thin film for enhanced light emission and extraction: Prof. Shivaprasad's group demonstrated that nanostructuring of GaN thin film significantly enhances the band-edge emission, due to structural and geometrical effects. Films of increasing roughness are formed by kinetic control in a PA-MBE system and their morphological, structural and optical properties are compared by complementary characterization probes. The nanowall configuration with largest pore size (≈ 215 nm) shows a two orders of magnitude enhancement of integrated PL intensity in comparison to a GaN epilayer. Finite difference time domain (FDTD) simulation is performed to explain the role of total internal reflection and scattering on light extraction. The extended defects terminate proximal to interface, leading to most regions of the nanowalls are defect free, enhancing light generation. The observation of broad HRXRD rocking curves is attributed to a mosaicity that originates due to mutual misorientation of the nanowalls. Thus, the low dislocation density in the nanowalls and their suitable geometry promotes high light emission and extraction, respectively, offering this nanostructure as a potential material for high brightness LED fabrication.

Electron mobility of self-assembled and dislocation free InN nanorods grown on GaN nano wall network template:

A kinetically controlled two-step growth process for the formation of an array of dislocation free high mobility InN nanorods (NRs) on GaN nanowall network (NWN) by Molecular Beam Epitaxy is demonstrated here. The epitaxial GaN NWN is formed on c-sapphire under nitrogen rich conditions, and then changing the source from Ga to In at appropriate substrate temperature yields the nucleation of a self-assembled spontaneous m-plane side faceted-InN NR. By HRTEM, the NRs are shown to be dislocation-free and have a low band gap value of 0.65 eV. Hall measurements are carried out on a single InN NR along with J-V measurements that yield mobility values as high as ≈ 4453 cm²/V s and the carrier concentration of $\approx 1.1 \times 10^{17}$ cm⁻³, which are unprecedented in the literature for comparable InN NR diameters.

Early stages of plasma induced nitridation of Si (111) surface and study of interfacial band alignment: a systematic study has been reported of the nitridation of the Si (111) surface by nitrogen plasma exposure. The surface and interface chemical composition and surface morphology are investigated by using RHEED, X-ray photoelectron spectroscopy, and atomic force microscopy (AFM). At the initial stage of nitridation two superstructures—"8×8" and "8/3×8/3"—form, and further nitridation leads to 1×1 stoichiometric silicon nitride. The interface is seen to have the Si¹⁺ and Si³⁺ states of silicon bonding with nitrogen, which suggests an atomically abrupt and defect-free interface. The initial single-crystalline silicon nitride layers are seen to become amorphous at higher thicknesses. The AFM image shows that the nitride nucleates at interfacial dislocations that are connected by sub-stoichiometric 2D-nitride layers, which agglomerate to form thick overlayers. The electrical properties of the interface yield a valence band offset that saturates at 1.9 eV and conduction band offset at 2.3 eV due to the evolution of the sub-stoichiometric interface and band bending.

New areas of research undertaken by this group were: 1. Confinement induced laser-like emission from GaN nanowall network; 2. Evaluation of GaN nanostructure as Transparent Conductor

Dr. Sridhar Rajaram

Biodegradable polymers are a class of materials that have found applications in drug delivery and in biocompatible stents. Currently, the material of choice is the polymer of lactic acid which is an α -hydroxy acid. The limited structure tenability of poly(lactide) has led to the search for other biocompatible polymers. In this context, Dr. Rajaram's research group has started exploring the possibility of living polymerization of β -hydroxy acid. Cyclic monomers that can polymerized with nucleophilic catalyst have been synthesized and the nucleophilic ring opening polymerization of these materials is currently being attempted.

In another project, the group focused on the development of dendritic materials for the efficient quantification of low viral loads in HIV infected individuals. Attachment of Raman markers to dendrimers is expected to enable the enhanced viral RNA using SERS technique.

Recently, the Group developed a cyanide free synthesis of amino acids using a carbonate as a source of carboxyl group. Transformation of the carbonate to a carboxyl group was accomplished via the use of a nucleophile. It was shown that this nucleophilic activation of carbonates is dependent on cation- π interactions. Currently, new reactions using this approach was developed.

Dr. Ranjani Viswanatha

Dr. Ranjani Viswanatha's research group worked on doping of magnetic ions into CdS nanocrystals and its corresponding magnetism. Spintronics is a new upcoming area of research for various applications. The most preferred material for these applications are semiconductors with a small percentage of magnetic dopants and are known as dilute magnetic semiconductors. The synthesis of these materials has been standardized. Diffusion of dopants or impurities in host nanocrystals out of the host has been used proactively to obtain uniformly doped QDs. It has been shown that uniform doping, specifically for magnetic impurities is crucial with up to two orders of magnitude increase in room temperature ferromagnetism. Studies are in progress on some extremely important and promising magnetic, optical and magneto-optical responses compared to earlier materials.

Secondly, the research group worked on the mechanism of Mn emission and uncovered an important long-standing puzzle regarding the Mn emission. Air stable Sn doped perovskite materials with excellent optical properties have also been synthesized.

The group also started working on advanced optical and magneto-optical techniques to study the electronic structure of QDs in detail.



Dr. Rajesh Ganapathy

Research in the Soft Matter Lab at ICMS focused on three key research themes namely (1) stochastic thermodynamics, (2) glass transition and (3) colloidal self-assembly. As a part of a collaborative effort, the research group of Dr. Rajesh Ganapathy designed and implemented a microscopic heat engine that is powered by bacterial activity. On the glass transition front, the Group devised new analysis techniques that allow the researchers to distinguish between competing mechanisms of glass formation. In the area of colloidal self-assembly, the research group developed special surfaces that not only aid in deciding the symmetry of the growing crystallites but also help in directing particles to specific sites prior to nucleation.

Dr. Premkumar Senguttuvan

After joining the Centre on November 2016, the faculty has dedicated his efforts to setup the group and laboratory. The primary focus of Dr. Senguttuvan's research group is to develop novel electrode and electrolyte materials for Li- and Beyond Li-ion Batteries. Since January 2017, the group started working on developing novel NASICON compounds as potential sodium ion cathodes, and the preliminary results were encouraging.

Following are the members of the Unit:

Director

C.N.R. Rao F.R.S. , Hon. F. R. S.C., Hon. F. Inst. P.,

Professors

C.N.R. Rao F.R.S. , Hon. F. R. S.C., Hon. F. Inst. P.,
S. M. Shivaprasad Ph.D., jointly with CPMU

Associate Professors

Ranjan Datta Ph D
Rajesh Ganapathy Ph D
Sridhar Rajaram Ph D

Faculty Fellows

Ranjani Viswanatha Ph.D., jointly with NCU
Premkumar Senguttuvan Ph D

Sr. Research Officer

Jay Ghatak

Technical Assistant

Mahesh J.I.

Student (PGDMS)

Ankit Sharma

MOLECULAR BIOLOGY AND GENETICS UNIT (MBGU)

Research Activities

Autophagy and autophagy related pathways in health and disease (Dr. Ravi Manjithaya)

Research undertaken by Dr. Ravi Manjithaya's research group on the characterization of autophagy pathways in yeast and mammalian cells has revealed novel signaling pathways that govern autophagy flux. In addition to these pathways, the Group has uncovered mechanisms that negatively regulate autophagosome lysosome fusion. The group could also achieve these insights as they employed both genetic and chemical biology approaches to address the questions related to regulation of autophagy flux. Two bodies of work from this laboratory have got accepted in the journal *Autophagy* and is expected to appear online soon. Two more manuscripts are currently under review.

Transcription regulation and chromatin dynamics (Prof. Tapas K Kundu)

The Transcription and Disease Laboratory is focusing on understanding the fundamental mechanisms of regulation of gene expression by epigenetic modifications and non-histone chromatin proteins, with special emphasis on disease and therapeutics. During the year 2016-2017, the research undertaken at this Laboratory were published in several high impact journals, and a patent has also been commercialized. Research collaboration was established and MoU signed between JNCASR and the University of Strasbourg, based on the discovery made by the research group of an activator of histone acetyltransferase p300 conjugated with CSP, to elucidate its effect in the Huntington Disease Model. Another license agreement is almost in place to be signed for the commercialization of one of the innovations of this Laboratory i.e., CTK7A, an inhibitor of lysine acetyltransferase with EMD Milipore Company. Furthermore, two international meetings and one science outreach program for the high school student were organised.

Stem cell potency and cardiovascular development (Prof. Maneesha S. Inamdar)

In the last year, Prof. Maneesha Inamdar's research group has identified novel metabolic regulators that maintain the stem cell state in human pluripotent stem cells and regulate differentiation. The Group has shown that oxidative phosphorylation status is key to determining cell fate. The Group also identified and published non-genetic means to modulate mesenchymal stromal cell response to the pro-inflammatory secretome in cardiac repair. New mouse models of leukemia which are currently being characterized were also established.

HIV-1 subtype-C strain: success story of the fittest viral subtype (Prof. Udaykumar Ranga)

Over the past few years, Research Group led by Prof. Udaykumar Ranga has been actively engaged in understanding how HIV-1 establishes and maintains viral latency. The research group found that the same viral protein Tat can activate as well as suppress transcription from viral promoter although how is this trick accomplished at the molecular level is yet under exploration. The research group has found some important leads in this direction. The research group has also found that the stronger the viral promoter, the faster the rate of latency establishment which appears to be paradoxical. However, the process of latency is controlled by Tat. The process of viral latency is more intriguing in the context of subtype C of HIV-1 as these viral strains are acquiring a greater magnitude of variation in the viral promoter. Subtype-specific genetic variations provide a powerful tool to examine how these variations offer a replication advantage to specific viral subtypes if any. Only in subtype C of HIV-1, two genetically distinct transcription factor binding sites are positioned at the most critical location of the viral promoter. Since a single promoter regulates viral gene expression, the promoter variations can play a key role in determining the replication fitness of the viral strains. For the first time, the work done by the research group provides a scientific explanation for the presence of a unique NF- κ B binding motif in subtype C, a major HIV-1 genetic family responsible for half of the global HIV-1 infections. The results offer compelling evidence that subtype C viral promoter is not only stronger but also is endowed with a qualitative-gain-of-function advantage. The genetically variant NF- κ B and the Sp1III motifs may be



responsive to specific cell signal pathways differentially, and these mechanisms must be examined. The group is actively pursuing these leads to unravel the most puzzling aspects of HIV-1 transcriptional latency.

Molecular genetics of hereditary, prelingual, sensorineural hearing impairment (Prof. Anuranjan Anand)

About one-fourth of the hereditary deafness seen in India is due to mutations in a single gene, Cx26. Interestingly, the high prevalence of a particular Cx26 mutant allele, W24X is attributable to an approximately 8000-year old founder effect in our population (Ram-Shankar et al. J. Med. Genet. 2003). Consistent with the critical role played by Cx26 (a gap-junction protein) a large number of Cx26 mutations have been described (Ram Shankar et al. EJHG 2008). On the other hand, mutations in Cx30, an equally important gene behind prelingual hearing loss are surprisingly rare. During 2016-17, Prof. Anuranjan Anand's research group has completed an analysis of a large multi-generation family in which severe-to-profound hearing loss is found associated with a variety of skin-related anomalies. Genome-wide analysis of the family showed that the locus maps to chromosome region 13ptel-q12.1 and that novel mutation, p.N54K in Cx30, cosegregates with the phenotype. Unlike wild-type Cx30, p.N54K Cx30 is predominantly localized in the cytoplasm and does not permit transfer of neurobiotin, suggesting improper cellular localization and abolishment of gap-junction activity.

Protein engineering and molecular parasitology (Prof. Hemalatha Balaram)

The central theme of research in Prof. Hemalatha Balaram's research group has been on metabolism in *P. falciparum* and on protein structure-function analysis of enzymes involved in purine nucleotide synthesis in the parasite. In collaboration with Drs. Balasubramanian and Prakash, using a combination of biochemical tools and MD simulation, the research group has deciphered the molecular basis of HGPRT activation and product release mechanisms. The study from this group on *M. jannaschii* GATase has led to the finding of a remarkably stable succinimide that plays a critical role in conferring hyperthermostability to the protein and opens up a novel route for enhancing protein stability. During last financial year, the group has also undertaken 3-dimensional structure solution using X-ray crystallography of numerous enzymes that are under investigation in the laboratory. These include the structures of MjGATase and MjATPPase-ligand complex solved using molecular replacement and apo-MjFH using Se-SAD. The group has also solved the structures of PflSN1 and complexes through a collaborative effort with Dr. Aghajari (France) using a combination of cryoEM and Se-SAD. The group has characterized PffH both biochemically and functionally. These results are in the process of communication.

Mechanisms underlying pathogenesis of human cerebral malaria (Prof. Namita Surolia)

The Molecular Parasitology lab focused its research activities last year on functional characterization of autophagy proteins in *Plasmodium falciparum*, which is relatively an unknown field. For the purpose, various GFP- autophagy fusion proteins have been constructed and using proteomics approach; the group tried to decipher the interacting partners of some of the *Plasmodium* autophagy proteins. The Group is also trying to characterize molecules which are highly upregulated in severe as well as cerebral malaria patients to explore the possibility of using these as biomarkers of the disease. During 2016-17, the Molecular Parasitology Laboratory has focused its efforts on understanding the role of Autophagy on growth and development of malaria parasite *Plasmodium falciparum*. The gene expression profiles of some of the representative Autophagy genes involved at various steps of the pathway are significantly upregulated during intra-erythrocyte stages of parasite proliferation. Further, the expression levels of the Autophagy marker proteins such as Pf Atg8 and PfAtg5 were found to be modulated by inhibitors and inducers of Autophagy. Under various stress conditions too, Autophagy seems to be mediating the parasite survival thus emphasizing that Autophagy is essential for the parasite growth. These studies are being pursued in detail.

Genetic and epigenetic definition of Centromeres (Dr. Kaustuv Sanyal)

Dr. Kaustuv Sanyal's laboratory identified centromeres of a human fungal pathogen *Candida tropicalis* (Chatterjee et al. , 2016, PLOS Genetics). This discovery revealed that centromeres in *C. tropicalis* diverged significantly

from its closely related *Candida* species but resemble those of a distantly related fission yeast. Another recent significant finding from his group is a *Candida* species-specific histone H3 variant that plays a major role in switching between the planktonic and biofilm mode of growth. His group is now investigating genome-wide occupancy of the core histone H3 and the variant one in different forms of growth of *Candida albicans*. His group has also identified centromeres of the *Cryptococcus* species complex. This work suggested that RNAi is required for maintaining retro-transposons at the centromere to stabilize the genome. The RNAi-deficient *Cryptococcus* species is found to have shorted centromeres with truncated retrotransposons as compared to the RNAi-proficient species. Moreover, discovery of centromeres in a non-pathogenic species, *Cryptococcus amyloletus* revealed the secret of transition of tetrapolar to biopolar mating system during the process of evolution (Sheng et al., 2017 PLOS Biology, in press). His group has also been studying efficacy of several antifungal compounds against *Candida* and *Cryptococcus* species in collaboration with scientists from JNCASR and elsewhere (Dutta et al, 2016 Biophysical Journal; Hoque et al., 2016 Molecular Pharmaceutics; Ghosh et al., 2017 ACS Infectious Disease).

Chromatin Biology and Genomics (Prof. MRS Rao)

Recent work from Prof. M.R.S. Rao's laboratory has identified various post-translational modifications on TH2B across the tetraploid and haploid stages of spermatogenesis. By computational analysis, it was also shown that the amino acid differences in the N-terminal tail and the post-translational modifications acquired by some of the residues could cause the destabilization of the nucleosomes. It is well established by now that meiotic recombination is triggered by DNA double strand breaks which require the chromatin reorganization but still the mechanism underlying this is not known. Currently, efforts are made to understand the role of serine-12 phosphorylation of TH2B (TH2BS12P) in meiotic prophase I. To address this, the phospho-specific TH2B (TH2BS12P) antibody was raised and characterized. Immunostaining revealed an enriched staining of TH2BS12P in the XY body compared to the result of the nucleus. This lead the group to the hypothesis that TH2BS12P may be involved in an XY body specific function like recombination, heterochromatin formation, etc. By colocalization studies, it was shown that TH2BS12P colocalizes with the major recombination proteins like DSB repair protein Spo11, strand invasion protein Rad51, H2A histone variant γ H2AX and meiotic recombination kinase pATM in the XY body during the pachytene spermatocytes.

New programmes launched during the year

- 11th Asian Epigenomics meeting held from September 30th to October 1st, 2016 at Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore. Organizing committee: Tapas K. Kundu, Rakesh K Mishra, Ullas L Kolthur, Jingde Zhu, Toshikazu Ushijima, Shyam Prabhakar, Li-Jung Juan, Young-Joon Kim.
- 6th Meeting of the Asian Forum of Chromosome and Chromatin Biology to be held from March 3rd to March 5th, 2017 at CSIR - Centre for Cellular and Molecular Biology, Hyderabad. Organizing committee: Rakesh K Mishra, Ullas L Kolthur Tapas K. Kundu, and Purnima Bharagava.
- "Stem Cells and Regenerative Medicine" a workshop in Malda West Bengal, 2016 for the high school students.

Following are the members of the Unit:

Chair

Ranga Udaykumar Ph D

Professors

V Nagaraja Ph.D., F A Sc, F N A Sc
Anuranjan Anand Ph.D., F A Sc
Hemalatha Balaram Ph.D., F A Sc



Namita Surolia	Ph.D., F A Sc, F N A Sc
Ranga Udaykumar	Ph D
Tapas Kumar Kundu	Ph.D., F A Sc, F N A Sc, F N A
Maneesha Inamdar	Ph D

Honorary Professor

M.R.S. Rao	Ph.D. F A Sc, F N A, F N A Sc, FTWAS
------------	--------------------------------------

Associate Professor

Kaustuv Sanyal	Ph D
----------------	------

Faculty Fellow

Ravi Manjithaya	Ph D
-----------------	------

Technical Officer(Veterinary)

R G Prakash	B V Sc & A.H.
-------------	---------------

Technical Staff

Suma B.S., Mohan V.	
---------------------	--

NEUROSCIENCE UNIT (NSU)

Research Activities

Dr. Sheeba Vasu

Dr. Sheeba's research group studies sleep arousal neural circuits and the interactions between circadian clock circuit and the sleep homeostat using the fruitfly, *Drosophila melanogaster*. The Group uncovered a role for a mechanosensor nanchung expressing cells in inducing daytime sleep in male flies. Using the *Drosophila* circadian pacemaker circuit as a model, studies were undertaken on behavioural, anatomical and cellular markers of the progression of Huntington's disease. Researchers were also engaged in studies to understand neuronal circuits that modulate rhythmic behaviour in response to thermal cues in *Drosophila melanogaster*.

A comparative study of rhythmic behaviour, putative circadian pacemaker neurons, circadian clock properties and sleep characteristics in a diurnal and a crepuscular species of *Drosophila* was carried out.

A study of the interactions between circadian oscillators modulating feeding and activity rhythms in fruit flies *Drosophila melanogaster* was done. A new study has been initiated to characterize features of *Drosophila* aggregation behaviour in the absence of food.

Dr. James Chelliah

A cardinal feature of the human brain development is that sensory, cognitive and emotional experiences shape synapses, neural-circuit development, memory formation and recall of stored memories. Several studies have shown that these features are altered in intellectual disability (ID) and Autism Spectrum Disorder (ASD). De novo heterozygous mutations in the gene that encode for synaptic *RasGAP*, *Syngap1*, has been shown to cause ID and increase the risk for developing ASD in young children. In the lab, Dr. James Chelliah's research group is trying to understanding the following functions of *SYNGAP1* in brain development: One of the questions explored is, how does *Syngap1* heterozygous mutation affects the function of GABA by modulating the switch of Cl⁻ transporters during development. Preliminary results show that this mutation advances the switch of Cl⁻ transporters during development, thereby regulating the function of GABA during development. The second question, that has been explored by the research group is, whether *SYNGAP1* can interact with the FMRP protein which is implicated in ID and ASD. Aspects of neuronal maturation in FMRP KO seem to be opposite to *Syngap1*. Heterozygous mutations i.e. delayed maturation in FMRP. This will help the research group to design therapeutic drugs targeting protein that regulate FMRP and reverse the behavioural and functional deficits observed in *SYNGAP1*. The third major question explored is to understand the role of astrocytes in neuronal maturation and how *Syngap1* Heterozygous mutation alters the function of astrocytes. Preliminary data collected by the group suggests that the astrocyte expression was reduced in *Syngap1* heterozygous mice, which can affect how the neurons (excitatory and inhibitory) neurons mature and function. The fourth major question, was studied (in collaboration with Prof. Vidita Vaidya, TIFR, Mumbai) to understand whether the phenotypes observed in *Syngap1* Het mutations can be rescued by targeting perineuronal nets that forms at the time of neuronal maturation (3-week mice). The preliminary results show that the number of perineuronal nets is reduced in *Syngap1* Hets. Dr. Chelliah has three collaborative projects with faculty members from the IISc., NCBS and RGCB with *Syngap1* not as the main theme and one collaborative project with Dr. Milos in the UK with *Syngap1* as a main theme. In collaboration with Dr. Milos, the UK, Dr. Chelliah started a project looking at the altered expression and function of SUMOylation and kainate receptors in *Syngap1* Het mice.



Dr. Ravi Manjithaya

Dr. Ravi Manjithaya's research group's work on characterization of autophagy pathways in yeast and mammalian cells, has revealed novel signaling pathways that govern autophagy flux. In addition to these pathways, the group has also uncovered mechanisms that negatively regulate autophagosome lysosome fusion. The group could achieve these insights as they employed both genetic and chemical biology approaches to address the questions related to regulation of autophagy flux. Two bodies of work from this laboratory has got accepted in the journal *Autophagy* and is expected to appear online soon. Two more manuscripts are currently under review.

Prof. K S Narayan**Synergetic combination of organic bioelectronics, sensor platforms and optogenetic tools for exploring neural systems**

The possibility of seamlessly integrating sense organs with device components and circuits consisting of soft electronic materials on biocompatible substrates offers useful options to monitor-enhance-augment natural response to various stimuli. In this regard, host of modern materials offer a unique combination of optoelectronic and mechanical properties as recently demonstrated for sensing and stimulating neuronal activity and evoking response in retinal ganglion cells. This possibility of triggering neuronal signals in a blind retina has opened up a route for utilizing these (intelligent) substrates as a prosthetic element. These promising initial results requires systematic deeper understanding to enable promising route for vision restoration targeted in retinitis pigmentosa and macular degeneration.

Quantitative assessment involving non-contact electrical methods without the involvement of microscopy can enable a remote user to monitor the cell growth and development at different stages. In this line of pursuit, Prof. Narayan's research group has examined the utility of ultra-high impedance, dry-contact capacitively coupled electric potential sensors. Standard cell lines have been used on a variety of substrates to demonstrate the efficacy of this sensor placed in close proximity without physical contact. Conventional imaging methods and multi-electrode array recordings are used in tandem to validate and ascertain this new method developed at JNCASR. This sensor platform is used to study neuronal cells in different model systems at different stages of development.

Rapid strides in the exciting field of optogenetics has opened up options, where cell signalling mechanism is light-controlled. The concept of “optogenetics” is essentially a combination of genetic and optical methods to cause or inhibit well-defined events in specific cells of living tissue. The research group expects that a simultaneous implementation of both the approaches (epiretinal implants and optogenetic) can generate interesting features and may be applicable in other context and systems also.

Prof. M.R.S. Rao

(i) *LncRNA Mrhl*: A new player in mouse embryonic neuronal development: The transcriptional landscape of all organisms is much more complex than imagined as majority of the genomic DNA is pervasively transcribed, both into protein-coding and non-coding transcripts. A class of regulatory non-coding transcripts is the long non-coding RNAs (*lncRNAs*). They exhibit important regulatory functions in various physiological phenomena, at the genomic, transcriptional, translational or post-transcriptional level. The current study involves one such *lncRNA* known as *Mrhl* (mouse recombination hotspot locus). *Mrhl* is 2.4 kb in length, intronic, single-exonic, polyadenylated and has tissue specific expression in the adult mouse. It is also syntenically conserved in humans. The role of *Mrhl* in regulating meiotic commitment during germ cell differentiation has been well established in Prof. MRS Rao's laboratory. By analyzing ENCODE datasets, the research group found that *Mrhl*

exhibits differential expression in the mouse embryonic and adult brain and it was shown that it is spatio-temporally expressed in the developing mouse embryonic brain. In the mammalian developing brain, a class of cells known as the radial glial cells, act as the progenitors for the neuronal lineage. Mouse embryonic stem cells was differentiated into the neuronal lineage with the help of retinoic acid to obtain a radial glia-like neuronal progenitors. In this context, the research group observed that *Mrhl* is significantly over-expressed in the neuronal progenitors with concomitant down regulation in early and late neurons. Mechanistic studies reveal *Pax6* as the major transcription factor that might be involved in regulating *Mrhl* RNA during neuronal differentiation. Furthermore, ChIP studies for histone modifications shows that *Mrhl* might be regulated epigenomically during mouse brain development. Current studies are being focused on decoding the mechanisms associated with regulation of neuronal differentiation/commitment by lncRNA *Mrhl*.

(ii) System analysis identifies distinct and common functional networks governed by transcription factor ASCL1, in glioma and small cell lung cancer: ASCL1 is a basic helix–loop–helix transcription factor (TF), which is involved in various cellular processes like neuronal development and signaling pathways. Transcriptome profiling has shown that ASCL1 over-expression plays an important role in the development of glioma and small cell lung carcinoma (SCLC) but distinct and common molecular mechanisms regulated by ASCL1 in these cancers are unknown. In order to understand how it drives the cellular functional network in these two tumors, a gene expression profile in a glioma cell line (U87MG) was generated to identify ASCL1 gene targets by an si RNA silencing approach and then compared this with a publicly available dataset of similarly silenced SCLC (NCI-H1618 cells). The research group constructed TF–TF and gene–gene interactions, as well as protein interaction networks of ASCL1 regulated genes in glioma and SCLC cells. Detailed network analysis uncovered various biological processes governed by ASCL1 target genes in these two tumor cell lines. The group found that novel ASCL1 functions related to mitosis and signaling pathways influencing development and tumor growth are affected in both glioma and SCLC cells. In addition, the group also observed ASCL1 governed functional networks that are distinct to glioma and SCLC.

Prof. Anuranjan Anand

(i) Microtubule associated defects caused by EFHC1 mutations in juvenile myoclonic epilepsy, a common form of adolescent epilepsy: Juvenile myoclonic epilepsy (JME) is a common form of epilepsy with substantial genetic basis to its etiology. While earlier studies have identified EFHC1 as a causative gene for JME, subsequent studies to examine the role of the gene in geographically distinct populations have been limited. Here, Prof. Anand's research group has reported contribution of EFHC1 in JME patients from India. The group examined the complete structure of the EFHC1 transcript from 480 JME patients and 700 control chromosomes by direct sequencing. Functional correlates of mutations were studied using immuno-localization experiments in cultured mammalian cells and in silico protein homology modeling studies. Thirteen mutations, of which 11 were previously not known, were identified in 28 JME patients. These mutations accounted for about 6% of the patients examined. Functional studies for the EFHC1 mutant proteins suggested varying extent of microtubule-related abnormalities during cell division. In silico analysis for a subset of mutations suggested that these may affect EFHC1 protein domains and their ability to interact with other proteins. Observations of the research group enhanced the evidence for the role of EFHC1 in JME in a population, ethnically and geographically distinct from the one in which the gene was identified and broaden the extent of its allelic heterogeneity.

(ii) SLC1A1 mutations in sensory human epilepsy syndrome triggered by tactile and temperature stimuli: Sensory or reflex epilepsies are characterized by seizures precipitated by a remarkably wide range of stimuli, among them contact with hot water. Hot water epilepsy (HWE) has been reported from New Zealand, Australia, the United States, the United Kingdom, Canada, Japan, Turkey and India. In India, this disorder is most prevalent in those parts of the country where hot water bathing following copious application of warm oil on the head, is a cultural custom. Its onset is usually during adolescence. The seizures are complex partial,



with or without generalization, and are characterized by a dazed look, sense of fear, irrelevant speech and visual and auditory hallucinations with complex automatisms. Spontaneous seizures are not commonly seen among patients with reflex epilepsies. The molecular basis of these disorders remains largely unknown. Familial clustering has suggested a genetic component and positive family histories have been reported among HWE patients in India and Turkey. Two HWE loci have been mapped to 10q21.3-q22.3 and 4q24-q28 in Indian families.

During 2016-17, Prof. Anand's research group has also reported identification of three mutations, p. Asp174Asn, p.Val251Ile and p.Ile304Met, in the SLC1A1 protein, a glutamate transporter. All three mutations affect glutamate uptake in cultured cells in a temperature-dependent manner. We take into account the known roles of SLC1A1 which comprise activation of NMDA receptors, altered GABA metabolism and the role of TRPV1 in temperature-responsive regulation of glutamate release, along with the observations on SLC1A1 mutations reported here to propose that a combination of these functions may underlie this unusual disorder.

Following are the members of this Unit:

Chair & Professor

Anuranjan Anand Ph.D., F A Sc

Honorary Professor

M.R.S. Rao Ph.D. F A Sc, F N A, F N A Sc, FTWAS

Faculty Fellow

James C. P. Chelliah PhD

Sheeba Vasu PhD

Associate Faculty

Anuranjan Anand Ph.D., F.A.Sc.

K S Narayan Ph.D., F.A.Sc., F.N.A., F.N.A.Sc.

Tapas Kumar Kundu Ph.D., F.A.Sc., F.N.A., F.N.A.Sc.

Ravi Manjithaya Ph.D.

Research Students

Abhik Paul, Iyengar Aishwariya Prasan, Iyer Aishwarya Ramakrishnan, Priyanka Mallick, Vijay Kumar M J, Vijaya Verma

NEW CHEMISTRY UNIT (NCU)

The New Chemistry unit was created by the Jawaharlal Nehru Centre for Advanced Scientific Research as part of the 11th Five Year Plan. The unit was inaugurated in the presence of Prof. A.K. Cheetam, Prof. M. L. Klein, Prof. W. Jones and Prof. E. W. Meijer on December 06, 2010 and works on interdisciplinary aspects of chemical science. The most important areas that are actively pursued are at the interface of chemical biology, chemical Science, and materials Science. Some of the specific areas of research are: solid state and materials chemistry, chemistry of metal chalcogenides, organic synthesis, biomaterials organic and supramolecular chemistry, antimicrobial therapeutics, drug delivery systems, patternable polymers, conducting polymers, semiconducting nanomaterials, renewable energy, liquid interfaces, multifunctional metal-Organic hybrids, medicinal chemistry, theoretical chemistry, carbon and oxide based materials and catalysis.

The Unit currently has a few core faculty members with Prof. C.N.R Rao as its Chairman. Several faculty members from other Units of the Centre are also associated with the NCU. The Unit admits students for the Ph.D. degree programme as well as integrated Ph.D. in Chemical Sciences. The Unit also admits students for integrated MS-Ph.D programme in Chemical Sciences through project-oriented chemical education (POCE). The students admitted for these programmes would undergo extensive course work and research training before continuing for dissertation work.

Research Activities

Prof. C. N.R. Rao's research group has initiated a few major programmes during the last year: one, related to artificial photosynthesis involving photocatalytic oxidation of water by nanoparticles of Mn and Co oxides and the other on photocatalytic H₂ generation by hybrid nanostructures by using the Z-scheme, Synthesis, characterization and properties of anions substituted metal oxides and chalcogenides where in oxygen is replaced by nitrogen and fluorine or sulfur by phosphorus chlorine research on 2D materials specially phosphorene.

Dr. T. Govindaraju's research group had mainly focused on the development of diagnostics and therapeutics for currently incurable neurodegenerative diseases such as Alzheimer's (AD) and Parkinson diseases (PD). Several solutions were explored to address issues related these diseases by elegantly combining the multidisciplinary chemical biology approaches. Hybrid peptoids an small molecule-based molecular tools were developed in his laboratory, which can clear the toxic plaques through the natural cellular process.

The Group's research interest in general is at the interface of chemistry, biology and (bio) materials science, and in particular, organic chemistry, peptide chemistry (peptidomimetics), functional and disease amyloids, molecular probes, nucleic acids and bioinspired (nano)architectonics. During the reporting period, major research efforts were in the development of diagnostics and therapeutics for currently incurable neurodegenerative diseases such as Alzheimer's (AD) and Parkinson diseases (PD). Several solutions were explored to address issues related to these diseases by elegantly combining the multidisciplinary-chemical biology approaches. Specifically, working on targeting multiple pathways involved in the pathogenesis of these diseases to develop peptide and small molecule-based therapeutic agents. Hybrid peptoids and small molecule based molecular tools were developed in his laboratory, which can clear the toxic plaques through the natural cellular process. The research group is in the process of developing molecular probes detecting AD biomarkers in cerebrospinal fluids, blood and brain tissue samples, to be used as viable tools for early diagnosis of AD. Another important area where work was undertaken extensively was the development of synthetic 48 technology to produce biomimetics of functional amyloids (e.g., silk) and their applications as biomaterials.

Dr. Jayanta Halder's research group: Multi-drug resistant Gram-positive bacteria like vancomycin resistant Enterococci (VRE) and Staphylococci (VISA and VRSA); as well as pan-drug resistant New Delhi metallo- β -lactamase-1 (NDM-1) producing Gram-negative bacteria have become a threat to the global public health.



The perennial persistence of bacterial resistance, calls for urgent need to develop more potent drugs having new mode of action, which would make bacterial resistance difficult to develop. Recently, Dr. Halder's research group has developed novel vancomycin analogues which not only overcome acquired resistance against VRE, VISA and VRSA but also took care of the inherent vancomycin resistance towards Gram-negative bacteria due to incorporation of novel membrane disrupting mechanism and pyrophosphate binding moiety in vancomycin. Unlike vancomycin, these vancomycin analogues showed the ability to stop the development of bacterial resistance. Additionally, the Group developed another strategy where the membrane-active molecules were found to re-sensitize the obsolete antibiotics such as tetracycline and inherently resistant antibiotic rifampicin to NDM-1 producing Gram-negative clinical isolates. It was observed that the membrane activity of the molecules provided a backdoor entry to these antibiotics which resulted in increased uptake. Researchers in his Group also created novel small molecular and macromolecular Antimicrobial Peptides Mimics (AMPs) and shown that they inactivate various wild-type and drug resistant pathogenic bacteria and are having no in-vitro and in-vivo toxicity. Additionally, the Group investigated anti-inflammatory properties of macromolecular mimic of AMPs and their ability to target intracellular pathogens by synergistic co-delivery of antibiotics in combination with antibiotics in targeting the persister cells that play an important role in biofilms. Some of the small molecular AMP mimics developed by the Group also showed significant level of activity against Ebola virus. Recently, the Group engineered new generation of polymeric biomaterials from synthetic and natural polymers to make any surface antimicrobial. These inactivate various pathogenic bacteria completely on contact and can be used to prevent the spread of infectious diseases. The Group also developed antibacterial hydrogels that could prevent bacterial infections at wound site without displaying any toxicity towards mice used as the model animal for the experiment.

Kanishka Biswas's research group is directed towards research in solid state chemistry; understanding (crystal and electronic) structure-property relationship and electronic and phonon transport properties of metal chalcogenides and metal halides. In last one year, the Group discovered several new classes of inorganic metal chalcogenides and developed new concepts to decrease the thermal conductivity (lone pair induced rattling, bonding asymmetry and phonon scattering due to intergrowth 2D nanostructures) which resulted in high thermoelectric performance (*J. Am. Chem. Soc.*, 2017, 139, 4350–4353; *Angew. Chem. Int. Ed.*, 2016, 55, 7592 and *Energy Environ. Sci.*, **2016**, 9, 20122). The low cost and earth abundant inorganic solids discovered in his laboratory can convert waste heat to electricity with 12-15 %. The Group has designed new concept to tailor the electronic structure of topological crystalline insulators (SnTe and $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$) and GeTe based materials, which resulted in significant improvement the thermoelectric performance. (*J. Am. Chem. Soc.*, 2016, 138, 13068 and *ACS Energy Lett.*, 2017, 2, 349–356).

Dr. Subi Jacob George's research Group has been directed towards spatio-temporal control over the self-assembly and functions of supramolecular systems for material applications such as development of novel functional organic and hybrid materials. For this, the Group's first approach was temporal control over supramolecular organization using a chemical fuel driven approach to precisely control the growth, steady state and decay of self-assembly and aim towards controlling the novel functions associated with the steady state assembly that features a unique class of living supramolecular polymerization and transient assemblies. The second approach was to design solution processable, organic-inorganic hybrids by the co-assembly of ionic dyes and nanoclay particles for properties such as room temperature phosphorescence for OLED applications.

Prof. Ranjani Viswanatha's research group worked on doping of magnetic ions into CdS nanocrystals and its corresponding magnetism. Spintronics is a new upcoming area of research for various applications. The most preferred material for these applications are semiconductors with a small percentage of magnetic dopants and are known as dilute magnetic semiconductors. The synthesis of these materials has been standardized. Diffusion of dopants or impurities in host nanocrystals out of the host has been used proactively to obtain uniformly doped QDs. It has been shown that uniform doping, specifically for magnetic impurities is crucial with up to two orders of magnitude increase in room temperature ferromagnetism. The Group now intends to

study some extremely important and promising magnetic, optical and magneto-optical responses compared to earlier materials.

Secondly, the Group worked on the mechanism of Mn emission and uncovered an important long-standing puzzle regarding the Mn emission. Air stable Sn doped perovskite materials with excellent optical properties was also synthesized.

Dr. Sebastian C. Peter's research group developed several stable and efficient non-Pt based compounds as electrode materials alternative to the state-of-the-art materials Pt or PtRu on carbon in fuel cell industry. The Group filed two patent applications and is in the process of scaling up the materials towards the commercialization in collaboration with various industries and national facilities. The Group also developed several low-cost materials for the efficient conversion of waste CO₂ into useful chemicals and fuels. The waste CO₂ produced at the coal power generation and cement factories are targeting in this research. The Group established collaboration with HPCL, SABIC, CCS, Thermax etc towards this research. Three international collaborative projects (Germany-DAAD, France-CEFIPRA and Poland-PMSR) with substantial financial support were obtained. The receipt of financial support from DST Nano Mission (Efficient conversion of CO₂ into fuel and chemicals using ordered nano intermetallics) and TRC (Device fabrication of efficient non-Pt based ordered intermetallic nanoparticles as electrode materials for fuel cell green energy production) were significant support for the ongoing research. During the year, Group members have made significant progress, two PhD students: Dr. Sumanta Sarkar and Dr. Udumula Subbareddy successfully defended their thesis. Ms. Sumanta joined as a Post-Doctoral Fellow at Northwestern University under the supervision of Prof. Mercuri Kanatzidis; and Dr. Udumula Subbareddy obtained the scientist job in defense section of the ordnance factory

Dr. Sarit S. Agasti's research group: The primary research focus of Dr. Sarit Agasti's research Group has been oriented towards engineering small molecules and programmable molecular materials to address challenges in bioimaging and to create novel approaches for diagnostic sensing and therapeutic delivery. In the field of bioimaging, it has been a challenging task to visualize biomolecules at nanoscopic resolution (~10-20 nm) as well as to track them while they function inside the cells. Over the last one year, Dr. Agasti's Group worked towards developing new techniques along with generating compatible molecular probes so that the diffraction limit (~200-300 nm) of light microscopy can be overcome and molecules inside cells be localized in nanometer precision. In addition, the Group integrated an important feature with this imaging technique i.e., the ability to simultaneously image and quantify 100s of target molecules from a single cell. The goal of the Group is to ultimately utilize these potentially transformative features, nanoscopic, quantitative and ultramultiplexed imaging, to address various biological questions. For example, going forward, the Group aims to understand the system level changes in synaptic protein compositions and their distribution during aging of neuronal system. Progress made towards this goal is highlighted below.

The Group is in a process of developing a novel method for super-resolution imaging that combines click chemistry based specific and autonomous target labeling approach with single molecule localization technique. This technique was named SISAC (Super-resolution Imaging using Stochastic and Autonomous Clicking). The method comprises of two key chemical components: (1) Docking unit: a small bioorthogonal click tag that is attached to the target molecule, and (2) Imager unit: a fluorogenic 'Click-On' dye that stochastically assembles with the docking unit via a highly selective click cycloaddition reaction to produce single fluorescence emitter from the target molecule. The idea is to construct the final super-resolution image from high-accuracy single molecule localization of the fluorescent emitters that are autonomously switched ON (by click reaction with target molecule) and turned OFF (by photobleaching) within the sample. Bioorthogonal click tag and fluorogenic 'Click-On' dye being the pivotal components of this super-resolution imaging method, a significant effort was dedicated towards developing these components. Now, 1,2,4,5-tetrazine based bioorthogonal click tags have been successfully synthesized. Studies showed that these molecules could undergo spontaneous strain promoted cycloaddition reactions with strained alkenes in biological environment. A series of fluorogenic



'Click-On' dyes has also been synthesized by taking advantages of efficient tetrazine quenching via through-bond energy transfer (TBET) and Förster resonance energy transfer (FRET) mechanism. In vitro bench marking of the SISAC imaging method using synthetic DNA-origami nanostructure and translation to live cell setting is underway.

In another approach, work has been carried out towards generating programmable DNA based molecular probes for super-resolution imaging. The objective is to utilize the transient and specific binding of fluorescently labeled short oligonucleotides (9-10 NT) with the complementary docking strands to obtain programmable and stochastic switching between fluorescence ON and OFF states for single molecule localization based super-resolution imaging. Utilizing this approach, currently the Group can obtain 8 colors super-resolution images from fixed cells. Next, the Group extending this capability to 100 targets imaging by synergistically combining DNA barcoding of cellular proteins with DNA-based super-resolution imaging. Concurrently, work is in progress towards translating this imaging method in more complex biological system (e.g. in neuronal system). Preparation of a manuscript to report a part of this study is also underway. The second part of the research activity has been directed towards developing stimuli responsive Drug Delivery Systems (DDSs) that minimizes side effects and enhance the efficacy of conventional pharmaceutical agents. Two concepts have been explored for this purpose: 1) Supramolecular interaction mediated actuation of therapeutic delivery system; and 2) Light actuated materials for spatiotemporally controlled drug release. An important feature of the design of these delivery systems is the capability to have an integrated sensing platform which allows understanding of therapeutic outcome. Highlights of research progress towards this goal is given below.

Supramolecular chemistry provides a versatile tool for assembling molecular components into functional structures and actuation of these assemblies for myriad applications. The reversibility of association between complementary molecular components enables numerous mechanisms for modular assembly and disassembly. Harnessing this concept, the research group has generated a functionalized gold nanoparticle based system that showed the ability to undergo supramolecular recognition mediated assembly and disassembly process. An important feature of this system is that in the assemble state it can incorporate various drug molecules. These drug molecules can then be released in the cells upon nanoparticle disassembly processes, mediated by the supramolecular trigger. In addition, given the generation of 'hot spots' during assembled state, this system is also currently under investigation for reversible SERS sensors application. Preparation of a manuscript to report this study is underway.

Delivery of drug in a spatiotemporally controlled fashion can serve to minimize side effects and increase its chemotherapeutics efficiency. In this respect, light, being a highly orthogonal external stimulus represents a distinctive way of controlling site-and time-specific delivery of pharmaceuticals. A light responsive charge switchable gold nanoparticle has recently been synthesized. Next, the Group would like to test if these nanoparticles are efficiently uptaken by the cancer cell upon light trigger. With this the Group, will get an ability to deliver drug molecules in a spatiotemporally controlled fashion.

Nanoparticle-stabilized capsules (NPSCs) represent a kind of microcapsule structural motifs whose shell consists of nanoparticles assembled at the interface of immiscible solvent droplets. Recently, the research group has also succeeded in developing two new strategies to fabricate NPSCs: 1) Bioorthogonal tetrazine cycloaddition mediated assembly at oil-water interface, and 2) Host-guest recognition mediated assembly of colloidal microcapsules using Cucurbituril 7 (CB[7]) host. Studies showed that these NPSCs have unique ability of simultaneous encapsulation of unmodified small molecules as well as macromolecular cargo (e.g. proteins) for co-delivery purpose. Preparation of a manuscript to report this study is underway.

Dr. Premkumar Senguttuvan's research group: After joining the Centre, Dr. Senguttuvan has dedicated his efforts to setup his research group and laboratory. The primary focus of his Group is to develop novel electrode and electrolyte materials for Li- and Beyond Li-ion Batteries. Since Jan 2017, along with the group's first student,

Mr. Subham Gosh, work has been undertaken to develop novel NASICON compounds as potential sodium ion cathodes and the preliminary results are encouraging.

Prof. H. Ila's research group work towards design and development of new general, highly efficient synthetic methods for biologically important five and six membered heterocyclic compounds using novel organosulphur building blocks/synthons derived from broad range of active methylene compounds. The various methodologies involve transition metal (especially palladium and copper) catalyzed C-C, C-N and C-S bond formation reactions, regio- and chemoselective C-C and C-heteroatom bond formations with various carbon and heteronucleophile on these synthons, heteroaromatic annulations with bifunctional heteronucleophiles and cycloadditions with activated isocyanomethylene compounds on these substrates.

Dr. Sridhar Rajaram's research group: Biodegradable polymers are a class of materials that have found applications in drug delivery and in biocompatible stents. Currently, the material of choice is the polymer of lactic acid which is an α -hydroxy acid. The limited structure tenability of poly(lactide) has led to the search for other biocompatible polymers. In this context, the possibility of living polymerization of β -hydroxy acid has been explored.

In another project, Dr. Rajaram's Research Group focused on the development of dendritic materials for the efficient quantification of low viral loads in HIV infected individuals. Attachment of Raman markers to dendrimers is expected to enable the enhanced viral RNA using SERS technique.

Recently, the Group had developed a cyanide free synthesis of amino acids using a carbonate as a source of carboxyl group. Transformation of the carbonate to a carboxyl group was accomplished via the use of a nucleophile. The Group has shown that this nucleophilic activation of carbonates is dependent on cation- π interactions. Currently, work is in progress for developing new reactions using this approach.

New Programmes and Highlights

The Seventh Annual Chemistry Lecture has been delivered by Prof. Richard N. Zare, Department of Chemistry, Stanford University, USA on "Mass Spectroscopy: Drop by Drop".

Prof. C.N.R. Rao, National Research Professor, Honorary President & Linus Pauling Research Professor, JNCASR delivered the *New Chemistry Unit Lecture Series* on "Exciting Story of Chemical Science" (Glorious Past and Challenging Future) on April 24, 2017.

Dr. Premkumar Senguttuvan joined the Unit as Faculty Fellow jointly with ICMS.

Dr. Kanishka Biswas launched a new research area on "Clean water" based on ppb level and selective sequestration of heavy metals (Pb, Hg, Cd, As) and nuclear waste (Cs, Sr, Ba, UO₂) from water body by open framework and layered chalcogenides based on the principle of hard soft Lewis acid base interactions (please see *J. Phys. Chem. C*, 2017, DOI: 10.1021/acs.jpcc.7b00908).

Dr. Ranjani Viswanatha started working on advanced optical and magneto-optical techniques to study the electronic structure of QDs in detail.

Dr. Sebastian C. Peter entered NRG COSIA carbon XPRIZE global competition prize worth 20 million USD. He has also initiated the Start-up venture "BREATHE Applied Sciences Pvt Ltd" on efficient conversion of CO₂ into fuels and chemicals.

Dr. Sarit S. Agasti established two new research facilities which include:

1. **Molecular biology facility:** The molecular biology facility has a set of basic equipment for carrying out molecular biology related and DNA nanotechnology based work. This facility includes thermal cycler, horizontal and vertical gel electrophoresis system, and temperature-controlled centrifuge.



-
-
2. **Tissue culture facility:** Work is in progress for establishing a tissue culture lab that will have facilities like, culture and processing of human and other eukaryotic cells for variety of biological experiments: biosafety cabinet, CO₂ incubators, fluorescence microscope with phase contrast, fluorescence and digital camera, temperature-controlled centrifuge, liquid N₂ storage, -80°C freezer, -20°C freezer, 4°C freeze, vacuum pump, water bath, stir-/hotplate.

Following are the members of this Unit:

Chair

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

Honorary Professor

H. Ila Ph D, F N A, F A Sc

Associate Professor

T. Govindaraju Ph D

Subi Jacob George Ph D

Jayanta Haldar Ph D

Faculty Fellow

Sebastian C. Peter Ph D

Ranjani Viswanatha Ph D

Kanishka Biswas Ph D

Sarit S. Agasti Ph D

Premkumar Senguttuvan Ph D

Research Students

Aditi Chiring, Amit, Amit Bhattacharya, Anand Acharya, Anand Kumar Roy, Ananya Banik, Ananya Mishra, Anusha Avadhani, Aritra Sarkar, Arjun C H, Arjun Kumar Chittoory, Arka Som, Arkamita Bandyopadhyay, Avijit Saha, Biswanath Maity, Brinta Bhattacharjee, Debasis Ghosh, Ekashmi Rathore, G. Krishnamurthy Grandhi, Geetika Dhanda, Harshit Arora, Jiaul Hoque, K. Rajasekhar, Krishnendu Jalani, Kushagra Gahlot, Lingampalli Srinivasa Rao, Madhulika Mazumder, Mahima Makkar, Manisha Samanta, Manjeet Chhetri, Manoj Kumar Jana, Manswee Barua, Mohd Monis Ayyub, Mohini Mohan Konai, Moinak Dutta, Paramita Sarkar, Payel Mondal, Pradeep K R, Pramoda K, Rajkumar Jana, Ramesh M S, Ranjan Sasmal, S. Yugandar, Santu Sinha, Satya Narayan Guin, Satyajit Pal, Saurav Chandra Sarma, Shikha Dhiman, Shreya Sarkar, Shubhajit Das, Soumyabrata Roy, Sourav Samanta, Sreyan Ghosh, Subhajit Roychowdhury, Subham Ghosh, Suchi Smita Biswas, Suman Kuila, Sumon Pratihar, Sushmita Chandra, Swagatam Barman, Yelisetty Venkata Suseela, Yogendra Kumar

THEORETICAL SCIENCES UNIT (TSU)

Research Accomplishments:

Members of the Materials Theory Group of **Prof. Umesh V Waghmare** were involved in improvement of the d-band model of catalysts for oxygen reduction reaction relevant to fuel cells, to uncover effects of magnetism, strain and charge transfer. In collaboration with experiments groups, the electronic and phonon-based mechanisms were identified for increasing thermoelectric performance of a material through enhancement of Seebeck coefficient and reduction of thermal conductivity. The efficacy of the newly developed SCAN metaGGA functional of density functional theory in prediction of transition temperatures of ferroelectric perovskite oxides was also demonstrated. The photo-catalytic performance of several 2-D materials was assessed for conversion of solar energy to chemical energy through splitting of water, and identified 2-D N-rich BCN and NbN as promising materials. Theoretical analysis of phosphorene, weak and strong electronic topological insulators and Dirac semi-metals, and complemented experimental works on their Raman spectra was presented. In addition, they developed a semi-empirical effective Hamiltonian for MD simulations of disordered perovskites

Dr. N. S. Vidhyadhiraja's research group - The Mott metal-insulator transition is known to be a first order phase transition. The Group found, for the first time, a lattice model that exhibits a whole surface of continuous quantum critical Mott transitions.

The Group also addressed a major theoretical challenge that hinders detailed investigations of real strongly correlated materials that is access to a well benchmarked, computationally feasible, and real-frequency based method. Researchers in this Group have developed a multi-orbital iterated perturbation theory method that has been shown to have these qualities. Furthermore, a completely open source implementation of this method, called MO-IPT along with detailed instructions, sample data and examples has been released, and is available at <http://www.institute.loni.org/lasigma/package/mo-ipt/>. Release of an updated version is expected soon. Open source access to such a method enables the community to take up theoretical investigations of real material systems.

Dr. Kavita Jain's research group performed the first quantitative study of the slow quench dynamics when a nonequilibrium system with isolated critical point is quenched in the critical region. This work has been included in the 'EPL highlights of 2016'. The Group obtained several analytical results for the dynamics of a phenotypic trait that are relevant to an understanding of polygenic adaptation.

Prof. Shobhana Narasimhan's research group has mainly progressed in identifying descriptors for several classes of problems and materials, including noble and transition metal catalysts, supramolecular host-guest assemblies and binary surface alloys. These are all quantities that can be computed rapidly, and can help one quickly identify a group of systems that are likely candidates for possessing the desired properties, and merit further investigation using abinitio techniques.

An important finding is that the oxidation of nanoparticles can be controlled by varying the substrate that they are deposited on. A new method has also been introduced for extracting oxidation states of metal centres from XANES spectra.

Ms. Nisha Mammen from this Group has obtained her PhD.

Prof. Swapan Pati's research group: Three-layer Phosphorene, which shows anisotropic mobility values has been studied in detail. With appropriate substitution, the Group found that the g-C₃N₄ Quantum Dots show photocatalytic behavior in Visible Light. It was also found that an improved catalytic activity of 25% Mn substituted Co₃O₄ Material for Water Oxidation Reaction (Oxygen Evolution Reaction). The Group discovered that a triangular lattice with dipolar Fermions can have several usual phases and triplet superfluid phase. A time



dependent density matrix renormalization method (tDMRG) has been developed. It was shown that N-doped Graphene system can efficiently trap several gaseous environmental pollutants.

Group led by **Dr. Subir Das** has been involved in problems related to equilibrium and nonequilibrium statistical mechanics. In this broad area, they have obtained significant new understanding on the following specific issues:

1. Active Matter -- influence of active particles on the phase behavior of demixing systems has been studied and obtained insight on how to map such nonequilibrium problems to equilibrium ones.
2. Ordering in Ferromagnets -- Dynamics of ordering and persistence of magnetic moments have been studied via Monte Carlo simulations of Ising model.
3. Kinetics of Phase Separation in Nanopore – Coarsening in phase separating binary fluid confined in nanochannels have been studied via Molecular Dynamics Simulations and the work has practical relevance in the technology related to extraction of oil and natural gas from porous rocks.

The research group of **Dr. Meher K. Prakash** has been involved in computational biophysics research at different scales. Some of the problems being addressed are related to the co-evolutionary patterns of amino acids in viruses which help them evade immune surveillance while remaining functional, bacterial strategies for nutrient acquisition and the relevance of chemotaxis mechanism for bacterial population multiplication, and quantitative structure activity relationships for a new class of drug candidates that disrupt the membranes and have smaller chances of developing resistance. This interdisciplinary research is being performed in collaborating with Biochemists, and Biologists at JNCASR.

Prof. Srikanth Sastry's research group has carried out research in 2016-17 in the areas of (i) shear jamming in granular matter, (ii) the yielding transition in amorphous solids, (iii) complex dynamics in glass forming liquids. In addition, collaborative research on research in physical biology has been initiated, including modeling of allosteric interactions in proteins, and big data methods in biomedical research.

Through extensive computer simulations and numerical calculations, the Group has been shown that the self-organization necessary for shear jamming occurs even for frictionless particles, and that jamming occurs at a precisely defined state at which the mean contact number reaches a value of $D + 1$ (D being the spatial dimension) and a percolation transition of stressed regions takes place, establishing new connections with analyses of rigidity in covalent glasses.

Yielding, or mechanical failure, in glasses has been probed with a cyclic deformation protocol, and it has been shown that yielding emerges as a sharply defined transition under such a protocol, which is characterized by a transition in plastic rearrangement events from being localized to system spanning, involving a discontinuous percolation transition.

Analyzing the dynamics of glass forming liquids, it has been shown that the Adam-Gibbs relation applies to diffusion, and not viscosity, and this observation has been employed in the analysis of the violation of the Stokes-Einstein relation.

New programmes launched during the year

Prof. Umesh V Waghmare's research group launched the following studies during the year:

- Organized an India-Korea bilateral workshop on computational materials science in response to a request and funding from the Department of Science and Technology (DST) with a goal to formulate and plan for setting up a Virtual Network Centre on Computational Materials Science (VNC-CMS).
- Cofounded a company "Breathe" to participate in the Carbon prize competition with a target to achieve efficient catalysis of chemical reduction of CO_2 into methanol.

Dr. N. S. Vidhyadhiraja's research group launched the following studies during the year:

- **Phonon localization:** An important route to the design of efficient thermoelectric materials is scattering of heat carrying phonons. The most destructive scattering mechanism known to us is that of coherent backscattering, which leads to Anderson localization. The Group adapted the method mentioned in the previous point, namely the TMDCA to study Anderson localization of phonons in real material systems. Through detailed benchmarking, researchers have established the exactness and computational feasibility of the method. Several new insights for enhancing Anderson localization of phonons have been obtained.
- **Quantum criticality with flow equation method:** Investigations of an extended periodic Anderson model have indicated a very unusual valence fluctuation induced quantum criticality of the Kondo destruction type. These investigations employ a class of renormalization group methods such as the flow equation method, poor man's scaling, and the Bloch-Feshbach method.
- **Periodically driven quantum many body systems :** The Group also initiated a Floquet Hamiltonian approach to investigate correlated systems subjected to periodic driving. The effective Hamiltonian thus obtained is then solved through dynamical mean field theory and RG based methods.

Dr. Kavita Jain's research group did a study on Coalescent theory and its applications.

Following are the members of this Unit:

Chair

Swapan K Pati Ph D, F A Sc, F N A Sc

Professors

Shobhana Narasimhan Ph D, F N A Sc
Srikanth Sastry Ph D
Swapan K Pati Ph D, F A Sc, F N A Sc
Umesh V Waghmare Ph D, F A Sc, F N A Sc

Associate Professors

N. S. Vidhyadhiraja Ph D
Kavita Jain Ph D
Subir Kumar Das Ph D

Faculty Fellow

Meher K Prakash Ph D

Research Students

Alok Kumar Dixit, Ananthu James, Anjali Singh, Arabinda Bera, Archana Devi, Arpita Paul, Bradraj Pandey, Debdipto Acharya, Dheeraj Kumar, Jiarul Midya, Jyoti Dalal, Kaushlendra Kumar, Koyel Das, Malay Ranjan Biswal, Meha Bhogra, Monoj Adhikari, Nalina V, Neha Bothra, Pallabi Das, Pawan Kumar, Rajdeep Banerjee, Raju Kumar Biswas, Rukhsan Ul Haq, Saikat Chakraborty, Sourav Mondal, Sruthi C K, Subhajit Paul, Sukanya Ghosh, Varghese Babu, Wasim Raja Mondal, Yagyik Goswami



CSIR CENTRE OF EXCELLENCE IN CHEMISTRY (CSIR-COE)

In January 1991, the CSIR established this person-based Centre of Excellence in Chemistry. The Centre works on various aspects of solid state and materials chemistry. The main activities of this Centre deal with the following aspects.

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

Inorganic analogues of graphene constitute an important area of research. Various chemical methods have been developed for the synthesis of layered transition metal dichalcogenides which includes MoS₂, WS₂, MoSe₂, WSe₂, NbS₂ and NbSe₂. Their applications in IR detectors, gas sensors, composites with polymers for mechanical properties and electrical properties, magnetic properties, have been studied. Micromechanical cleavage method has been used for obtaining the single-layers of MoS₂, GaS and GaSe and studied their applications in transistors, detectors and sensors. Functionalization of MoS₂ nanosheets and MoS₂ covalently bonded to nanosheets of other materials are being pursued.

High Surface area borocarbonitrides were synthesized from low cost starting materials like urea, boric acid and activated charcoal. Graphene-like B_xC_yN_z samples exhibit surface area in the range 1500-1900 m²/g, with large uptakes values of CO₂ and shows good performance characteristics as supercapacitor electrodes and as ORR catalysts. Several other aspects of borocarbonitrides are being examined.

Photocatalytic water splitting using powder catalyst dispersed in water by simply shining light is one of the most energy effective and easiest ways to obtain H₂ and O₂. Generation of hydrogen by using semiconductor heterostructures and dyes is being investigated. Thermochemical decomposition of H₂O by perovskite oxide is another area of active exploration. Besides photochemical and thermochemical methods, photoelectrochemical means of splitting water is being pursued.

Aliovalent anion substitution in metal oxides and sulfides causes major changes in electronic properties and structure. Several oxides including ZnO and TiO₂ substituted by N and F have been investigated. P, Cl substituted CdS and ZnS are being examined. Analogues of ZnO and Cds such as Zn₂NF and Cd₄P₂Cl₃ are being investigated.

Following are the members of this Centre:

Linus Pauling Research Professor and Chair

C N R Rao, FRS, FASc, FNA, FTWAS, Hon FRS(C), Hon F Inst P, Hon. FRSC

Glass Blower (Temporary)

Nandha Kishore

Office Staff

Victor Sathish D.G. (Lab Helper)

Research Staff

S. Rajesh, R&D Assistant

THEMATIC UNIT OF EXCELLENCE ON COMPUTATIONAL MATERIALS SCIENCE (TUE-CMS)

Research Activities

CO₂ adsorption in a metal organic framework (TKL MOF series) with flexible ligands has been studied. It has been demonstrated that the linker flexibility can modulate gas uptake via kinetic barriers. Gated adsorption behavior in a MOF has been studied using DFT calculations. The desolvated structure of this MOF was first predicted from the calculations which was later verified by in-situ single crystal XRD measurements. The proton hopping mechanism in a protic organic ionic plastic crystal (POIPC) was studied using ab initio MD simulations which revealed the individual contributions from ion and proton transport to the electrical conductivity of the material.

Ab initio MD simulations of the POIPC compound revealed a new defect induced mechanism of proton transfer between cations rather than between the cation and the anion. The observation has spurred researchers to predict a novel compound whose plastic crystalline phase should have a much higher electrical conductivity than the parent compound.

Identifying descriptors for several classes of problems and materials, including noble and transition metal catalysts, supramolecular host-guest assemblies and binary surface alloys. These are all quantities that can be computed rapidly, and can help one quickly identify a group of systems that are likely candidates for possessing the desired properties, and merit further investigation using ab initio techniques.

It has been shown that the oxidation of nanoparticles can be controlled by varying the substrate that they are deposited on.

Researchers also worked on shear jamming in granular matter, yielding transition in amorphous solids and complex dynamics in glass forming liquids. Collaborative research has been initiated on physical biology including modeling of allosteric interactions in proteins, and big data methods in biomedical research.

Through extensive computer simulations and numerical calculations, it has been shown that the self-organization necessary for shear jamming occurs even for frictionless particles, and that jamming occurs at a precisely defined state at which the mean contact number reaches a value of $D + 1$ (D being the spatial dimension) and a percolation transition of stressed regions takes place, establishing new connections with analyses of rigidity in covalent glasses.

Yielding or mechanical failure, in glasses has been probed with a cyclic deformation protocol, and it has been shown that yielding emerges as a sharply defined transition under such a protocol, which is characterized by a transition in plastic rearrangement events from being localized to system spanning, involving a discontinuous percolation transition.

Analysis of the glass forming liquids dynamics has shown that the Adam-Gibbs relation applies to diffusion, and not viscosity, and this observation has been employed in the analysis of the violation of the Stokes-Einstein relation.

Three-layer Phosphorene, which show anisotropic mobility values have been studied in detail. It was demonstrated that with appropriate substitution, the g-C₃N₄ Quantum Dots show photocatalytic behavior in Visible Light. It was also shown that improved catalytic activity of 25% Mn substituted Co₃O₄ Material for Water Oxidation Reaction (Oxygen Evolution Reaction). Triangular lattice with dipolar Fermions can have several usual phases and triplet superfluid phase was also demonstrated. Time dependent density matrix renormalization method (tDMRG) has been developed. It has been shown that N-doped Graphene system can efficiently trap several gaseous environmental pollutants.



Researchers were also involved in improvement of the d-band model of catalysts for oxygen reduction reaction relevant to fuel cells, to uncover effects of magnetism, strain and charge transfer. In collaboration with experiments groups, identified the electronic and phonon-based mechanisms for increasing thermoelectric performance of a material through enhancement of Seebeck coefficient and reduction of thermal conductivity. It was demonstrated that the efficacy of the newly developed SCAN metaGGA functional of density functional theory in prediction of transition temperatures of ferroelectric perovskite oxides. The photo-catalytic performance of several 2-D materials for conversion of solar energy to chemical energy through splitting of water was assessed, and identified 2-D N-rich BCN and NbN as promising materials. A theoretical analysis of phosphorene, weak and strong electronic topological insulators and Dirac semi-metals, and complemented experimental works on their Raman spectra was presented. In addition, the researchers developed an improved d-band model of magnetic catalysts, and semi-empirical effective Hamiltonian for MD simulations of disordered perovskites.

At present the statistical mechanics of how to combine the data from different simulations is being worked out. The results are showing a promise when the free-energy surface of the wild type protein was looked at, and juxtapose it with the non-equilibrium forces introduced by mutations, the trends in the free-energy surface of the mutants can be predicted.

From the non-equilibrium force data, the researchers predicted whether the mutant can destabilize the protein fold, at a very minimal computational cost.

TUE-CMS Visitors Programmes and Meetings

1. Dr. Henu Sharma, University of Liege (Belgium), Visiting Scientist with Prof. Waghmare, March 1- May 31, 2016. Area of research interest: First-principles calculations, biophysics, material science, oxides.
2. Dr. Richard Charles Remsing, Institute for Computational Molecular Science, Temple University, Philadelphia, USA. He received the APS-IUSSTF Travel Fellowship to spend a month in India. He visited JNCASR (primarily) as well as IMSc-Chennai & IIT-D. He stayed at JNCASR during March 31 – April 10 and April 14 – April 30, 2016. During his visiting period, he delivered a talk in seminar titled “The Role of Frustration in Electron Transfer Reactions Confined within Layered Manganese Dioxides” on April 6, 2016”.
3. Dr. Sathya Narayana Bonkala, JNCASR Alumni, Visiting Researcher with Prof. S. Balasubramanian, January 1-31, 2017.

New programmes launched during the year

Prof. Umesh V. Waghmare organized an India-Korea bilateral workshop on computational materials science in response to a request and funding from the DST with a goal to formulate and plan for setting up a Virtual Network Centre on Computational Materials Science (VNC-CMS). He also co-founded a company “Breathe” to participate in the Carbon prize competition with a target to achieve efficient catalysis of chemical reduction of CO₂ into methanol.

Following are the members of TUE-CMS

Prof. Balasubramanian Sundaram

Prof. Shobhana Narasimhan

Prof. Srikanth Sastry

Prof. Swapan K Pati

Prof. Umesh V Waghmare

Prof. Meher K Prakash

Research Staff

Mr. Soutick Saha, Junior Research Fellow, TUE-CMS, from 01.06.2016 with Dr. Meher K Prakash

MS. Bhupalee Kalita, Junior Research Fellow, TUE-CMS from June 2016 with Prof. Umesh V Waghmare

Support Staff

Venkatesh K, Programme Assistant

Basavaraj T, Helper

Anoop S, Research Scientist B

Suresh J, Research Scientist B

Former R&D Personnel trained and relieved during 2016-2017:

Dr. Sandhya Shenoy U, Research Associate, TUE-CMS, from 01.01.2016 to 17.06.2016, with Prof. Umesh V Waghmare

Dr. Somesh Kr. Bhattacharya, Research Associate, TUE-CMS, from 08.01.2015 to 30.06.2016 with Prof. Shobhana Narasimhan

Dr. Saibal Jana, R&D Assistant, TUE-CMS, from 09.03.2016 to 30.09.2016, with Prof. S. Balasubramanian

Mr. Premkumar Leishangthem, Research Associate (Provisional), TUE-CMS, from 25.11.2014 to 02.03.2015 upgraded to Research Associate from 03.03.2015 to 30.11.2016, with Prof. Srikanth Sastry

Dr. Sebastiano Bernini, Scientist, TUE-CMS, from 01.06.2016 to 30.11.2016 with Prof. Srikanth Sastry

Ex-Support Staff who had served and have been relieved during 2016-2017

Vijay Amirtharaj A, Research Scientist B

Anandaraman A, Research Scientist B



THEMATIC UNIT OF EXCELLENCE IN NANOCHEMISTRY (TUE-NANO)

New synthetic strategies for nanomaterials and investigating properties leading to applications are the two important aspects, currently pursued in the Unit. The synthesized nanomaterials include size and shape controlled metal and semiconductor nanocrystals, functionalized carbon nanotubes, graphene and its derivatives as well as analogues, metal and semiconductor nanowires, nanocomposites, semiconductor wall-like structures, organic as well as biomaterials.

Various wet chemical routes are being employed for the synthesis of pristine and doped semiconductor Nanocrystals. Their size-dependent electronic and optical behavior are being investigated in detail. Nanoparticles of several oxides, chalcogenides, nitrides and carbides have also been synthesized.

Catalysis using porous materials is important both in terms of shape-selective and green chemistry points of view. Porous nanomaterials and metal/metal oxide nanoparticles have been synthesized which are being used in catalytic reactions such as NO_x removal, methane conversion and selective oxidation of hydrocarbons. Synthesis and structural characterization of new classes of porous metal-organic frameworks solids is another area of study being pursued. These crystalline solids are examined for their potential applications in gas storage, separation and catalysis; they also possess interesting optical and magnetic properties.

Nanotubes filled with inorganic guests provide an interesting platform to study materials in one dimensional confinement. Nanostructures of metals, superconductors, oxides, sulfide and nitrides are being produced inside CNTs. Other unique materials being investigated are graphene and functionalized graphene. Inorganic graphene analogues such as metal sulfides and BCN have also been synthesized and well characterized. Properties of some of these materials are being investigated in devices, e.g. supercapacitor, field emitter, and radiation detectors. Nanocarbons as potential materials for storage of hydrogen and other gases are being studied. Various photocatalytic nanocomposites have been made and demonstrated to have high activity in water splitting.

Transparent conductors are ubiquitous among optoelectronic devices. As alternate to ITO, new generation transparent conductor in the form of highly interconnected metal (Au, Ag, Cu etc.) wire networks have been developed, invisible to the naked eye, on common substrates such as glass. Unlike the conventional method of dropping nanowires on a substrate, these conducting electrodes (TCEs) are produced employing a newly developed recipe termed as "crackle lithography". The TCEs thus formed exhibit optoelectronic properties that are superior in many ways, to those of conventional ITO films and other alternate materials. The performance characteristics of the TCEs as well as of devices- solar cells, transparent heaters, transparent capacitor and transparent strain sensor fabricated using the TCEs, have been measured. Many non-optoelectronic devices related to transparent electronics such as transparent capacitors, strain sensors, have also been fabricated.

Supramolecular nanofibres have been made via self-assembly in water. The nanofibres are built via self-assembly of donor and acceptor molecules (coronenetetra-carboxylate and dodecyl methyl viologen respectively) involved in charge transfer interactions. The fibres have been employed as active channel in field effect transistors and from such devices, high mobility values have been derived. The devices work in ambient conditions and can regenerate in the presence of a single drop of water. This aspect has been exploited in fabricating a sensitive humidity sensor. The conductivity of the nanofibre was found to vary sensitively over a wide range of relative humidity (RH) with unprecedented fast response and recovery times. Based on UV-vis, XRD and AFM measurements, it is found that the stacking distance in the nanofibre decreases slightly while the charge transfer band intensity increases, all observations implying enhanced charge transfer interaction and hence the conductivity. It is demonstrated to be as a novel breath sensor which can monitor the respiration rate. Using

two humidity sensors, a breath flow sensor was made which could simultaneously measure RH and flow rate of exhaled nasal breath. The integrated device was used for monitoring RH in the exhaled breath from volunteers undergoing exercise and alcohol induced dehydration.

Following are the members of the Unit:

Faculty

Prof. C.N.R. Rao
Prof. G.U. Kulkarni
Prof. A. Sundaresan
Prof. K.S. Narayan
Prof. S.M. Shivaprasad
Prof. M. Eswaramoorthy
Dr. Rajesh Ganapathy
Dr. Subi Jacob George
Dr. T. Govindaraju
Dr. Jayanta Haldar
Dr. Tapas Kumar Maji
Dr. Sridhar Rajaram
Dr. Ranjan Datta
Dr. Ranjani Viswanatha
Dr. Sebastian C. Peter

Research Staff

Dr. K. S. Subrahmanyam (Research Scientist-C)
Mr. Sanjit Parida (Research Scientist-B)
Ms. Amala M. (R & D Assistant)



LIBRARY

The Library has a collection of over 9336 books and access to over 5000 scientific journals. Journal articles were procured on request under document delivery service from CSIR and DST Institutions across the country and from neighbouring libraries within the city. It is equipped with network scanners and copiers, Wi-Fi and Desktop PCs for browsing online journals and library catalogue.

Collection Development

The library has procured books, journals and e-resources as per the recommendations of faculty members. The documents and resources procured during 2016-17 are following:

Collection (Types of resources)	Added during 2016-17	Total as on March 31, 2017	Amount spent (in Rs.)
Books	209	9336	2,62,675.00
Scientific and technical books	76 (purchased) 66 (gratis)		
Hindi books	1 (gratis)		
Ebooks			
Theses & dissertations	66		
Bound volumes of journals	-	11,799	
CD collection	-		
Subscription to current journals		168	1,67,02,407.00
Online journals	1 (Jove online)	164	
Print journals	-	4	
Subscription through consortium (NKRC)	-	5000+	
Journals on gratis	-	25	
Abstracting & indexing databases	1 (Scopus)	4 (Scopus, Web of Science, SciFinder & Cambridge Crystallographic Data Centre)	
Patent database	-	1 (Derwent Innovations Index)	

Document Delivery Service (DDS)

Journal articles on request from faculty and students were procured from libraries across the country and abroad under Document Delivery Service. Total 123 article requests have been fulfilled through inter-library cooperation.

Following are the library staff members:

Sr Library-cum-Information Officer

Nabonita Guha

Sr Library cum Information Assistants(Gr.I)

Nandakumari E., Nagesh Hadimani

Library cum Information Assistant

Senthil Kumar N.

Helper

Rajeeva J.

CompLab (COMPUTER LAB)

Network: JNCASR has a high speed Local Area Network (LAN) which can support up to 10Gbps Intranet connectivity. In year 2016-2017, efforts have been made to ensure integrated Internet bandwidth of 430 Mbps. Infrastructural upgrades were done to increase the bandwidth to 600 Mbps in the year 2017-2018. This increased bandwidth should ensure an average bandwidth of 10 Mbps per person in the campus.

Central Storage facility: a centralized storage of 10 TB has been added to better manage data storage requirements in the campus. For critical data, such as email, a DeDuplication mechanism via Veeam software has been installed and a secondary storage has been created to ensure redundancy in the system.

Mail Migration: To overcome the technical limitations of the enterprise version of ZIMBRA mail server, the mail server has been migrated to new open-source version of Zimbra.

Secured and Enhanced Wi-Fi: High speed Wireless network with 802.11 b/g/n/ac has been successfully installed in our Campus. Entire Campus has been covered with 70 Instant Access Points. Each Access Point can provide 350Mbps to 500Mbps network connectivity with 802.11 b/g/n/ac. Campus Wi-Fi is fully configured with high-end security modules. Wi-Fi Users and visitors are authenticated via our centralized LDAP and CPPM Server.

Enhanced Network Management system: The network management system has been set up to ensure security and redundancy of servers and other interconnecting devices like core switch, firewall etc. All critical network components have been put on Active-Active redundancy mode to increase the network performance and provide continuous network connectivity in the campus.

Following are the members of CompLab:

Head, CompLab

Dr. Santosh Ansumali, Ph D

Consultant

Avinash

Trainees

Udhya Kumar, Chandan Kumar

Onsite Engineers:

Vikas Mohan Bajpai, Rajeev Ranjan, Manjunath



ENDOWED RESEARCH PROFESSORS

Linus Pauling Research Professor

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

Jawaharlal Nehru Centre for
Advanced Scientific Research, Bangalore

(Term: Life time)

D S Kothari Chair

Prof. M.M. Sharma F R S, F A Sc, F N A

Emeritus Professor of Eminence,
Mumbai University, Mumbai

(Term: 30/11/2014 to 30/11/2017)

Hindustan Lever Research Professor

Prof. H. Ila

Honorary Professor, Jawaharlal Nehru Centre for
Advanced Scientific Research, Bangalore

(Term: 01/01/2015 to 31/12/2017)

ACADEMIC PROGRAMMES

Academic Activities

At JNCASR, an interdisciplinary research in materials and biology is carried out in eight Units: Chemistry and Physics of Materials Unit (CPMU), Evolutionary and Integrative Biology Unit (EIBU), Engineering Mechanics Unit (EMU), International Centre for Materials Science(ICMS), Molecular Biology and Genetics Unit (MBGU), New Chemistry Unit (NCU), Neuro Science Unit (NSU) and Theoretical Sciences Unit (TSU).

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

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

(a) Research Admissions

During 2016-17, 52 students joined various degree programmes at JNCASR in the August session, and, 11 students joined in the January 2017 session. The current student strength at JNCASR is 305. The advertisement for the regular admissions to the Integrated Ph.D., Ph.D. and M.S. programmes in the 2017-18 session was released in many prominent national and regional newspapers and announced on our website.

(b) Degrees Awarded

The Centre is a Deemed University, and awards Ph.D. and M.S degrees. Following students were awarded degrees under the various degree programmes during April 2016- March 2017:

Ph.D. Degree

Chidambar Kulkarni	Sumanta Sarkar	Dhanya R	Varun Thakur
K. Hima Nagamanasa	S. R. K. Chaitanya Sharma Y	Shilpee Sharma	Sudeshna Sen
Yarlagadda Venkateswarlu	Shetty Ronak Kutty	Satyanarayana Bonakala	Amritroop Achari
Arpan Hazra	Venkata Suresh Mothika	Divakara S. S. Murthy Uppu	Pallavi Bothra
Manpreet Kaur	Nagamalleswara Rao Dasari	Mohammed Istaful Haque Ansari	Amrutha Swaminathan
Summayya Kouser	Rajesh Ranjan	Nisha Mariam Mammen	Kalpita Rashmi Karan
Nagarjun N	M. Pandeewar	Nikhil K. L.	Ujjayan Paul
Gangaiah Mettela	Udumula Subba Rao	Dibyajyoti Ghosh	M.H. Lakshminarayana Reddy
B. Loukya Chowdary	S. Vijay Kumar	Antara Das	



M.S.(Engg.) Degree	Master of Science (M.S.) in Materials Science of Integrated Ph.D. Degree	Master of Science (M.S.) in Biological Sciences of Integrated Ph.D. degree	Master of Science (M.S.) in Chemical Sciences of Integrated Ph.D. degree
Rishav Harsh	Priyank Singh	Shubhangini Kataruka	Saurav Chandra Sarma
Jumpal Shashikiran Reddy	Abhiroop Lahiri	Priya Jaitly	Amit Bhattacharya
Achal Mahajan	Nikita Gupta	Veena A	Paramita Sarkar
		Shambhavi Chidambaram	Mahima Makkar
		K. Ratna	Suchi Smita Biswas
		Siddharth Singh	
		Pallabi Mustafi	

Postgraduate Diploma in Materials Science
Danish Shamoon
Rajesh S
Vidyanshu Mishra

(c) Best Thesis Awards

- Dr. K. Hima Nagamanasa received Best Thesis Award in Physical Sciences in the year 2015-16;
- Dr. Nikhil K. L. received Best Thesis Award in Biological Sciences in the year 2015-16;
- Dr. Mohammed Istafaul Haque Ansari received the Roddam Family Award for the Best Ph.D. thesis in Engineering Mechanics;
- Mr. Achal Mahajan received the Roddam Family Award for the Best M.S. (Engg.) thesis in Engineering Mechanics.

(d) Short term Academic Programmes (2016-17)

Mr. Ankit Sharma joined the Centre's Postgraduate Diploma programme in Materials Science (PGDMS) under Dr. Ranjan Datta. He is presently undergoing course work and will be completing his course requirements by July 2017. On successful completion of the course requirements, he will be awarded a Postgraduate Diploma of the Centre.

The advertisement for the Postgraduate Diploma in Materials Science and Postgraduate Diploma in Science Education will be released during May 2017.

DISCUSSION MEETINGS

1. Three-day Symposium on Contemporary Issues in Condensed Matter Systems, convened by Prof. V. Venkataraman, June 13-15, 2016.
2. Group Research Conference, convened by Prof. Roddam Narasimha, Engineering Mechanics Unit, June 30, 2016.
3. Conference on Emerging Materials (CEMAT) 2016, convened by Prof. Arun M. Umarji, IISc, July 18-19, 2016.
4. Workshop on "Modern Approach to Materials", Christ University, Bangalore, August 29-30, 2016.
5. 11th Asian Epigenomics Meeting, Prof. Tapas K Kundu, JNCASR, September 30 - October 01, 2016.
6. Sixth Annual Materials lecture by Prof. Sir Richard Friend, Cavendish Laboratory, Department of Physics, University of Cambridge, June 14, 2016.
7. Symposium on Contemporary Issues in Condensed Matter Systems at IISc during June 13-15, 2016.
8. Central Instrument Facility Meeting, convened by Dr. Kaustuv Sanyal, Molecular Biology and Genetics Unit, August 25, 2016.
9. Chemical Frontiers-2016, convened by Prof. R. Murugavel, August 25-28, 2016.
10. 12th JNC Research Conference on "Chemistry of Materials", convener: Dr. Subi J. George, JNCASR, September 23-25, 2016 at Trivandrum.
11. Ninth International Materials Lecture by Prof. Clément Sanchez, Collège de France, September 29, 2016.
12. 19th Transcription Assembly Meeting, Prof. Chandrima Das, Bose Institute, Kolkata, November 8-9, 2016.
13. International Symposium on Solid State Chemistry, December 1-3, 2016.
14. Winter School Conference, December 5-9, 2016.
15. IUMRS-ICYRAM 2016, Prof. P.S. Anil Kumar, IISc, December 11-15, 2016.
16. 3rd Chromosome Stability Meeting, Dr. Kaustuv Sanyal, JNCASR, December 15-18, 2016.
17. 42nd Annual Meeting of the Indian Society of Human Genetics (ASHG2017), Prof. Arun Kumar, IISc, March 2-4, 2017.
18. DBT-JNCASR Partnership Proposal Expert Committee Meeting, March 15, 2017.

ENDOWMENT LECTURES

A.V. Rama Rao Foundation Lecture in Chemistry: Intramolecular Electronic Coupling at the Mixed Valent States. Fact or Fiction, Prof. G.K. Lahiri, Chemistry Department, Indian Institute of Technology Bombay, Powai, Mumbai; **Prize Lecture:** Natural Products Synthesis: Efficient Methods & Innovative Strategies, Dr. C.V. Ramana, Division of Organic Chemistry, CSIR-National Chemical Laboratory, Pune, May 04, 2016.

Sixth Annual Materials Lecture of ICMS: Radiative and Non-Radiative Processes in Photovoltaics, Professor Sir Richard Friend, FRS, Cavendish Laboratory, Cambridge, June 14, 2016.

Prof. C.N.R. Rao Oration Award Lecture (17th in the series): Earthquake generation along the Himalayan Arc: knowns and unknowns, Prof. C. P. Rajendran, Geodynamics Unit, August 16, 2016.



DAE-Raja Ramanna Lectures in Physics: Down-to-Earth String Theory, Prof. Rajesh Gopakumar, Director, ICTS (TIFR), Bengaluru; **Prize Lecture:** Spin-Spin Correlations at Different Length Scales in Crystalline Systems, Dr. S M Yusuf, Head-Magnetism Section & Scientific Officer, Solid State Physics Division, BARC, Mumbai, September 28, 2016.

International Materials Lecture of ICMS: Integrative Materials Chemistry: from

Nanostructures to Hierarchical structures, Prof. Clement Sanchez, Chair, Chemistry of Hybrid Materials, Laboratoire de Chimie de la Matiere Condensee de Paris, Universite Pierre et Marie Curie Collège de France, Paris, September 29, 2016.

SPECIAL LECTURE

Science Start-ups from R&D Institutions, Mr. Kaushik Gala, India Science Venture Fund, VC Community, August 08, 2016.

SYMPOSIA / WORKSHOPS / CONFERENCES / WINTER SCHOOL

1. Flow Cytometry Workshop: The Flow Cell at MBGU, along with Flow cytometry Solutions Pvt. Ltd conducted a 3-day workshop "Experimental designing, data analysis and presentation" from July 12-14, 2016.
2. School on optical microscopy and spectroscopy was organized at SSCU auditorium, IISc, July 18th-22nd, 2016.
3. Biotechnology Ignition Grant (BIG) Workshop, July 20, 2016.
4. TSU In-House symposium, August 03, 2016.
5. JNCASR-Cambridge University -SSL Winter School – 2016 on Frontiers of Materials Science, December 05 - 09, 2016.
6. An International Symposium on Solid State Chemistry on December 01-03, 2016.
7. NGS Workshop (Next Generation Sequencing) by Clevergene Biocorp Pvt. Ltd, March 23 – 24, 2017.

FLUID DYNAMICS COLLOQUIA

1. Ideas from 19th Century to their 21st Century Computational Solvers by TchebyFlow, Dr. Gerard Labrosse, TchebyFlow, France, November 16, 2016.
2. Evaporative Instabilities in Pure and Binary Mixtures, Dr. Dipin S. Pillai, University of Florida, November 18, 2016.
3. Boundary layer instabilities in near-critical fluids, Prof. Sakir Amiroudine, Universite Bordeaux, France, December 26, 2016.
4. Theoretical models for compressible vortex streets, Mr. Vikas Krishnamurthy, Imperial College London, UK, February 20, 2017.

SEMINARS AND LECTURE SERIES

Chemistry and Physics of Materials Unit Seminars

1. Nature Inspired Computational Architectures, Dr. Saurabh K. Bose, University of Canterbury, New Zealand, April 13, 2016.
2. Multiple Colossal Phenomena in Magnetolectric Eu (Ba, La) TiO₃, Prof. Ramanathan Mahendiran, Department of Physics, National University of Singapore, June 14, 2016.
3. Covalent Organic Frameworks as Ingredient for novel heterogeneous Catalysts- Old wine in a new bottle?”, Prof. Ramanathan Vaidhyanathan, Department of Chemistry, Indian Institute of Science Education and Research, Pune, July 08, 2016.
4. Kelvin Probe: A Powerful technique for non-destructive surface and interface studies”, Prof. A. Subramanyam, Department of Physics, IIT Madras, Chennai. August 17, 2016.
5. The Nobel Prizes in Science (2016): An Appreciation”, Dr. S. T. Lakshmikumar, National Physical Laboratory, (NPL), New Delhi. November 10, 2016.
5. Investigation of some New Sulfides Based Thermoelectric Materials: A Comparison with Oxides, Prof. Antoine Maignan, Laboratoire CRISMAT – ENSICAEN/CNRS, France, November 29, 2016.
6. Mixed Potential Electrochemical Sensors for Exhaust Gas Monitoring in Various Applications, Dr. Ramaiyan Kannan, Rutgers University, USA, December 14, 2016.
7. Biophotonics: A new Dawn in personalized Medicine and Personal Health, Dr. Ishan Barman, Johns Hopkins University, USA, December 22, 2016.
8. Tuneable sieving of ions using graphane oxide membranes & Van der Waals pressure and its effect on trapped interlayer molecules, Dr. Siddeswara Vasu Kalangi, University of Manchester, UK, January 5, 2017.

Engineering Mechanics Unit Seminars

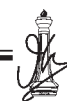
1. Mechanics of non-woven fibrous matrices and their interactions with cells, Prof. Sovan Das, Indian Institute of Technology Kanpur, September 16, 2016.
2. Use of 3D photoelastic model to extract three components of traction, Dr. Dhiraj Kumar Singh, Graduate University Okinawa, Japan, September 28, 2016.
3. Marangoni Instabilities and Pattern Selection in Layered Flows, Mr. Jason R. Picardo, Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, October 5, 2016.

Evolutionary and Integrative Biology Unit (EIBU) Seminar

1. Perceptual and cognitive processes in developmental prosopagnosia: why some mothers can't recognize their children from their face, Dr. Garga Chatterjee, Indian Statistical Institute (ISI), Kolkata, January 8, 2017.

International Centre for Materials Science Seminar

1. Semiconductor Nanowires for Optoelectronics and Energy Applications, Prof. Chennupati Jagadish, Research School of Physics and Engineering, the Australian National University, Australia, October 26, 2016.



Molecular Biology & Genetics Unit Seminars

1. Wisdom of Crowds: Linking Collective Protein Interactions to Cellular Function, Dr. Sivaraj Sivaramakrishnan Protein Acrobatics Lab University of Minnesota, Twin-Cities, July 04, 2016.
2. A tale beyond (Histone) tails: Enhancer identification using Histone H3 tail and globular domain acetylation marks, Dr. Pradeepa Madapura, School of Biological Sciences, University of Essex, UK, August 24, 2016.
3. Understanding chikungunya induced disease and approaches to vaccines and therapeutics, Dr. Suresh Mahalingam, Institute for Glycomics, Griffith University, August 26, 2016.
4. Why HIV-1 clade C is less fit – and yet highly successful in the global AIDS epidemic?, Prof. Vinayaka Prasad, Department of Microbiology and Immunology, Albert Einstein College of Medicine, USA, September 26, 2016.
5. HIV-1 host-virus interactions and persistence-- Novel single cell assays to monitor latent HIV-1 reservoirs, Prof. Ganjam V Kalpana, Department of Microbiology and Immunology, Department of Genetics, Albert Einstein College of Medicine, USA, September 27, 2016.
6. LSM with Airyscan: The present and the future with Cryo Airyscan, Dr. Vimal Gangadharan, Applications Scientist, Zeiss Microscopy Labs New York (ZMLNY), Carl Zeiss Microscopy, New York, USA, September 30, 2016.
7. Engineering Cardiac Ion channels with new approaches in order to illuminate mechanisms of cardiac function and disease, Dr. Prakash Subramanyam, Columbia University, New York, October 06, 2016.
8. Composition and conformation of peptide: an implication to de novo sequencing in tandem mass spectrometry, Dr. Raja Banerjee, Department of Biotechnology, Department of Bioinformatics, Maulana Abul Kalam Azad University (WBUT), West Bengal, November 04, 2016.
9. Human TRIM5 is a potent restriction factor for tick-borne flaviviruses, Abhilash Chiramel, Laboratory of Virology, NIAID (National Institute of Allergy and Infectious Diseases), USA, November 07, 2016.
10. Understanding HIV-Mycobacteria synergism through comparative proteomics, Dr. Sharmistha Banerjee, University of Hyderabad, Hyderabad, November 24, 2016.
11. Epigenetic strategies: nucleosome remodeling and histone variants, Prof. Stefan Dimitrov, Institute Albert Bonniot, France November 28, 2016.
12. RNAi-dependent epimutations evoke transient antifungal drug resistance, Dr. Joseph Heitman, Duke University, USA, December 13, 2016.
13. Kinetochore specifica/on and assembly in vertebrate cells, Dr. Tatsuo Fukagawa, Osaka University, Japan, December 14, 2016.
14. Gene duplication and sub functionalization regulates germ-line stem cell fate in the Drosophila Ovary Dr. Girish Ratnaparkhi, IISER Pune, December 16, 2016.
15. Gene Therapy of Human Hemoglobinopathies: A Personal Odyssey, Prof. Arun Srivastava, University of Florida, USA, December 22, 2016.
16. No More Missed Connections: Identifying Novel Interactors of the Insulin-like Growth Factor-1 Receptor by Proximity Labeling, Dr. Akshay Bareja, Duke University, USA, January 3, 2017.
9. *Salvia divinorum*: A Unique CNS Active Plant, Thomas E. Prisinzano, University of Kansas, US, February 16, 2017.
17. Role of Epigenetics and non-coding RNAs in Diabetic Complications and Metabolic Memory, Dr. Rama Natarajan, Beckman Research Institute of City of Hope, February 28, 2017.

-
-
18. RNA regulation in development and disease, Dr. Ruthrotha Selvi B, MRC Genetics and Molecular Medicine, University of Edinburgh, UK, March 1, 2017.
 19. Neuro AIDS and Drug Abuse go hand in HAND: Blaming the messengers, Dr. Shilpa Buch, University of Nebraska Medical Center, USA, March 7, 2017.
 20. Single-cell Measurement of Microbial Stress-response Dynamics in Complex Growth Conditions, Dr. Somenath Bakshi, Harvard Medical School, USA, March 20, 2017.

MBGU Lecture Series

1. Cellular Roles of Restriction Endonucleases -Primitive Immune System to Programmed Cell Death, Prof. V. Nagaraja, President, JNCASR, November 11, 2016.
2. A Beautiful Mind! Social Cognition in Wild Bonnet Macaques, Prof. Anindya 'Rana' Sinha, National Institute of Advanced Studies, Bangalore, February 10, 2017.
3. Careers - The Right Track for you, Sandhya Sriram, SciGlo Pte. Ltd. April 7, 2017.

New Chemistry Unit (NCU) Seminars

1. Transient and Adaptive Organization in Nanosystems, Dr. Subhabrata Maiti, University of Padova, Italy, January 12, 2017.
2. Time-dependent evolution of metastable supramolecular assemblies, Prof. Kazunori Sugiyasu, National Institute for Materials Science, Japan, January 13, 2017.
3. Generating LnPd(0) Catalysts for 21st Century Organic Synthesis: Understanding the Reduction Mechanism of Pd(II) to LnPd(0)(n = 1 and 2), Dr. Thomas J. Colacot, Johnson Matthey Global R & D Manager, Johnson Matthey, New Jersey, February 6, 2017.
4. Carbon nanotube grows long – Synthesis and Application, Dr. Supriya Chakrabarti, Ulster University, UK, February 7, 2017.
5. Mass Spectroscopy: Drop by Drop, Prof. Richard N. Zare, Stanford University, USA, February 15, 2017.
6. Recent developments in the synthesis of carbo and heterocycles with fluorinated side chains, Prof. Rene Gree, Institut des Sciences Chimiques de Rennes, CNRS UMR, France, March 1, 2017.
7. Peptide based artificial fluorescent probes for biological targets and their bioimaging application, Dr. Debabrata Maity, University of Duisburg-Essen, Germany, March 20, 2017.
8. Optoelectronic properties of low-dimensional nanomaterials and heterostructures, Dr. Chandan Biswas, University of Texas, March 22, 2017.
9. Boron, Borophenes and Borospherenes, Prof. E. Jemmis, IISc, Bangalore, March 28, 2017.

Neuroscience Unit Seminars

1. If we can make computers play chess, why can't we make them see?, Dr. Arun Sripati, Centre for Neuroscience, Indian Institute of Science (IISc), Bangalore, April 29, 2016.
2. Rhesactome → protein network as a “molecular brake” for motor behaviors in mice”, Dr. Srinivasa Subramaniam, Department of Neuroscience, The Scripps Research Institute, Florida, USA, July 25, 2016.
3. “Adult Neurogenesis: Targeting new neuron formation to regulate mood”, Vidita Vaidya, Department of Biological Sciences, Tata Institute of Fundamental Research, Mumbai, August 23, 2016.



-
-
4. Gene Regulatory Networks Guiding Retinal Development Evolution and Disease, Dr. Anand Swaroop, National Institutes of Health Bethesda, USA November 30, 2016.
 5. Molecular mechanisms regulating cell fate specification in the developing cerebral cortex, Dr. Bhavana Muralidharan, Tata Institute of Fundamental Research, Mumbai, January 13, 2017.
 6. Developmental mechanisms of projection neurons in the forebrain Dhananjay Huilgol, Cold Spring Harbor Laboratory, New York, USA, January 13, 2017.

Theoretical Sciences Unit (TSU) Seminars

1. Effect of Macromolecular Crowding on an Enzymatic Reaction: Experimental Results and Theoretical Model, Prof. R. Swaminathan, Department of Biosciences and Bioengineering, IIT Guwahati, Guwahati, May 27, 2016.
2. How does the closed state of β 3 Integrin destabilized by mutations? Multiscale Molecular Dynamics Study, Dr. Anirban Polley, The University of Chicago, Illinois, USA, August 02, 2016.
3. Localized Operator Partitioning Method for Electronic Energy Transfer, Dr. Jayashree Nagesh, Chemical Physics Theory Group, University of Toronto, August 24, 2016.
4. Rheology of dense emulsions – a shear start-up and steady state study, Dr. Vishwas Vasisht, Georgetown University, USA, November 8, 2016.
5. Stochastic thermodynamics in small systems, estimation of dissipation and feedback control, Dr. Anupam Kundu, International Centre for Theoretical Sciences, Bengaluru, November 29, 2016.
6. Correlation effects in Real Materials, Prof. Tanusri Saha-Dasgupta, S.N. Bose National Centre for Basic Sciences, Kolkata, November 30, 2016.
7. Kagome Spin-Liquids and Herbertsmithites, Prof. Rajiv R. P. Singh, University of California, USA, December 27, 2016.
8. Stress Response of Granular Systems, Dr. Kabir Ramola, Brandies University, January 3, 2017.
9. A theoretical model for Scanning Tunneling Microscopy: applications in bi-dimensional materials and molecular electronics, Dr. Yannick J. Dappe, Universita Paris-Saclay, France, January 10, 2017.
10. Towards controlled assemblies of ligand-stabilized noble metal nanoclusters, Prof. Hannu Hakkinen, University of Jyvaskyla, Finland, January 24, 2017.
11. Synchronization and survival of connected bacterial populations, Dr. Shreyas Gokhale, Massachusetts Institute of Technology, February 7, 2017.
12. From soft matter to 2D electron gases: Anomalous transport phenomena in heterogeneous media, Prof. Juergen Horbach, Heinrich-Heine-Universitat Dasselndorf, February 16, 2017.
13. Phase Ordering Studies and Ground States of the Random Field Ising Model, Dr. Varsha Banerjee, Indian Institute of Technology, New Delhi, February 20, 2017.
14. Accuracy-energy trade-off in a cellular signaling cascade, Dr. Bhaswar Ghosh, Max Planck Institute for Terrestrial Microbiology, Marburg, Germany, February 21, 2017.
15. Two-dimensional melting in systems of soft-deformable particles, Prof. Massimo Pica Ciamarra, Nanyang Technological University, Singapore, February 28, 2017.
16. Phase bands for periodically driven integrable quantum systems, Prof. Krishnendu Sengupta, Indian Association for the Cultivation of Science, Kolkata, March 8, 2017.
17. A geometrical description of granular physics, Dr. Shankar Ghosh, Tata Institute of Fundamental Research Mumbai, India, March 28, 2017.

ANNUAL FACULTY MEETING

Lectures delivered at the Annual Faculty Meeting, 2016

Talks delivered by Centre's faculty members and other eminent scientists during Annual Faculty Meeting and In-House Symposium held during November 21 – 22, 2016:

1. Non-Coding RNA as Regulators of Gene Function - Mrhl RNA: Discovery to Function by Prof. M.R.S. Rao, NSU/MBGU, JNCASR
2. Structure Dynamics in Molecular Zinc Phosphates, by Prof. R. Murugavel, IIT Bombay.
3. Why ecology should take a long – Term View, by Prof. R. Sukumar, CES, IISc.
4. Electronic structure of quantum dots in the eyes of a laser light by Dr. Ranjani Viswanatha, NCU/ICMS, JNCASR.
5. Towards super - efficient LEDs, Prof. S.M. Shivaprasad, CPMU/ICMS.

OTHER PROGRAMMES

Hindi Workshop

Hindi Workshop on "Verbal Communication in Hindi", Shri. Srinivas Rao, BEL, Bengaluru, June 20, 2016.

International Day of Yoga

The 2nd International Day of Yoga was celebrated in the Centre on June 21, 2016. Prof. K S Narayan, Dean R & D inaugurated the Yoga Posters displayed by the JNCASR group. A lecture was organized on Healthy eating habits, Diet & Nutrition by Dr. Supritha. K.M. Specialist Physician, Dietitian and Nutritionist, followed by Yoga Demonstration by JNCASR group, led by Smt. Shwetha (Yoga trainer) at the Kanada Hall, Jakkur Campus. During the programme, Certificates were distributed to the Yoga Performers of JNCASR, by Grandmaster Yoga Bhushana, Smt. Rajashree Prasad, Swami Vivekananda Seva Kendra, Bangalore.

AEBS Orientation Programme

An orientation programme has been arranged on July 28, 2016 to familiarize the staff on Aadhaar Enabled Biometric System (AEBS).

Hindi Week

The Centre organized week long activities from 14-21 September, 2016 under the Hindi Saptah. These include talks by scientists from JNC and NAL; most prominently, the inaugural talk on "अतीत की एक महान नदी सरस्वती और हरप्पा सभ्यता" by Prof. K.S. Valdiya, Honorary Professor, GDU, JNCASR. Workshop on the importance of learning Hindi for official correspondence, quiz competition and various other cultural activities. A talk in Hindi on 'Science of Speech Coding', Shri Sanjeev Gupta, DRDO Bangalore, was organized on September 16, 2016. Staff and students enthusiastically participated in all the events and won prizes.

Rashtriya Ekta Diwas

The Centre organized a marathon titled 'Run for the Unity' on Monday, October 31, 2016 to observe the "Rashtriya Ekta Diwas (National Unity Day)". The run started from the security main gate of Jakkur Campus was participated by faculty, students and staff of the Centre.



Vigilance Awareness Week

On account of Vigilance Awareness Week from October 31 – November 05, 2016, the "Vigilance Pledge" was taken by all Faculty, Students and Staff of the Centre on November 02, 2016 and was administered by Justice Santosh Hegde, Former Justice of Supreme Court of India, and Former Lokayukta of Karnataka. A Vigilance lecture on "Public Participation in promoting Integrity and eradicating Corruption" was delivered by Shri. Shiva Kumar, Chief Vigilance Officer, BEL, Bangalore on November 03, 2016 in the Kanada Auditorium Jakkur Campus.

Staff Orientation Programme

Two Staff Orientation Programme have been arranged for the administrative staff under the Staff Development Programme. The first was on Importance of self-motivation at work by Dr. P Chiranjeevi, JNCASR on July 26, 2016 and another on Communication Skills and English Language by Mr. Sreenivas Krishna, October 14, 2016.

Orientation Programme for Students

Workshop on Prohibition of Sexual Harassment of Women at Work Place, Ms. Kanti Joshi, Support against Sexual Harassment (SASHA), March 13, 2017.

FELLOWSHIPS AND EXTENSION PROGRAMMES

EVENTS AND PROGRAMMES HELD DURING THE YEAR 2016-17

Orientation Programme for POBE-POCE 2016 students.

An orientation programme was conducted for the 2016 batch of POBE and POCE programme students on 03 June 2016 and was also attended by SRFP students. Inaugural address by Prof. C.N.R. Rao for students of POBE-POCE and SRFP programmes 2016 was held on June 03, 2016.

Student Buddy Programme

The aim of this programme is to expose class XI/XII students to a day in the life of a research scholar, through individual interactions. Under this programme, 94 students from Jawahar Navodaya Vidyalaya and Kendriya Vidyalaya have benefitted for the year 2016. Detailed feedback was collected from participating students, buddies and teachers. The response was very positive and enthusiastic. JNC faculty and students wholeheartedly participated and the programme was immensely appreciated by the school students and their teachers.

Award of Diploma Certificates Ceremony for the award of diploma certificates to POBE-POCE (2014 to 2016) batch of students was held on July 01, 2016.

ONGOING PROGRAMMES

Visiting Fellowship Programme

Fifteen scientists from research institutions across the country were selected for the Visiting Fellowships programme 2016-17. They will be hosted by the faculty of CPMU, EIBU, MBGU, NCU, NSU, and TSU. The following is the status of their fellowship:

SL. No.	Name & Present Position/Employment	Proposed to work with (Name of the Faculty)	Status
1	Dr. Bhaskarjyoti Borah Assistant Professor, Charotar University of Science & Technology, Anand, Gujarat	Prof. S. Balasubramanian	Yet to join
2	Dr. S. Arungalai Vendan Associate Professor, VIT University, Vellore, TN	Prof. K.S. Narayan	The first spell completed
3	Dr. Anita R. Warriar Assistant Professor, AMET University Chennai, TN	Prof. Chandrabhas Narayana	Yet to join
4	Dr. Ann Mary K.A. Assistant Professor, St. Thomas' College Thrissur, Kerala	Dr. Sebastian C. Peter	Yet to join
5	Dr. M. Venkatesh Perumal Assistant Professor, Bannari Amman Institute of Tech., Sathymangalam, TN	Prof. K.S. Narayan	The first spell completed
6	Dr. H.T. Srinivasa Sci. Asst., Raman Research Institute Bangalore, Karnataka	Dr. T. Govindaraju	Completed



SL. No.	Name & Present Position/Employment	Proposed to work with (Name of the Faculty)	Status
7	Dr. Debashis Mallick Assistant Professor, Mrinalini Datta Mahavidyapith, Kolkata, West Bengal	Dr. Tapas K. Maji	Yet to join
8	Dr. S. Harish Assistant Professor, PSG Inst. Of Tech. & Applied Research, Coimbatore, TN	Prof. M. Eswaramoorthy	The first spell completed
9	Dr. Jinu George Assistant Professor, Sacred Heart College Kochi, Kerala	Dr. Subi J. George	Yet to join
10	Dr. G. Nagaraju Assistant Professor, Siddaganga Institute of Technology, Tumakuru, Karnataka	Prof. M. Eswaramoorthy	The first spell completed
11	Dr. H. Dhanalakshmi Assistant Professor, Veterinary College KVAFSU, Hassan, Karnataka	Prof. Hemalatha Balaram	Yet to join
12	Dr. Tani Agarwal Assistant Professor, Amity University Haryana Manesar, Gurgaon	Prof. Tapas K. Kundu	Yet to join
13	Dr. Venkata Rao D.K. Senior Scientist, CSIR-CIMAP Research Centre Bangalore, Karnataka	Dr. Ravi Manjithaya	Completed
14	Dr. Soorej M. Basheer Assistant Professor, Kannur University Kasargod, Kerala	Prof. P. Balaram, Honorary Fellow, Chemical Biology, JNCASR	Yet to join
15	Dr. M. Manikannan Scientist C, Sathyabama University Chennai, TN	Prof. Udaykumar Ranga	Yet to join

Summer Research Fellowship Programme (SRFP)

For SRFP 2016, 63 students (list given in pg. 80) availed the scholarship and received research training in various areas of Physics, Chemistry, Biology or Engineering at research institutes in Bangalore, and elsewhere in the country.

The advertisement of SRFP 2017 was announced on the JNCASR website and emailed to around 150 college principals in the country. A total of 1396 applications were received and 94 offers have been sent.

Category	No. of applications received (for 2017)	No. of fellowships offered in 2017	No. of applications received (2016)	No. of fellowships utilized in 2016
Life Sciences	710	35	753	19
Engineering Sciences	158	13	183	07
Physical Sciences	256	14	410	12

Chemical Sciences	167	29	160	23
Mathematics	054	03	115	02
Materials Science	051	01	060	00
Total	1396	95	1681	63

Project Oriented Chemistry Education (POCE)

Advertisement for POCE-2017 was released in 6 newspapers and announced on our website. In addition, a copy of the form and information sheet was sent to over 200 college principals of small towns to expand the reach of POCE and encourage students to apply for the programme.

Eight students of POCE-2014-16 completed the program successfully. Seven of them are doing M.Sc. in different institutions in the country, whereas one student is doing his Master's programme in Ruhr University, Germany.

Project Oriented Biology Education (POBE)

Advertisement for POBE-2017 was released in 6 newspapers and announced on our website. In addition, a copy of the form and information sheet was sent to over 200 college principals of small towns to expand the reach of POBE and encourage the students to apply for the programme. Eight students of POBE-2014-16, who had completed the programme successfully, are doing M.Sc. in different institutions in the country.



INTELLECTUAL PROPERTY

IP assets (IPAs) are collections of intellectual properties – patents, trademarks, copyrighted works, industrial designs, geographical indications, trade secrets, etc. IP assets have economic value because of their ability to enhance the value and financial return from technologies, products and services.

Realising the importance of IPAs created by research personnel and to foster Academia-Industry Partnership, the Centre encourages and facilitates the creation, development, protection and management of commercially exploitable IP and its enforcement. The Centre has so far filed 241 (PCT-49, Australia-5, Brazil-3, Canada-5, China-6, Europe-22, Germany-2, Hong Kong-2, India-78, Israel-1, Japan-8, Korea-2, Singapore-1, S. Africa-3, S.Korea-3, USA-50 and Vietnam-1) National and International Patent Applications and obtained 63 (Australia-2, China-4, Europe-9, India-10, Japan-4, Korea-1, S.Africa-2, S.Korea-1 and USA-30) patent grants, in addition to registering Copyright-1, Industrial Design-1 and Trade Mark-1.

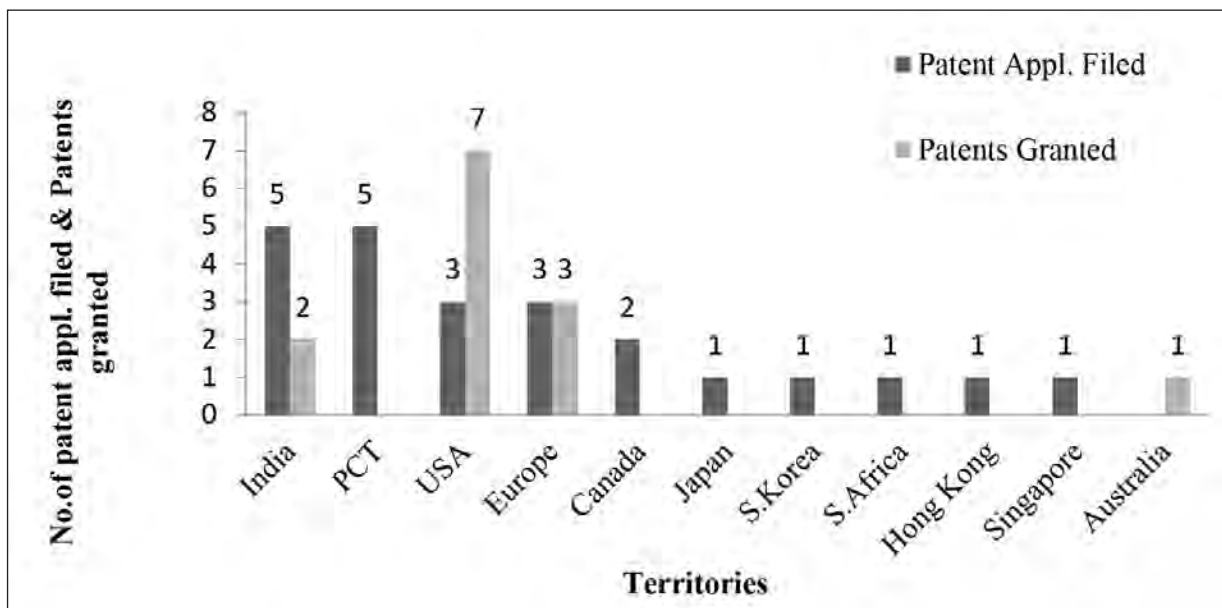
During the reporting year, the researchers at the Centre developed several new inventions. The Dean, R&D reviewed strategically and recommended filing of 23 patent applications (PCT-5, Canada-2, Europe-3, Hong Kong-1, India-5, Japan-1, Singapore-1, S. Africa-1, S. Korea-1, USA-3) for commercialisable inventions meeting the patentability criteria. The Centre has also obtained 13 (Australia-1, Europe-3, India-2 and USA-7) patent grants.

Copyright application has been submitted (Diary No. 12289/2016-CO/SW, dated 20-10-2016) for computer software titled '*ANUROOP: A compressible DNS code to simulate and study flow over turbine blades*' developed by Prof. Roddam Narasimha, Shri Suresh Madhusudan Deshpande and Shri Rajesh Ranjan.

Technology Transfer:

'*A Composition and Methods Thereof*' developed by Prof. Eswaramoorthy Muthusamy of JNCASR and Dr. Kesavan Subaharan and Bosukonda Veera Venkata Surya Pavan Kumar of CPCRI-ICAR has been licensed to 3 companies.

Graphical Representation of the Patent Applications Filed and Granted (2016-2017)



Patent Applications Filed (April 2016- March 2017)

Title of the invention	Inventors	Territory	Application No	Date of filing
Indian Patent Applications				
Self-Cleaning Nanoscale Metal-Organic Frameworks and Process of Preparation Thereof	Tapas Kumar Maji, Syamantak Roy, Venkata Suresh Mothika	India	201641040976	30-Nov-2016
	Jayanta Halder, Jiaul Hoque	India (Prov)	201641026116	29-Jul-2016
	Sebastian Chirambatte Peter, Rajkumar Jana	India (Prov)	201741010595	25-Mar-2017
	Sebastian Chirambatte Peter, Saurav Chandra Sarma	India (Prov)	201741010611	25-Mar-2017

International Phase Patent Applications Filed Under PCT

Luminescent Conjugates Microporous Polymer with Lewis Acidic 'Boron' Sites on the Pore Surface: Ratiometric Sensing and Capture of F ⁻ Ions	Tapas Kumar Maji, Venkata Suresh M, Swapan K. Pati, Arkamita Bandyopadhyay	PCT	PCT/IB2016/051961	07-Apr-16
Compounds as DNA Probes, Methods and Applications Thereof	Govindaraju Thimmaiah, Nagarjun Narayanaswamy	PCT	PCT/IB2016/055113	26-Aug-2016
Compounds as Stimuli-Responsive Probes, Methods and Applications Thereof	Govindaraju Thimmaiah, Nagarjun Narayanaswamy	PCT	PCT/IB2016/055114	26-Aug-2016
Method For Modulating Autophagy and Applications Thereof	Ravi Manjithaya, Piyush Mishra, Suresh Santhi Natesan, Somya Bats, Veena Ammanathan, Aravinda Chavalmane	PCT	PCT/IB2016/057498	9-Dec-2016
A Composite, Scaffold and Applications Thereof	Govindaraju Thimmaiah, Shivaprasad Manchineella	PCT	PCT/IB2017/050734	10-Feb-2017

National Phase Patent Applications

Vancomycin-Sugar Conjugates and Uses Thereof	Jayanta Halder, Yarlagadda Venkateswarlu, Goutham Belagula Manjunath, Mohini Mohan Konai	Europe	14796240.1	20-Apr-2016
		South Korea	10-2016-7009601	12-Apr-2016



Chitin Derivatives, Method for Production and Uses Thereof	Jayanta Halder, Jiaul Hoque, Goutham Belagula Manjunath, Padma Akkapeddi	USA	15/105153	16-Jun-2016
Antimicrobial Conjugates, Method For Production And Uses Thereof	Jayanta Halder, Mohini Mohan Konai, Miles Carroll	India	201647034069	5-Oct-2016
		USA	15/125214	5-Oct-2016
		Europe	15714003.9	4-Nov-2016
		Hong Kong	17102845.4	20-Mar-2017
		Japan	2016-574508	13-Sep-2016
Small Molecular Probes, Processes and Use Thereof	Govindaraju Thimmaiah, Nagarjun Narayanaswamy, Kolla Rajasekhar	Canada	2941933	20-Sep-2016
		USA	15/301,952	4-Oct-2016
		Europe	15723043.4	3-Nov-2016
		Canada	2,944,763	3-Oct-2016
		South Africa	2016/07051	13-Oct-2016
		Singapore	11201608296P	4-Oct-2016

Patents Granted (April 2016 - March 2017)

Title of the invention	Inventors	Territory	Patent No.	Granted on
A Nanosphere-Histone Acetyltransferase (HAT) Activator Composition And Process Thereof	Tapas Kumar Kundu, Anne-Laurence Boutillier, Snehajyoti Chatterjee, Muthusamy Eswaramoorthy, Puspak Mizar, Chantal Mathis, Jean-Christophe Cassel, Romain Neidl, Mohankrishna Dalvoy Vasudevarao, Vedamurthy Bhusainahalli Maheswarappa	USA	9314539 B2	19/04/2016
		Europe {Validation in Germany, France and UK}	2841111	01/06/2016
Inhibition of Histone Acetyltransferases by CTK7A and Methods Thereof	Tapas Kumar Kundu, Mohammed Arif, Kempgowda Mantelingu, Gopinath Kodaganur Srinivasachar	Europe (Validation in France and Germany)	2475769	18/01/2017
Polynucleotide Sequences of Candida dubliniensis and probes for Detection	Kaustuv Sanyal, Sreedevi Padmanabhan, Jitendra Thakur	USA	9334535	10/05/2016
Cationic Antibacterial Composition	Jayanta Halder, Yarlagadda Venkateswarlu, Akkapeddi Padma	Australia	2012338461	13/10/2016

Intrinsically Fluorescent Carbon Nanospheres And A Process Thereof	Tapas Kumar Kundu, Es-waramoorthy Muthusamy, Selvi Bharatha Ruthrotha Vikru, Dinesh Jagadeesan	India	272637	13/04/2016
		Europe	Received communication reg. 'Intention to Grant Patent'	17/11/2016
Artificial Retina Device (Bulk heterojunction/electrolyte polymers as novel biocompatible photoactive multi color-sensing technology)	Kavassery Sureswaran Narayan, Vini Gautam, Monijit bag	USA	9322713 B2	26/04/2016
Chromophores for Detection of Volatile Organic Compounds	Subi Jacob George, Mohit Kumar	USA	9376435B2	28/06/2016
Antimicrobial Compounds, Their Synthesis and Applications Thereof	Jayanta Haldar, Chandradhish Ghosh, Gautham Belagula Manjunath, Padma Akkapeddi	USA	Received 'Notice of Allowance'	25/11/2016
Manufacturing Strain Sensitive Sensors and/or Strain Resistant Conduits From a Metal and Carbon Matrix	Kulkarni Giridhar Udapi Rao, BoyaRadha, Abhay A Sagade	USA	9562814	07/02/2017
Nanoparticle Compositions Of Antibacterial Compounds And Other Uses Thereof	Jayanta Haldar, Divakara Siva Sathyanarayana Murthy Uppu, Akkapeddi Padma, Goutham Belagula Manjunath	USA	Received 'Notice of Allowance' on 11.01.2017	11/01/2017
A Synthetic Cyclic Dipeptide And A Process Thereof	Govindaraju Thimmaiah	India	281909	28/03/2017

Following are the members of this Unit

Dean, Research & Development

Prof. K.S. Narayan

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

Technical Officer Gr. I

A.V. Nagarathnamma

M.Sc.

Technical Staff

Yadati Rajyalakshmi

B.E.



RESEARCH PROGRAMMES

RESEARCH AREAS

1. Chemistry and Physics of Materials Unit (CPMU)

- Computational molecular science
- Programmable molecular materials in imaging and diagnostics
- Raman, brillouin spectroscopy and high pressure research
- Nanomaterials and catalysis
- Nanomaterials, nanofabrication and devices
- Functional organic/organic-inorganic hybrid materials
- Organic electronics, photovoltaics, device physics and bio-electronics
- Chemistry of materials
- Novel low-dimensional properties of GaN thin films
- Magnetism, superconductivity and multiferroicity
- Engineering Mechanics Unit (EMU)
- Fluid mechanics and heat transfer
- Mechanics of granular matter and nonlinear dynamics
- Computational physics
- Aerospace and atmospheric fluid mechanics
- Complex fluids and flows

2. Evolutionary and Integrative Biology Unit (EIBU)

- Circadian rhythms in fruit flies and ants
- Evolutionary genetics, life-history evolution and population dynamics
- Animal behavior and sociogenetics

3. Geodynamics Unit

- Neotectonics and environmental geology
- Fault zone studies, active tectonics and seismic hazard

4. Molecular Biology and Genetics Unit (MBGU)

- Molecular and cellular mechanisms of human genetic disorders
- Molecular parasitology and molecular enzymology
- Stem cell potency and cardiovascular development

-
-
- Transcription regulation and chromatin dynamics
 - Autophagy and autophagy related pathways
 - Chromatin biology and genomics
 - Genetic and epigenetic definition of centromeres
 - Mechanisms underlying pathogenesis of human cerebral malaria
 - The HIV-1 subtype-C strain

5. Neuroscience Unit (NSU)

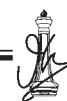
- Molecular pathways in gliomagenesis
- SynGAP1 in neuronal function and in Intellectual disability
- Neuronal circuits in fruit flies

6. New Chemistry Unit (NCU)

- Engineering molecular systems for biological applications
- Thermoelectrics and metal chalcogenides
- Supramolecular functional (organic and hybrid) materials
- Bioorganic chemistry
- Chemical biology and medicinal chemistry
- Designing new ways to small molecule heterocyclic scaffolds
- Solid state inorganic chemistry
- Semiconductor nanocrystals

7. Theoretical Science Unit (TSU)

- Theory and simulations of materials
- Statistical physics of systems at and away from equilibrium
- Nonequilibrium phenomena in physics and biology
- Computational nanoscience
- Advanced quantum theory: from molecules to materials
- Computational studies of protein-protein interactions
- Phase transformations and dynamics of soft matter
- Non-commutative probability and geometry: mathematics of quantum mechanics
- Coorelated electron systems and organic electronics



8. International Centre for Materials Science (ICMS)

- HRTEM, HREELS, semiconductors, thin film growth
- Experimental soft condensed matter research
- Organic semiconductors and asymmetric catalysis
- Obtaining high mobility indium nitride and InGaN thin films
- Semiconductor nanocrystals: electronic structure study

RESEARCH FACILITIES

- Jeol 600 MHz. NMR spectrometer
- Micro plate reader
- Electrical measurement system for IV/CV
- Low temperature manual probe station
- Chemiluminescence gel documentation system
- LabRamII Raman Spectrometer
- Optical tables, standard isolator, air compressor, table top plate
- Dr. Sinter lab Spark plasma sintering system SPS211Lx
- Combiflash Rf+ Automated flash chromatography system
- SpectraMax i3X multimode microplate reader
- Diode pumped solid state laser
- Labconco Benchtop freeze dry system
- Shimadzu HPLC system
- Boston HP servers etc
- Electrochemical workstation with biopotentiostat/galvanostat
- QX200droplet digital PCR system & CFX touch real-time PCR
- Leica fully motorized Microtome
- Electrochemical workstation with biopotentiostat/galvanostat +bcycler
- High resolution and sensitive confocal microscope
- Modular glove box
- Typhoon FLA 7000 IPA
- Cyclic voltametry system with electrochemical workstation

SPONSORED ONGOING RESEARCH PROJECTS

Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
1	J C Bose Fellowship	SERB	Amitabh Joshi	10	0
2	Congenital deafness in Dhadkai Village of Doda of Jammu & Kashmir	ICMR	Anuranjan Anand	4	0
3	Towards identification of novel genes for a reflex epilepsy (hot water epilepsy) triggered by tactile & temperature stimuli	ICMR	Anuranjan Anand	3	0
4	Thematic Unit of Excellence on "Computational Materials Science" at JNCASR	DST	Balasubramanian S	6	0
5	Geological & geomorphic characterization of the frontal thrust fault at central & northeast Himalaya	MOES	C P Rajendran	2	11
6	Post Doctoral Fellowship Programme entitled "Nano Science and Technology (NS &T) Overseas Visiting Fellowships" under the guidance of Prof. C.N.R. Rao	DST	C.N.R. Rao	1	0
7	MOU between RAK-CAM and JNCASR	SSL	C.N.R. Rao	6	0
8	MOU between DRDO and JNCASR	DRDO	C.N.R. Rao	5	0
9	CSIR Center for Excellence in Chemistry	CSIR	C.N.R. Rao	5	0
10	Evaluating earthquake tsunami recurrence along the Adaman Arc from the study of shallow cores	INCOIS	C P Rajendran	4	0
11	Development of a beam line at PETRA III & assured access to all PETRA III beam lines & flash facility at Desy, Hamburg, Germany	DST	Chandrabhas Narayana	1	5
12	Controlled release dispensers for delivery of semiochemicals	DBT	Eswaramoorthy M	3	0
13	Clay satblized metal nanoprtical for catalysis	SHELL	Eswaramoorthy M	2	0
14	Development of biomimetic materials as substitutes for natural fibers using designed modular peptides	DBT	Govindaraju T	6	0
15	Developing novel chemosensors of metal ions in aqueous media for environmental & biological applications	CSIR	Govindaraju T	3	0
16	Development of nucleic acid hybrid nanosystems & materials for durg targeting delivery & biosensing applications	DBT	Govindaraju T	3	0



Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
17	Deciphering the role of purine nucleotide cycle in plasmodium by metabolic rewiring using genetic strategies	DBT	Hemalatha Balam	3	0
18	Significance of fumarate metabolism in plasmodium examination of the growth phenotype of FH MQO & AAT knockout parasites	SERB	Hemalatha Balam	3	0
19	Malarial parasite biology: an avenue to discover new drug targets (phase II) under the category II Outstanding Scientist Research Programme in Biotechnology of Centre of Excellence and Innovation	DBT	Hemalatha Balam	5	0
20	Start up grant for young scientists entitled "Holocene climate change & tracking the impact of anthropogenic activity in Wular or Mansar Lake in Kashmir Himalaya: appraisal of human influence"	SERB	Jaishri Bhatt	2	0
21	Impact of SYANGAP 1 heterozygous mutations on the maturation & function of GABAergic interneurons during development	SERB	James Chelliah	3	0
22	Collaborative research work with Public Health of England	PHE	Jayanta Haldar	2	0
23	Development of novel organic-inorganic antimicrobial with hydroxyapatite & antimicrobial polymer	DST	Jayanta Haldar	3	0
24	Develop a powerful new antibiotic that kills all resistant bacteria	SRISTI	Jayanta Haldar	2	0
25	Development of new class of glycopeptide antibiotics for tackling drug resistant bacterial infections	BIRAC	Jayanta Haldar	2	0
26	Development of laboratory setup to evaluate the performance of drag reducers for refinery streams pipeline transportation	HPCL	K R Sreenivas	1	0
27	Improving organic solar cell performance in large area architecture by use of active encapsulation & aging studies	DST	K S Narayan	3	0
28	Advancing the efficiency & production potential of excitonic solar cells (apex phase II)	DST	K S Narayan	2	0

Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
29	Setting up of Technical Research Center at the Jawaharlal Nehru Center for Advanced Scientific Research Bangaluru	DST	K S Narayan	5	0
30	SERB Distinguished Fellow	SERB	Kalyan Bidhan Sinha	3	0
31	Ramanujan Fellowship	SERB	Kanishka Biswas	5	0
32	DAE Young Scientist Research award entitled "Efficient waste heat to electrical energy conversion in chalcopyrite AGINX2"	DAE	Kanishka Biswas	3	0
33	Financial assistance for Indian scientists to carry out experiments at International synchrotron radiation facilities & neutron facilities for materials science research	DST	Kanishka Biswas	5	0
34	Structure-function analysis of centromeres of a pathogenic budding yeast <i>Candida Tropicali</i>	DBT	Kaustuv Sanyal	4	0
35	Characterization of the fungal specific DAM1 complex as an attractive target for safer and more potent antifungal drug to treat candidiasis	DBT	Kaustuv Sanyal	4	0
36	Identification of centromeres of the budding yeast <i>Saccharomyces Castellii</i>	DBT	Kaustuv Sanyal	3	0
37	Role of histone H3 variants in genome indexing in <i>Candida Albicans</i>	SERB	Kaustuv Sanyal	3	0
38	J C Bose Fellowship	SERB	K S Narayan	5	0
39	Postdoctoral Fellowship in Nanoscience & Technology	DST	Kulkarni G U	10	0
40	Thematic Unit of Excellence on Nanochemistry at JNCASR, Bangalore	DST	Kulkarni G U	5	0
41	Assured access to all the beam lines of isis neutron scattering facility at Rutherford Appleton Laboratory (RAL), UK for carrying out research in nanoscience and technology	DST	M. K. Sanyal, SINP & Jayachandra A N	5	0
42	Indo - Denmark titled "Genetics towards future genetics towards future cell therapy in diabetes & cardiovascular disease understanding embryonic stemparcreatic beta cells & cardiomyoc"	DBT	Maneesha S Inamdar	4	0
43	Analysis of human development emt in vitro & establishment of ex vivo models of embryogenesis	DBT	Maneesha S Inamdar	3	0



Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
44	Elucidation of conserved molecular signatures and regulators for blood cell prgenitor maintenance	CEFIPRA	Maneesha S Inamdar	3	0
45	Analysis of factors regulating self renewal and differentiation to aid generation of lineage restricted stem cells/progenitors for cell replacement therapy	DBT	Maneesha S Inamdar & Hemalatha Balaram	4	5
46	Experiments using salt water / fresh water test facility for buyoancy induced flow studies	BARC	Meheboob alam	3	4
47	SERB Distinguished Fellow	SERB	M R S Rao	3	0
48	Chromatin biology research - phase II	DBT	M R S Rao	5	0
49	Analysis of in vivo transcription of plasmodium falciparum from indian patents suffering from cerebral malaria and its comparision with cerebral malaria and its comparision with (mod) symptoms	ICMR	Namita Surolia	3	0
50	The Year of Science Professorship	DST	Narasimha R	5	0
51	Numerical simulation of cloud flow and mixing layers	INTEL	Narasimha R	5	0
52	HPC simulations with ANUROOP: code acceleration, optimization and benchmarking	DRDO	Narasimha R	2	0
53	DST-INSPIRE Faculty Award	DST	Rajani Garg	5	0
54	Research work in HIV lab	MDPL	Ranga Udaykumar	1	0
55	A multi- centric observational study to examine replicative fitness & pathogenic proper ties of the emerging new viral strains of HIV-1 in India	DBT	Ranga Udaykumar	3	0
56	The biological significance of unique NF-KB binding site in the viral promoter of HIV -1 sub type C	SERB	Ranga Udaykumar	3	0
57	Synthesis and study of the otical magnetic and electrical properties of co-doped II-IV semiconductor nanocrystals	DST	Ranjani Viswanatha	3	0
58	Small molecule modulators of autophagy and autophagy related pathways	WT-DBT	Ravi Manjithaya	5	0
59	MoU between JNCASR & HPCL development of microbial catalyts (biocatalyts) for fermentative butanol production	HPCL	Ravi Manjithaya	3	9

Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
60	Multiscale modeling of complex fluids	SERB	Ravi Manjithaya	3	0
61	Structure-property relations in the RE2TSI3(RE= RARE EARTHS: T= transition metals) compounds	CSIR	Sebastain C Peter	3	0
62	Experimental realization of the topological insulators from the heusler compounds	SERB	Sebastian C Peter	3	0
63	A study of the interactions between the circadian clock & homeostatic mechanisms regulating sleep & arousal in drosophila melanogaster	SERB	Sheeba Vasu	3	0
64	Magentism of self - organized structures at surfaces	CEFIPRA	Shobhana Narasimhan	3	0
65	Extending the D-band model of transaction metal Ca catalyts to S and P bands	IKST	Shobhana Narasimhan	1	0
66	Computational modeling on fuels cells for clean & efficient energy storage	SERB	Siamkhanthang Neihisial	3	0
67	J C Bose Fellowship	SERB	Srikanth Sastry	3	0
68	Exploring A-site magnetic & a-site ordered spinel oxides for magnetoelectric & multiferroic properties	SERB	Sundaresan A	3	0
69	J C Bose Fellowship	DST	Swapam K Pati	5	0
70	Nano 2 Fun	EU	Swapam K Pati	4	0
71	Theranostic approach for mechanistic understanding & discovery of novel inhibitors of neurodegenerative diseases	SERB	T. Govindaraju	3	0
72	J C Bose Fellowship	DST	Tapas Kumar Kundu	10	0
73	Regulation of chromatin associated proteins by mirnas: implications in breast cancer	DBT	Tapas Kumar Kundu	4	6
74	Investigating the role of BLM helicase as a global tumor suppressor: undersatnding its regulatory LOO Loops & using the knowledge for therapeutic & clinical applications in cancer biology	DBT	Tapas Kumar Kundu	5	0
75	Development of nano-particle based directed delivery systems for peptide therapeutics	DST	Tapas Kumar Kundu	3	0
76	Programme support on chromatin and disease (chromatin dynamics and transcription regulations: implications in disease and therapeutics)	DBT	Tapas Kumar Kundu & Ranga Udaykumar	5	6



Sl. No.	Project Title	Funded by	Principle/ project investigator	Years	Months
77	Encapsulation and stabilization of metal or metal- complexes in nanoscale Metal-Organic Frameworks (MOFs) for gas storage, magnetism and heterogeneous catalysis	SERB	Tapas Kumar Maji	3	0
78	Between - group encounters & its correlates in female Asian elephants	NGS	T N C Vidya	3	2
79	Between - group encounters & its correlation in female asian elephants	CSIR	T N C Vidya	3	0
80	Ramanujan Fellowship	DST	Ujjal K Gautam	5	0
81	J C Bose Fellowship	DST	Umesh V Waghmare	5	0
82	Tuning coupled dynamics of electrons & phonons in MoS ₂ with strain, substrate & electrodes	AOARD	Umesh V Waghmare	3	0
83	Plasticity of covalent nanoprticles	CEFIPRA	Umesh V Waghmare	3	0
84	Consultancy & Collaborative Research Work	SHELL	Umesh V Waghmare	1	0
85	Raman Charpak Fellowship Mr. Bel Haj Salah Selim, Visiting Student	CEFIPRA	Umesh V Waghmare	0	4
86	J C Bose Fellowship	SERB	V Nagaraja	5	0
87	Design & development of new synthetic methods for novel heterocyclic motifs via multicomponent & domino reactions	SERB	Vibha Gautam	3	0
88	Molecular genetic & neuronal analysis of early & late emergence chronotypes in drosophila melanogaster populations	SERB	Vijay Kumar Sharma	3	0

NEW SPONSORED PROJECTS STARTED DURING 2016-17

Sl. No.	Project Title	Funded By	Principle/ project investigator	Years	Months
1	National Postdoctoral Fellowship	SERB	Amit Gupta	2	0
2	From disease phenotype to the molecular mechanisms underlying juvenile myoclonic epilepsy	ICMR	Anuranjan Anand	3	0
3	National Postdocotral Fellowship	SERB	Ashish Singh	2	0
4	Implementaion of phase II of Indian Beamline at Photon Factory, Kek, Tskuba, Japan	DST	Chandrabhas Narayana	5	0
5	Amplification-free molecular detection of nucleic acids using Surface-Enhanced Raman Spectroscopy	TRC	Chandrabhas Narayana	2	0
6	Develop a novel compound restores obsolete antibiotics to NDM-1 superbugs	SRISTI	Diwakar S S Murthy	2	0
7	Molecular probes for in vitro and in cellulo detection of toxic-amyloid beta aggregation species found in Alzheimer's disease	DST	Govindaraju T	1	0
8	Multifunctional probes and inhibitors to study and alleviate multifaceted toxicity in Alzheimer's disease	DST	Govindaraju T	5	0
9	Prevention is better than cure: biodegradable antimicrobial paint that kills bacteria and fungi and prevents infection	SRISTI	Jayanta Haldar	1	0
10	Development of cationic cleavable amphiphiles and study aggregation and antibacterial properties	DAE	Jayanta Haldar	3	0
11	Acyclic and cyclic lipopeptides to combat bacterial resistance and eradicate biofilms	SERB	Jayanta Haldar	3	0
12	Temperature and pressure dependent studies on Metal Organic Frameworks (MOFs) and evaluation of their performance for gas storage by Raman sepectroscopy and X-Ray diffraction	SERB	Kamali Kesavan	2	0
13	Scale-up synthesis of low cost high performance P and N-type thermoelectric (TE) materials and development of TE module for "waste heat to electrical energy conversion"	TRC	Kanishka Biswas	2	0
14	PB-free thermoelectric energy conversion: enhancement of thermoelectric performance of snite by alliovalent doping, valence band convergence and nanostructuring	SERB	Kanishka Biswas	3	0
15	A PCR-based approach for rapid detection of the human pathogenic candida species	TRC	Kaustuv Sanyal	2	0



Sl. No.	Project Title	Funded By	Principle/ project investigator	Years	Months
16	Women Scientist Scheme A (WOS-A) "Interdependence of ubiquitin proteasome system and autophagy in cellular proteostasis and its relevance in neurodegenerative disorders"	SERB	Lakshmi Garimella	3	0
17	National Postdoctoral Fellowship	SERB	M Shivanna	2	0
18	Understanding the cross-talk between cellular compartments for regulation of drosophila blood cell homeostasis	SERB	Maneesha S Inamdar	3	0
19	SERB National Postdoctoral Fellowship	SERB	Nagaraja K K	2	0
20	Development of novel antituberculosis compounds	DST	Nagaraja V	2	0
21	National Postdoctoral Fellowship	SERB	Nandu Gopan	2	0
22	Photovoltaics-printing solar cells, packaged instrumentation for scanning and solar-simulator, designing prototype of smart-cart for outdoor vendors	DST	Narayan K S	1	6
23	National Postdoctoral Fellowship	SERB	Provas Pal	2	0
24	Evaluation of tsunami hazard for the eastern seaboard of India	DAE	Rajendran C P	3	0
25	Collaborative work on "Characterization of materials -pressure sensitive adhesive and optically clear resin"	SAMSUNG	Rajesh Ganapathy	2	0
26	Designer granular matter for probing the physics of non-equilibrium glass transition(s)	DST	Rajesh Ganapathy	5	0
27	Engineering of HIV-1 subtype C and subtype B infectious molecular clones and examine the significance of natural polymorphic variations on drug resistance	CSIR	Ranga Udaykumar	3	0
28	The combinatorial effects of oplates and the emerging promoter-variant strains of HIV-1 subtype C on HIV neuropathogenesis and latency	NIH-UNMC	Ranga Udaykumar	4	11
29	Diffusion of dopants in semiconducting nanocrystals leading to diverse optical and magnetic properties	INSA	Ranjani Viswanatha	3	0
30	SERB Women Excellence Award	SERB	Ranjani Viswanatha	3	0
31	Molecular mechanisms underlying the clearance of cytotoxic protein aggregates associated with parkinsonism through induction of autophagy by small molecule modulations	SERB	Ravi Manjithaya	3	0

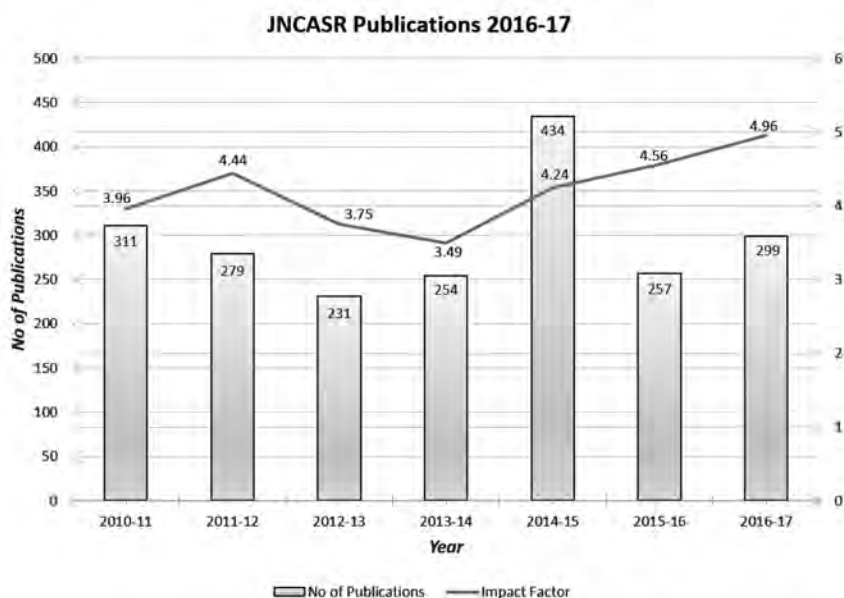
Sl. No.	Project Title	Funded By	Principle/ project investigator	Years	Months
32	National Postdoctoral Fellowship	SERB	Sajad Ahmed Bhat	2	0
33	Tailoring the properties of InGaN/TiO ₂ nano-heterostructures for the fabrication of efficient water splitters	DST	Saraswathi C	3	0
34	Innovative Young Biotechnology Award - "Optical nanoscopy using fluorogenic click-on dyes"	DBT	Sarit S Agasti	3	0
35	Microfluidics assisted fabrication of bio-orthogonal colloidal microcapsules for single cell analysis	SERB	Sarit S Agasti	3	0
36	Nanosopic imaging with DNA for network level understanding of cytoskeletal alterations during aging	WT-DBT	Sarit S Agasti	5	0
37	Indo-German(DST-DAAD) Joint Research Project "Structure and physical properties of Yb based indides"	DST	Sebastian C Peter	2	0
38	Efficient conversion of Co ₂ into fuel and chemicals using ordered nano intermetallics	DST	Sebastian C Peter	3	0
39	Device fabrication of efficient non-PT based ordered intermetallic nanoparticles as electrode materials for fuel green energy production	DST	Sebastian C Peter	2	0
40	Indo-French Collaboration Project "Studies on the topological insulator behavior in heavy metal based ternary chalcogenides"	CEFIPRA	Sebastian C Peter	3	0
41	National Postdoctoral Fellowship	SERB	Shafeekh Kulathinte Meethal	2	0
42	Thematic project entitled "Chemical physics of functional nanostructures and interfaces"	DST	Shivaprasad S M	3	0
43	Mathematical modelling of thin film coating flows	SERB	Siamkhanthang Neihisial	3	0
44	NBHM Postdoctoral Fellowship	DAE	Soumalya Joardar	3	0
45	DST INSPIRE Faculty Award	DST	Soumalya Joardar	2	0
46	National Postdoctoral Fellowship	SERB	Sreedevi P	2	0
47	Energy efficient polyhouse and aeroponic system for mini tuber production of tissue cultured potato	ICAR	Sreenivas K R	3	0
48	National Postdoctoral Fellowship	SERB	Sreenivasulu Bandi	2	0



Sl. No.	Project Title	Funded By	Principle/ project investigator	Years	Months
49	A tunable strong base catalyst and its applications	SERB	Sridhar Rajaram	3	0
50	Synthesis of metal free triplet phosphors with tunable emission	TRC	Subi Jacob George	2	0
51	National Postdoctoral Fellowship	SERB	Sukanta Mondal	2	0
52	Indo-Russian Project entitled "layered pervoskite - related oxide materials: synthesis structure and properties"	DST	Sundaresan A	2	0
53	Modeling charge carrier transport properties and rechargeable batter components on a large class of layered materials by accurate computational tools	SERB	Swapan K Pati	3	0
54	Self-fluorescent cell permeable glucose derived carbon nanospheres as a brain targeting vehicle: implications in drug delivery and imaging	DBT	Tapas Kumar Kundu	3	0
55	Donor-acceptor porous organic polymers for H ₂ storage and photocatalytic H ₂ generation	DST	Tapas Kumar Maji	2	0
56	High-throughput virtual screening for accelerated materials discovery: DFT descriptor generation for Co ₂ electroreduction catalyst screening	SHELL	Umesh V Waghmare	1	0
57	National Postdoctoral Fellowship - design and development of ordered intermetallic supported nanocatalysts for the conversion of bio-renewable feedstock	SERB	Vijaykumar S Marakatti	2	0

PUBLICATIONS

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



Chemistry and Physics of Materials Unit (CPMU)

1. Vijayan, R.; Swathi, K.; Narayan, K. S., Synergistic Effects of Electric-Field-Assisted Annealing and Thermal Annealing in Bulk-Heterojunction Solar Cells. *ACS Applied Materials & Interfaces* **2016**, <http://dx.doi.org/10.1021/acsmi.6b09480>
2. Avinash, M. B.; Swathi, K.; Narayan, K. S.; Govindaraju, T., Molecular Architectonics of Naphthalenediimides for Efficient Structure-Property Correlation. *ACS Applied Materials & Interfaces* **2016**, *8* (13), 8678-8685 <http://dx.doi.org/10.1021/acsmi.6b00011>
3. Gokhale, S.; Sood, A. K.; Ganapathy, R., Deconstructing the glass transition through critical experiments on colloids. *Advances in Physics* **2016**, *65* (4), 363-452 <http://dx.doi.org/10.1080/00018732.2016.1200832>
4. Karadan, P.; John, S.; Anappara, A. A.; Narayana, C.; Barshilia, H. C., Evolution mechanism of mesoporous silicon nanopillars grown by metal-assisted chemical etching and nanosphere lithography: correlation of Raman spectra and red photoluminescence. *Applied Physics a-Materials Science & Processing* **2016**, *122* (7), <http://dx.doi.org/10.1007/s00339-016-0203-8>
5. Rajaji, V.; Malavi, P. S.; Yamijala, Ssrkc; Sorb, Y. A.; Dutta, U.; Guin, S. N.; Joseph, B.; Pati, S. K.; Karmakar, S.; Biswas, K.; Narayana, C., Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe₂. *Applied Physics Letters* **2016**, *109* (17), <http://dx.doi.org/10.1063/1.4966275>
6. Swathi, K.; Narayan, K. S., Image pixel device using integrated organic electronic components. *Applied Physics Letters* **2016**, *109* (19), <http://dx.doi.org/10.1063/1.4967505>
7. Kumar, P.; Devi, P.; Kumar, M.; Shivaprasad, S. M., Optimization of energy and fluence of N²⁽⁺⁾ ions in the conversion of Al₂O₃ surface into AlN at room temperature. *Applied Surface Science* **2016**, *361*, 265-268 <http://dx.doi.org/10.1016/j.apsusc.2015.11.180>



-
-
8. Santhosh, V.; Voggu, R.; Chaturbedy, P.; Ganapathy, R.; Rao, C. N. R., Mechanical properties of C-60 thin films at the air-water interface. *Carbon* **2016**, *96*, 1-5 <http://dx.doi.org/10.1016/j.carbon.2015.08.098>
 9. Karthigeyan, D.; Surabhi, S.; Mizar, P.; Soumik, S.; Banerjee, A.; Sinha, S. H.; Dasgupta, D.; Narayana, C.; Kundu, T. K., A Dual Non-ATP Analogue Inhibitor of Aurora Kinases A and B, Derived from Resorcinol with a Mixed Mode of Inhibition. *Chemical Biology & Drug Design* **2016**, *87* (6), 958-967 <http://dx.doi.org/10.1111/cbdd.12728>
 10. Chakraborty, A.; Achari, A.; Eswaramoorthy, M.; Maji, T. K., MOF-aminoclay composites for superior CO₂ capture, separation and enhanced catalytic activity in chemical fixation of CO₂. *Chemical Communications* **2016**, *52* (76), 11378-11381 <http://dx.doi.org/10.1039/c6cc05289d>
 11. Chakraborty, A.; Bhattacharyya, S.; Hazra, A.; Ghosh, A. C.; Maji, T. K., Post-synthetic metalation in an anionic MOF for efficient catalytic activity and removal of heavy metal ions from aqueous solution. *Chemical Communications* **2016**, *52* (13), 2831-2834 <http://dx.doi.org/10.1039/c5cc09814a>
 12. Sutar, P.; Maji, T. K., Bimodal self-assembly of an amphiphilic gelator into a hydrogel-nanocatalyst and an organogel with different morphologies and photophysical properties. *Chemical Communications* **2016**, *52* (89), 13136-13139 <http://dx.doi.org/10.1039/c6cc06971a>
 13. Sutar, P.; Maji, T. K., Coordination polymer gels: soft metal-organic supramolecular materials and versatile applications. *Chemical Communications* **2016**, *52* (52), 8055-8074 <http://dx.doi.org/10.1039/c6cc01955b>
 14. Roy, S.; Suresh, V. M.; Maji, T. K., Self-cleaning MOF: realization of extreme water repellence in coordination driven self-assembled nanostructures. *Chemical Science* **2016**, *7* (3), 2251-2256 <http://dx.doi.org/10.1039/c5sc03676c>
 15. Siddhanta, S.; Zheng, C.; Narayana, C.; Barman, I., An impediment to random walk: trehalose microenvironment drives preferential endocytic uptake of plasmonic nanoparticles. *Chemical Science* **2016**, *7* (6), 3730-3736 <http://dx.doi.org/10.1039/c6sc00510a>
 16. Uppu, Dssm; Konai, M. M.; Baul, U.; Singh, P.; Siersma, T. K.; Samaddar, S.; Vemparala, S.; Hamoen, L. W.; Narayana, C.; Haldar, J., Isosteric substitution in cationic-amphiphilic polymers reveals an important role for hydrogen bonding in bacterial membrane interactions. *Chemical Science* **2016**, *7* (7), 4613-4623 <http://dx.doi.org/10.1039/c6sc00615a>
 17. Hazra, A.; Bonakala, S.; Bejagam, K. K.; Balasubramanian, S.; Maji, T. K., Host-Guest 2+2 Cycloaddition Reaction: Postsynthetic Modulation of CO₂ Selectivity and Magnetic Properties in a Bimodal Metal-Organic Framework. *Chemistry-a European Journal* **2016**, *22* (23), 7792-7799 <http://dx.doi.org/10.1002/chem.201505131>
 18. Kanoo, P.; Haldar, R.; Reddy, S. K.; Hazra, A.; Bonakala, S.; Matsuda, R.; Kitagawa, S.; Balasubramanian, S.; Maji, T. K., Crystal Dynamics in Multi-stimuli-Responsive Entangled Metal-Organic Frameworks. *Chemistry-a European Journal* **2016**, *22* (44), 15864-15873 <http://dx.doi.org/10.1002/chem.201602087>
 19. Sikdar, N.; Bonakala, S.; Haldar, R.; Balasubramanian, S.; Maji, T. K., Dynamic Entangled Porous Framework for Hydrocarbon (C₂-C₃) Storage, CO₂ Capture, and Separation. *Chemistry-a European Journal* **2016**, *22* (17), 6059-6070 <http://dx.doi.org/10.1002/chem.201505217>
 20. Haldar, R.; Prasad, K.; Samanta, P. K.; Pati, S.; Maji, T. K., Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al³⁺ Sensing. *Crystal Growth & Design* **2016**, *16* (1), 82-91 <http://dx.doi.org/10.1021/acs.cgd.5b01448>

-
-
21. Chakraborty, A.; Escuer, A.; Ribas, J.; Maji, T. K., A discrete Cu-6(II) cluster and a 3D Mn-II-Cu-II framework based on assembly of Mn₂Cu₄ clusters: synthesis, structure and magnetic properties. *Dalton Transactions* **2016**, 45 (39), 15523-15531 <http://dx.doi.org/10.1039/c6dt03094g>
 22. Palimar, S.; Kaushik, S. D.; Siruguri, V.; Swain, D.; Viegas, A. E.; Narayana, C.; Sundaram, N. G., Investigation of Ca substitution on the gas sensing potential of LaFeO₃ nanoparticles towards low concentration SO₂ gas. *Dalton Transactions* **2016**, 45 (34), 13547-13555 <http://dx.doi.org/10.1039/c6dt01819j>
 23. Banik, A.; Vishal, B.; Perumal, S.; Datta, R.; Biswas, K., The origin of low thermal conductivity in Sn_{1-x}Sb_xTe: phonon scattering via layered intergrowth nanostructures. *Energy & Environmental Science* **2016**, 9 (6), 2011-2019 <http://dx.doi.org/10.1039/c6ee00728g>
 24. Haldar, R.; Inukai, M.; Horike, S.; Uemura, K.; Kitagawa, S.; Maji, T. K., Cd-113 Nuclear Magnetic Resonance as a Probe of Structural Dynamics in a Flexible Porous Framework Showing Selective O₂/N₂ and CO₂/N₂ Adsorption. *Inorganic Chemistry* **2016**, 55 (9), 4166-4172 <http://dx.doi.org/10.1021/acs.inorgchem.5b02873>
 25. Roy, S.; Sarkar, S.; Pan, J.; Waghmare, U. V.; Dhanya, R.; Narayana, C.; Peter, S. C., Crystal Structure and Band Gap Engineering in Polyoxometalate-Based Inorganic-Organic Hybrids. *Inorganic Chemistry* **2016**, 55 (7), 3364-3377 <http://dx.doi.org/10.1021/acs.inorgchem.5b02718>
 26. Sadhu, A.; Salunke, H. G.; Shivaprasad, S. M.; Bhattacharyya, S., Extensive Parallelism between Crystal Parameters and Magnetic Phase Transitions of Unusually Ferromagnetic Praseodymium Manganite Nanoparticles. *Inorganic Chemistry* **2016**, 55 (16), 7903-7911 <http://dx.doi.org/10.1021/acs.inorgchem.6b00815>
 27. Loukya, B.; Negi, D. S.; Sahu, R.; Pachauri, N.; Gupta, A.; Datta, R., Structural characterization of epitaxial LiFe₅O₈ thin films grown by chemical vapor deposition. *Journal of Alloys and Compounds* **2016**, 668, 187-193 <http://dx.doi.org/10.1016/j.jallcom.2016.01.217>
 28. Dileep, K.; Sahu, R.; Sarkar, S.; Peter, S. C.; Datta, R., Layer specific optical band gap measurement at nanoscale in MoS₂ and ReS₂ van der Waals compounds by high resolution electron energy loss spectroscopy. *Journal of Applied Physics* **2016**, 119 (11), <http://dx.doi.org/10.1063/1.4944431>
 29. Joshya, R. S.; Rajaji, V.; Narayana, C.; Mascarenhas, A.; Kini, R. N., Anharmonicity in light scattering by optical phonons in GaAs_{1-x}Bi_x. *Journal of Applied Physics* **2016**, 119 (20), <http://dx.doi.org/10.1063/1.4952381>
 30. Shetty, S.; Shivaprasad, S. M., Early stages of plasma induced nitridation of Si (111) surface and study of interfacial band alignment. *Journal of Applied Physics* **2016**, 119 (5), <http://dx.doi.org/10.1063/1.4941102>
 31. Tangi, M.; De, A.; Ghatak, J.; Shivaprasad, S. M., Electron mobility of self-assembled and dislocation free InN nanorods grown on GaN nano wall network template. *Journal of Applied Physics* **2016**, 119 (20), <http://dx.doi.org/10.1063/1.4952380>
 32. Karmakar, T.; Roy, S.; Balaram, H.; Balasubramanian, S., Structural and dynamical correlations in PfHGXPRT oligomers: A molecular dynamics simulation study. *Journal of Biomolecular Structure & Dynamics* **2016**, 34 (7), 1590-1605 <http://dx.doi.org/10.1080/07391102.2015.1085441>
 33. Karmakar, T.; Roy, S.; Balaram, H.; Prakash, M. K.; Balasubramanian, S., Product Release Pathways in Human and Plasmodium falciparum Phosphoribosyltransferase. *Journal of Chemical Information and Modeling* **2016**, 56 (8), 1528-1538 <http://dx.doi.org/10.1021/acs.jcim.6b00203>



-
-
34. Radhakrishnan, D.; Narayana, C., Guest dependent Brillouin and Raman scattering studies of zeolitic imidazolate framework-8 (ZIF-8) under external pressure. *Journal of Chemical Physics* **2016**, *144* (13), <http://dx.doi.org/10.1063/1.4945013>
 35. Rana, M.; Patil, P. K.; Chhetri, M.; Dileep, K.; Datta, R.; Gautam, U. K., Pd-Pt alloys nanowires as support-less electrocatalyst with high synergistic enhancement in efficiency for methanol oxidation in acidic medium. *Journal of Colloid and Interface Science* **2016**, *463*, 99-106 <http://dx.doi.org/10.1016/j.jcis.2015.10.042>
 36. Reddy, G. R.; Avadhani, A. S.; Rajaram, S., Activation of Benzyl Aryl Carbonates: The Role of Cation- π Interactions. *Journal of Organic Chemistry* **2016**, *81* (10), 4134-4141 <http://dx.doi.org/10.1021/acs.joc.6b00441>
 37. Bonakala, S.; Balasubramanian, S., Structure-Property Relationships in Amorphous Microporous Polymers. *Journal of Physical Chemistry B* **2016**, *120* (3), 557-565 <http://dx.doi.org/10.1021/acs.jpcc.5b08842>
 38. Das, S.; Karmakar, T.; Balasubramanian, S., Molecular Mechanism behind Solvent Concentration-Dependent Optimal Activity of Thermomyces lanuginosus Lipase in a Biocompatible Ionic Liquid: Interfacial Activation through Arginine Switch. *Journal of Physical Chemistry B* **2016**, *120* (45), 11720-11732 <http://dx.doi.org/10.1021/acs.jpcc.6b08534>
 39. Karmakar, T.; Balasubramanian, S., Molecular Dynamics and Free Energy Simulations of Phenylacetate and CO₂ Release from AMDase and Its G74C/C188S Mutant: A Possible Rationale for the Reduced Activity of the Latter. *Journal of Physical Chemistry B* **2016**, *120* (45), 11644-11653 <http://dx.doi.org/10.1021/acs.jpcc.6b07034>
 40. Mondal, A.; Balasubramanian, S., Understanding SO₂ Capture by Ionic Liquids. *Journal of Physical Chemistry B* **2016**, *120* (19), 4457-4466 <http://dx.doi.org/10.1021/acs.jpcc.6b02553>
 41. Dutta, D.; Gope, S.; Negi, D. S.; Datta, R.; Sood, A. K.; Bhattacharyya, A. J., Pressure-Induced Capillary Encapsulation Protocol for Ultrahigh Loading of Sulfur and Selenium Inside Carbon Nanotubes: Application as High Performance Cathode in Li-S/Se Rechargeable Batteries. *Journal of Physical Chemistry C* **2016**, *120* (51), 29011-29022 <http://dx.doi.org/10.1021/acs.jpcc.6b11017>
 42. Kumar, P.; Muthu, C.; Nair, V. C.; Narayan, K. S., Quantum Confinement Effects in Organic Lead Tribromide Perovskite Nanoparticles. *Journal of Physical Chemistry C* **2016**, *120* (32), 18333-18339 <http://dx.doi.org/10.1021/acs.jpcc.6b06545>
 43. Mondal, A.; Balasubramanian, S., Proton Hopping Mechanisms in a Protic Organic Ionic Plastic Crystal. *Journal of Physical Chemistry C* **2016**, *120* (40), 22903-22909 <http://dx.doi.org/10.1021/acs.jpcc.6b08274>
 44. Sikdar, N.; Dutta, D.; Haldar, R.; Ray, T.; Hazra, A.; Bhattacharyya, A. J.; Maji, T. K., Coordination-Driven Fluorescent J-Aggregates in a Perylenetetracarboxylate-Based MOF: Permanent Porosity and Proton Conductivity. *Journal of Physical Chemistry C* **2016**, *120* (25), 13622-13629 <http://dx.doi.org/10.1021/acs.jpcc.6b04347>
 45. Roy, S.; Hazra, A.; Bandyopadhyay, A.; Raut, D.; Madhuri, P. L.; Rao, D. S. S.; Ramamurty, U.; Pati, S. K.; Prasad, S. K.; Maji, T. K., Reversible Polymorphism, Liquid Crystallinity, and Stimuli-Responsive Luminescence in a Bola-amphiphilic π -System: Structure-Property Correlations Through Nanoindentation and DFT Calculations. *Journal of Physical Chemistry Letters* **2016**, *7* (20), 4086-4092 <http://dx.doi.org/10.1021/acs.jpcclett.6b01891>

-
-
46. Sharada, G.; Mahale, P.; Kore, B. P.; Mukherjee, S.; Pavan, M. S.; De, C. D.; Ghara, S.; Sundaresan, A.; Pandey, A.; Row, T. N. G.; Sarma, D. D., Is CH₃NH₃PbI₃ Polar? *Journal of Physical Chemistry Letters* **2016**, 7 (13), 2412-2419 <http://dx.doi.org/10.1021/acs.jpcclett.6b00803>
 47. De, A.; Shivaprasad, S. M., Epitaxy, phase separation and band-edge emission of spontaneously formed InGaN nanorods. *Journal of Physics D-Applied Physics* **2016**, 49 (35), <http://dx.doi.org/10.1088/0022-3727/49/35/355304>
 48. Sorb, Y. A.; Rajaji, V.; Malavi, P. S.; Subbarao, U.; Halappa, P.; Peter, S. C.; Karmakar, S.; Narayana, C., Pressure-induced electronic topological transition in Sb₂S₃. *Journal of Physics-Condensed Matter* **2016**, 28 (1), <http://dx.doi.org/10.1088/0953-8984/28/1/015602>
 49. Tomar, M.; Ashar, A. Z.; Narayan, K. S.; Mullen, K.; Jacob, J., Tuning the HOMO energy levels in quinoline and biquinoline based donor-acceptor polymers. *Journal of Polymer Research* **2016**, 23 (3), <http://dx.doi.org/10.1007/s10965-016-0945-1>
 50. Sarkar, S.; Borah, R.; Santhosha, A. L.; Dhanya, R.; Narayana, C.; Bhattacharyya, A. J.; Peter, S. C., Heterostructure composites of rGO/GeO₂/PANI with enhanced performance for Li ion battery anode material. *Journal of Power Sources* **2016**, 306, 791-800 <http://dx.doi.org/10.1016/j.jpowsour.2015.12.094>
 51. Dicko, H.; Pages, O.; Hussein, R. H.; Pradhan, G. K.; Narayana, C.; Firszt, F.; Marasek, A.; Paszkowicz, W.; Maillard, A.; Jobard, C.; Broch, L.; Hassan, F. E., Near-forward/high-pressure-backward Raman study of Zn_{1-x}BexSe (x similar to 0.5) - evidence for percolation behavior of the long (Zn?Se) bond. *Journal of Raman Spectroscopy* **2016**, 47 (3), 357-367 <http://dx.doi.org/10.1002/jrs.4817>
 52. Kumari, G.; Patil, N. R.; Bhadram, V. S.; Haldar, R.; Bonakala, S.; Maji, T. K.; Narayana, C., Understanding guest and pressure-induced porosity through structural transition in flexible interpenetrated MOF by Raman spectroscopy. *Journal of Raman Spectroscopy* **2016**, 47 (2), 149-155 <http://dx.doi.org/10.1002/jrs.4766>
 53. Subbarao, U.; Marakatti, V. S.; Amshumali, M. K.; Loukya, B.; Singh, D. K.; Datta, R.; Peter, S. C., Size and morphology controlled NiSe nanoparticles as efficient catalyst for the reduction reactions. *Journal of Solid State Chemistry* **2016**, 244, 84-92 <http://dx.doi.org/10.1016/j.jssc.2016.09.020>
 54. Gokhale, S.; Nagamanasa, K. H.; Sood, A. K.; Ganapathy, R., Influence of an amorphous wall on the distribution of localized excitations in a colloidal glass-forming liquid. *Journal of Statistical Mechanics-Theory and Experiment* **2016**, <http://dx.doi.org/10.1088/1742-5468/2016/07/074013>
 55. Pandeewar, M.; Senanayak, S. P.; Narayan, K. S.; Govindaraju, T., Multi-Stimuli-Responsive Charge-Transfer Hydrogel for Room-Temperature Organic Ferroelectric Thin-Film Devices. *Journal of the American Chemical Society* **2016**, 138 (26), 8259-8268 <http://dx.doi.org/10.1021/jacs.6b03811>
 56. Kumar, M.; Kumar, P.; Devi, P.; Shivaprasad, S. M., Formation of low-dimensional GaN on trenched Si(5512), probed by STM and XPS. *Materials Research Express* **2016**, 3 (3), <http://dx.doi.org/10.1088/2053-1591/3/3/035010>
 57. Jungmann, R.; Avendano, M. S.; Dai, M. J.; Woehrstein, J. B.; Agasti, S. S.; Feiger, Z.; Rodal, A.; Yin, P., Quantitative super-resolution imaging with qPAINT. *Nature Methods* **2016**, 13 (5), 439-+ <http://dx.doi.org/10.1038/nmeth.3804>
 58. Krishnamurthy, S.; Ghosh, S.; Chatterji, D.; Ganapathy, R.; Sood, A. K., A micrometre-sized heat engine operating between bacterial reservoirs. *Nature Physics* **2016**, 12 (12), 1134-+ <http://dx.doi.org/10.1038/nphys3870>
 59. Swathi, K.; Narayan, K. S., Solution processed integrated pixel element for an imaging device. In *Organic Sensors and Bioelectronics IX*, Kymissis, I.; Shinar, R.; Torsi, L., Eds. 2016; Vol. 9944, 978-1-5106-0280-9.



-
-
60. Saha, R.; Vasu, K.; Negi, D. S.; Datta, R.; Sundaresan, A.; Rao, C. N. R., Exchange bias at low fields exhibited by the interface between epitaxial layers of ferromagnetic and charge-ordered rare-earth manganites. *Physica Status Solidi-Rapid Research Letters* **2016**, *10* (8), 622-626 <http://dx.doi.org/10.1002/pssr.201600155>
 61. Mondal, A.; Sunda, A. P.; Balasubramanian, S., Thermal phase behavior and ion hopping in a 1,2,4-triazolium perfluorobutanesulfonate protic organic ionic plastic crystal. *Physical Chemistry Chemical Physics* **2016**, *18* (3), 2047-2053 <http://dx.doi.org/10.1039/c5cp05701a>
 62. Rao, K. V.; Haldar, R.; Maji, T. K.; George, S. J., Dynamic, conjugated microporous polymers: visible light harvesting via guest-responsive reversible swelling. *Physical Chemistry Chemical Physics* **2016**, *18* (1), 156-163 <http://dx.doi.org/10.1039/c5cp05052a>
 63. Narayan, B.; Sorb, Y. A.; Loukya, B.; Samanta, A.; Senyshyn, A.; Datta, R.; Singh, A. K.; Narayana, C.; Ranjan, R., Interferroelectric transition as another manifestation of intrinsic size effect in ferroelectrics. *Physical Review B* **2016**, *94* (10), <http://dx.doi.org/10.1103/PhysRevB.94.104104>
 64. Saha, R.; Ghara, S.; Suard, E.; Jang, D. H.; Kim, K. H.; Ter-Oganessian, N. V.; Sundaresan, A., Magnetolectric effect in simple collinear antiferromagnetic spinels. *Physical Review B* **2016**, *94* (1), <http://dx.doi.org/10.1103/PhysRevB.94.014428>
 65. Gokhale, S.; Ganapathy, R.; Nagamanasa, K. H.; Sood, A. K., Localized Excitations and the Morphology of Cooperatively Rearranging Regions in a Colloidal Glass-Forming Liquid. *Physical Review Letters* **2016**, *116* (6), <http://dx.doi.org/10.1103/PhysRevLett.116.068305>
 66. Adalikwu, S. A.; Chakraborty, A.; Hazra, A.; Ghosh, D.; Pati, S. K.; Maji, T. K., 2D coordination polymer composed of 1D {Ni-II(μ -O)(μ -H₂O)Ni-II}(n) ferromagnetic chains: Modulation of magnetic properties based on dehydration and rehydration. *Polyhedron* **2016**, *115*, 276-281 <http://dx.doi.org/10.1016/j.poly.2016.05.011>
 67. Mishra, C. K.; Sood, A. K.; Ganapathy, R., Site-specific colloidal crystal nucleation by template-enhanced particle transport. *Proceedings of the National Academy of Sciences of the United States of America* **2016**, *113* (43), 12094-12098 <http://dx.doi.org/10.1073/pnas.1608568113>
 68. Karadan, P.; Anappara, A. A.; Moorthy, V. H. S.; Narayana, C.; Barshilia, H. C., Improved broadband and omnidirectional light absorption in silicon nanopillars achieved through gradient mesoporosity induced leaky waveguide modulation. *RSC Advances* **2016**, *6* (110), 109157-109167 <http://dx.doi.org/10.1039/c6ra20467h>
 69. Deb, S.; Bhasker, H. P.; Thakur, V.; Shivaprasad, S. M.; Dhar, S., Polarization induced two dimensional confinement of carriers in wedge shaped polar semiconductors. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep26429>

Engineering Mechanics Unit (EMU)

1. Singh, S. K.; Thantanapally, C.; Ansumali, S., Gaseous microflow modeling using the Fokker-Planck equation. *Physical Review E* **2016**, *94* (6), <http://dx.doi.org/10.1103/PhysRevE.94.063307>
2. Saha, S.; Alam, M., Normal stress differences, their origin and constitutive relations for a sheared granular fluid. *Journal of Fluid Mechanics* **2016**, *795*, 549-580 <http://dx.doi.org/10.1017/jfm.2016.237>
3. Prakash, Vivek N.; Sreenivas, K. R.; Arakeri, Jaywant H., The role of viscosity contrast on plume structure in laboratory modeling of mantle convection. *Chemical Engineering Science* **2016**, *158*, 245-256 <http://dx.doi.org/10.1016/j.ces.2016.10.012>

-
-
4. Namburi, M.; Krithivasan, S.; Ansumali, S., Crystallographic Lattice Boltzmann Method. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep27172>
 5. Dabade, V.; Marath, N. K.; Subramanian, G., The effect of inertia on the orientation dynamics of anisotropic particles in simple shear flow. *Journal of Fluid Mechanics* **2016**, *791*, 631-703 <http://dx.doi.org/10.1017/jfm.2016.14>
 6. Brysev, A. P.; Zoueshtiagh, F.; Pernod, P.; Preobrazhensky, V. L.; Diwakar, S. V.; Makalkin, D., Excitation of standing gravity-capillary waves at an interface between two immiscible liquids by a periodic sequence of ultrasound pulses. *Physics of Wave Phenomena* **2016**, *24* (2), 155-160 <http://dx.doi.org/10.3103/s1541308x16020114>

Conference Papers

1. Rao, Samrat; Prasanth, P.; Deshpande, S. M.; Narasimha, R. In *A DNS Study of a Transient Diabatic Plume as a Model for a Cumulus Cloud*, 8th Annual CFD Symposium, Bangalore, Bangalore, 2016;
2. Ranjan, Rajesh; Deshpande, S M; Narasimha, Roddam In *A Critical Comparison of RANS, LES, Hybrid LES/RANS and DNS Studies of the Flow Past a Low Pressure Turbine Blade in a Cascade*, 18th AeSI CFD Symposium, Bangalore, Bangalore, 2016;
3. Ranjan, Rajesh; Deshpande, S M; Narasimha, Roddam In *Quasi-laminar theory for relaminarization in a highly accelerated high-Re turbulent boundary layer*, 8th European Postgraduate Fluid Dynamics Conference Poland, Poland, 2016;
4. K R, Sreenivas ; Rafiuddin, Mohammad In *Modeling Radiation Fog*, APS Division of Fluid Dynamics 2016;

Book / Book Chapter

1. Narasimha, R, Rockets in India. In *Encyclopaedia of the History of Science, Technology and Medicine in Non-Western Cultures.*, Springer: 2016.
2. Ranjan, R.; Deshpande, S. M.; Narasimha, R., *A High-Resolution Compressible DNS Study of Flow Past a Low-Pressure Gas Turbine Blade*. 2016; p 291-301 978-981-4635-16-5; 978-981-4635-15-8.

Evolutionary and Integrative Biology Unit

1. Nikhil, K. L.; Ratna, K.; Sharma, V. K., Life-history traits of *Drosophila melanogaster* populations exhibiting early and late eclosion chronotypes. *BMC Evolutionary Biology* **2016**, *16*, <http://dx.doi.org/10.1186/s12862-016-0622-3>
2. Nikhil, K. L.; Vaze, K. M.; Ratna, K.; Sharma, V. K., Circadian clock properties of fruit flies *Drosophila melanogaster* exhibiting early and late emergence chronotypes. *Chronobiology International* **2016**, *33* (1), 22-38 <http://dx.doi.org/10.3109/07420528.2015.1108981>
3. Gupta, Manan; Ravindranath, Shruthi; Prasad, Deepika; Vidya, T. N. C., Short-Term Variation in Sex Ratio Estimates of Asian Elephants Due to Space Use Differences between the Sexes. *Gajah* **2016**, *44*, 5-15
4. Vidya, T N C, Evolutionary History and Population Genetic Structure of Asian Elephants in India. *Indian Journal of History of Science* **2016**, *51* (2.2), 391-405 <http://dx.doi.org/10.16943/ijhs/2016/v51i2.2/48453>
5. Das, A.; Holmes, T. C.; Sheeba, V., dTRPA1 in Non-circadian Neurons Modulates Temperature-dependent Rhythmic Activity in *Drosophila melanogaster*. *Journal of Biological Rhythms* **2016**, *31* (3), 272-288 <http://dx.doi.org/10.1177/0748730415627037>



-
-
6. Nikhil, K. L.; Abhilash, L.; Sharma, V. K., Molecular Correlates of Circadian Clocks in Fruit Fly *Drosophila melanogaster* Populations Exhibiting early and late Emergence Chronotypes. *Journal of Biological Rhythms* **2016**, *31* (2), 125-141 <http://dx.doi.org/10.1177/0748730415627933>
 7. Abhilash, L.; Sharma, V. K., On the relevance of using laboratory selection to study the adaptive value of circadian clocks. *Physiological Entomology* **2016**, *41* (4), 293-306 <http://dx.doi.org/10.1111/phen.12158>
 8. Shindey, R.; Varma, V.; Nikhil, K. L.; Sharma, V. K., Evolution of robust circadian clocks in *Drosophila melanogaster* populations reared in constant dark for over 330 generations. *Science of Nature* **2016**, *103* (9-10), <http://dx.doi.org/10.1007/s00114-016-1399-3>
 9. Abhilash, Lakshman; Sharma, Vijay Kumar, Time Measurement in Living Systems: Human Understanding and Health Implications. In *Space, Time and the Limits of Human Understanding*, Wuppuluri, S.; Ghirardi, G., Eds. Springer: 2016; pp 337-352, 978-3-319-44417-8

Geodynamics Unit

1. Kotlia, Bahadur Singh; Singh, Anoop Kumar; Waseem, Jaishri Sanwal; Ahmad, Raza Syed Masood; Joshi, Lalit Mohan; Sirohi, Manisha; Sharma, Arun Kumar; Sagar, Netramani, Stalagmite Inferred High Resolution Climatic Changes through Pleistocene-Holocene Transition in Northwest Indian Himalaya. *Journal of Earth Science & Climatic Change* **2016**, *7* (3), <http://dx.doi.org/10.4172/2157-7617.1000338>
1. Rajendran, C. P.; John, B.; Rajendran, K.; Sanwal, J., Liquefaction record of the great 1934 earthquake predecessors from the north Bihar alluvial plains of India. *Journal of Seismology* **2016**, *20* (3), 732-745 <http://dx.doi.org/10.1007/s10950-016-9554-z>
2. Rajendran, C. P.; Sanwal, J.; Morell, K. D.; Sandiford, M.; Kotlia, B. S.; Hellstrom, J.; Rajendran, K., Stalagmite growth perturbations from the Kumaun Himalaya as potential earthquake recorders. *Journal of Seismology* **2016**, *20* (2), 579-594 <http://dx.doi.org/10.1007/s10950-015-9545-5>
3. Sanwal, J.; Dudwadkar, N. L.; Thirumurugan, A.; Tripathi, S. C.; Gandhi, P. M.; Satyam, P. V.; Sengupta, P., Adsorption of Ru, Ce and Eu radionuclides within naturally precipitated polycrystalline calcium carbonate under acidic environment. *Journal of Radioanalytical and Nuclear Chemistry* **2016**, *309* (2), 751-760 <http://dx.doi.org/10.1007/s10967-015-4672-6>
4. Sanwal, J.; P., Sengupta; L., Dudwadkar N.; C., Tripathi S.; M, Gandhi P, Adsorption of ¹⁰⁶Ru, ¹⁴⁴Ce and ¹⁵²⁺¹⁵⁴Eu within cave deposits and its relevance in nuclear waste disposal. *Journal of Radio-analytical and Nuclear Chemistry* **2016**, <http://dx.doi.org/10.1007/s10967-015-4672-6>.
5. Sengupta, P.; Sanwal, J.; Dudwadkar, N. L.; Tripathi, S. C.; Gandhi, P. M., Adsorption of actinides within speleothems. *Mineralogical Magazine* **2016**, *80* (5), 765-780 <http://dx.doi.org/10.1180/minmag.2016.080.013>
6. Valdiya, K. S., Geological marvels, hallowed shrines and unification of people of India. *Current Science* **2016**, *110* (6), 987-995.

Books

1. Valdiya, K.S., *Prehistoric River Saraswati, Western India*. Springer International Publishing: 2016; ISBN: 978-3-319-44223-5.
2. Valdiya, K.S., *The Making of India*. Springer International Publishing: 2016; <http://dx.doi.org/10.1007/978-3-319-25029-8>.

International Centre for Materials Science (ICMS)

1. Vasu, K.; Sreedhara, M. B.; Ghatak, J.; Rao, C. N. R., Atomic Layer Deposition of p-Type Epitaxial Thin Films of Undoped and N-Doped Anatase TiO₂. *ACS Applied Materials & Interfaces* **2016**, *8* (12), 7897-7901 <http://dx.doi.org/10.1021/acsami.6b00628>
2. Dey, S.; Rao, C. N. R., Splitting of CO₂ by Manganite Perovskites to Generate CO by Solar Isothermal Redox Cycling. *ACS Energy Letters* **2016**, *1* (1), 237-243 <http://dx.doi.org/10.1021/acsenergylett.6b00122>
3. Gokhale, S.; Sood, A. K.; Ganapathy, R., Deconstructing the glass transition through critical experiments on colloids. *Advances in Physics* **2016**, *65* (4), 363-452 <http://dx.doi.org/10.1080/00018732.2016.1200832>
4. Kumar, R.; Raut, D.; Ramamurty, U.; Rao, C. N. R., Remarkable Improvement in the Mechanical Properties and CO₂ Uptake of MOFs Brought About by Covalent Linking to Graphene. *Angewandte Chemie-International Edition* **2016**, *55* (27), 7857-7861 <http://dx.doi.org/10.1002/anie.201603320>
5. Kumar, P.; Devi, P.; Kumar, M.; Shivaprasad, S. M., Optimization of energy and fluence of N-2(+) ions in the conversion of Al₂O₃ surface into AlN at room temperature. *Applied Surface Science* **2016**, *361*, 265-268 <http://dx.doi.org/10.1016/j.apsusc.2015.11.180>
6. Sandoval, S.; Kumar, N.; Oro-Sole, J.; Sundaresan, A.; Rao, C. N. R.; Fuertes, A.; Tobias, G., Tuning the nature of nitrogen atoms in N-containing reduced graphene oxide. *Carbon* **2016**, *96*, 594-602 <http://dx.doi.org/10.1016/j.carbon.2015.09.085>
7. Santhosh, V.; Voggu, R.; Chaturbedy, P.; Ganapathy, R.; Rao, C. N. R., Mechanical properties of C-60 thin films at the air-water interface. *Carbon* **2016**, *96*, 1-5 <http://dx.doi.org/10.1016/j.carbon.2015.08.098>
8. Santhosh, V.; Voggu, R.; Chaturbedy, P.; Ganapathy, R.; Rao, C. N. R., Mechanical properties of C-60 thin films at the air-water interface. *Carbon* **2016**, *96*, 1-5 <http://dx.doi.org/10.1016/j.carbon.2015.08.098>
9. Chhetri, M.; U. Gupta, L. Yadgarov; Rosentsveig, R.; Tenne, R.; Rao, C.N.R., Noteworthy effects of p- and n-type doping in IF-MoS on the hydrogen evolution reaction. *ChemElectroChem* **2016**, *3* (11), <http://dx.doi.org/10.1002/celec.201600291>
10. Shenoy, U. S.; Gupta, U.; Narang, D. S.; Late, D. J.; Waghmare, U. V.; Rao, C. N. R., Electronic structure and properties of layered gallium telluride. *Chemical Physics Letters* **2016**, *651*, 148-154 <http://dx.doi.org/10.1016/j.cplett.2016.03.045>
11. Sreedhara, M. B.; Gopalakrishnan, K.; Bharath, B.; Kumar, R.; Kulkarni, G. U.; Rao, C. N. R., Properties of nanosheets of 2D-borocarbonitrides related to energy devices, transistors and other areas. *Chemical Physics Letters* **2016**, *657*, 124-130 <http://dx.doi.org/10.1016/j.cplett.2016.05.064>
12. Dey, S.; Naidu, B. S.; Rao, C. N. R., Beneficial effects of substituting trivalent ions in the B-site of La(0.5)Sr(0.5)Mn(1-x)A(x)O(3) (A = Al, Ga, Sc) on the thermochemical generation of CO and H₂ from CO₂ and H₂O. *Dalton Transactions* **2016**, *45* (6), 2430-2435 <http://dx.doi.org/10.1039/c5dt04822b>
13. Jana, M. K.; Gupta, U.; Rao, C. N. R., Hydrazine as a hydrogen carrier in the photocatalytic generation of H₂ using CdS quantum dots. *Dalton Transactions* **2016**, *45* (38), 15137-15141 <http://dx.doi.org/10.1039/c6dt02505f>
14. Pramoda, K.; Kaur, M.; Gupta, U.; Rao, C. N. R., Nanocomposites of 2D-MoS₂ nanosheets with the metal-organic framework, ZIF-8. *Dalton Transactions* **2016**, *45* (35), 13810-13816 <http://dx.doi.org/10.1039/c6dt02667b>



-
-
15. Banik, A.; Vishal, B.; Perumal, S.; Datta, R.; Biswas, K., The origin of low thermal conductivity in Sn_{1-x}Sb_xTe: phonon scattering via layered intergrowth nanostructures. *Energy & Environmental Science* **2016**, *9* (6), 2011-2019 <http://dx.doi.org/10.1039/c6ee00728g>
 16. Chhetri, M.; Maitra, S.; Chakraborty, H.; Waghmare, U. V.; Rao, C. N. R., Superior performance of borocarbonitrides, B_xC_yN_z, as stable, low-cost metal-free electrocatalysts for the hydrogen evolution reaction. *Energy & Environmental Science* **2016**, *9* (1), 95-101 <http://dx.doi.org/10.1039/c5ee02521d>
 17. Sadhu, A.; Salunke, H. G.; Shivaprasad, S. M.; Bhattacharyya, S., Extensive Parallelism between Crystal Parameters and Magnetic Phase Transitions of Unusually Ferromagnetic Praseodymium Manganite Nanoparticles. *Inorganic Chemistry* **2016**, *55* (16), 7903-7911 <http://dx.doi.org/10.1021/acs.inorgchem.6b00815>
 18. Loukya, B.; Negi, D. S.; Sahu, R.; Pachauri, N.; Gupta, A.; Datta, R., Structural characterization of epitaxial LiFe₅O₈ thin films grown by chemical vapor deposition. *Journal of Alloys and Compounds* **2016**, *668*, 187-193 <http://dx.doi.org/10.1016/j.jallcom.2016.01.217>
 19. Dileep, K.; Sahu, R.; Sarkar, S.; Peter, S. C.; Datta, R., Layer specific optical band gap measurement at nanoscale in MoS₂ and ReS₂ van der Waals compounds by high resolution electron energy loss spectroscopy. *Journal of Applied Physics* **2016**, *119* (11), <http://dx.doi.org/10.1063/1.4944431>
 20. Sahu, R.; Bhat, U.; Batra, N. M.; Sharona, H.; Vishal, B.; Sarkar, S.; Aravindh, S. A.; Peter, S. C.; Roqan, I. S.; Costa, Pmfj; Datta, R., Nature of low dimensional structural modulations and relative phase stability in RexMo(W)(1-x)S-2 transition metal dichalcogenide alloys. *Journal of Applied Physics* **2017**, *121* (10), <http://dx.doi.org/10.1063/1.4977111>
 21. Shetty, S.; Shivaprasad, S. M., Early stages of plasma induced nitridation of Si (111) surface and study of interfacial band alignment. *Journal of Applied Physics* **2016**, *119* (5), <http://dx.doi.org/10.1063/1.4941102>
 22. Tangi, M.; De, A.; Ghatak, J.; Shivaprasad, S. M., Electron mobility of self-assembled and dislocation free InN nanorods grown on GaN nano wall network template. *Journal of Applied Physics* **2016**, *119* (20), <http://dx.doi.org/10.1063/1.4952380>
 23. Rana, M.; Patil, P. K.; Chhetri, M.; Dileep, K.; Datta, R.; Gautam, U. K., Pd-Pt alloys nanowires as support-less electrocatalyst with high synergistic enhancement in efficiency for methanol oxidation in acidic medium. *Journal of Colloid and Interface Science* **2016**, *463*, 99-106 <http://dx.doi.org/10.1016/j.jcis.2015.10.042>
 24. Dey, S.; Rajesh, S.; Rao, C. N. R., Significant reduction in the operating temperature of the Mn(II)/Mn(III) oxide-based thermochemical water splitting cycle brought about by the use of nanoparticles. *Journal of Materials Chemistry A* **2016**, *4* (43), 16830-16833 <http://dx.doi.org/10.1039/c6ta06271g>
 25. Pramoda, K.; Gupta, U.; Ahmad, I.; Kumar, R.; Rao, C. N. R., Assemblies of covalently cross-linked nanosheets of MoS₂ and of MoS₂-RGO: synthesis and novel properties. *Journal of Materials Chemistry A* **2016**, *4* (23), 8989-8994 <http://dx.doi.org/10.1039/c6ta00645k>
 26. Sreedhara, M. B.; Santhosha, A. L.; Bhattacharyya, A. J.; Rao, C. N. R., Composite of few-layer MoO₃ nanosheets with graphene as a high performance anode for sodium-ion batteries. *Journal of Materials Chemistry A* **2016**, *4* (24), 9466-9471 <http://dx.doi.org/10.1039/c6ta02561g>
 27. Reddy, G. R.; Avadhani, A. S.; Rajaram, S., Activation of Benzyl Aryl Carbonates: The Role of Cation-pi Interactions. *Journal of Organic Chemistry* **2016**, *81* (10), 4134-4141 <http://dx.doi.org/10.1021/acs.joc.6b00441>

-
-
28. Dutta, D.; Gope, S.; Negi, D. S.; Datta, R.; Sood, A. K.; Bhattacharyya, A. J., Pressure-Induced Capillary Encapsulation Protocol for Ultrahigh Loading of Sulfur and Selenium Inside Carbon Nanotubes: Application as High Performance Cathode in Li-S/Se Rechargeable Batteries. *Journal of Physical Chemistry C* **2016**, *120* (51), 29011-29022 <http://dx.doi.org/10.1021/acs.jpcc.6b11017>
 29. Grandhi, G. K.; Arunkumar, M.; Viswanatha, R., Understanding the Role of Surface Capping Ligands in Passivating the Quantum Dots Using Copper Dopants as Internal Sensor. *Journal of Physical Chemistry C* **2016**, *120* (35), 19785-19795 <http://dx.doi.org/10.1021/acs.jpcc.6b04060>
 30. Roy, A.; Shenoy, U. S.; Manjunath, K.; Vishnoi, P.; Waghmare, U. V.; Rao, C. N. R., Structure and Properties of Cd₄P₂Cl₃, an Analogue of CdS. *Journal of Physical Chemistry C* **2016**, *120* (28), 15063-15069 <http://dx.doi.org/10.1021/acs.jpcc.6b04058>
 31. Saha, A.; Chattopadhyay, S.; Shibata, T.; Viswanatha, R., Core-Shell to Doped Quantum Dots: Evolution of the Local Environment Using XAFS. *Journal of Physical Chemistry C* **2016**, *120* (33), 18945-18951 <http://dx.doi.org/10.1021/acs.jpcc.6b06803>
 32. Saha, A.; Shetty, A.; Pavan, A. R.; Chattopadhyay, S.; Shibata, T.; Viswanatha, R., Uniform Doping in Quantum-Dots-Based Dilute Magnetic Semiconductor. *Journal of Physical Chemistry Letters* **2016**, *7* (13), 2420-2428 <http://dx.doi.org/10.1021/acs.jpclett.6b01099>
 33. De, A.; Shivaprasad, S. M., Epitaxy, phase separation and band-edge emission of spontaneously formed InGaN nanorods. *Journal of Physics D-Applied Physics* **2016**, *49* (35), <http://dx.doi.org/10.1088/0022-3727/49/35/355304>
 34. Rao, C. N. R.; Dey, S., Generation of H₂ and CO by solar thermochemical splitting of H₂O and CO₂ by employing metal oxides. *Journal of Solid State Chemistry* **2016**, *242*, 107-115 <http://dx.doi.org/10.1016/j.jssc.2015.12.018>
 35. Subbarao, U.; Marakatti, V. S.; Amshumali, M. K.; Loukya, B.; Singh, D. K.; Datta, R.; Peter, S. C., Size and morphology controlled NiSe nanoparticles as efficient catalyst for the reduction reactions. *Journal of Solid State Chemistry* **2016**, *244*, 84-92 <http://dx.doi.org/10.1016/j.jssc.2016.09.020>
 36. Gokhale, S.; Nagamanasa, K. H.; Sood, A. K.; Ganapathy, R., Influence of an amorphous wall on the distribution of localized excitations in a colloidal glass-forming liquid. *Journal of Statistical Mechanics-Theory and Experiment* **2016**, <http://dx.doi.org/10.1088/1742-5468/2016/07/074013>
 37. Lingampalli, S. R.; Manjunath, K.; Shenoy, S.; Waghmare, U. V.; Rao, C. N. R., Zn₂NF and Related Analogues of ZnO. *Journal of the American Chemical Society* **2016**, *138* (26), 8228-8234 <http://dx.doi.org/10.1021/jacs.6b04198>
 38. Kumar, M.; Kumar, P.; Devi, P.; Shivaprasad, S. M., Formation of low-dimensional GaN on trenched Si(5512), probed by STM and XPS. *Materials Research Express* **2016**, *3* (3), <http://dx.doi.org/10.1088/2053-1591/3/3/035010>
 39. Krishnamurthy, S.; Ghosh, S.; Chatterji, D.; Ganapathy, R.; Sood, A. K., A micrometre-sized heat engine operating between bacterial reservoirs. *Nature Physics* **2016**, *12* (12), 1134-+ <http://dx.doi.org/10.1038/nphys3870>
 40. Jana, M. K.; Rao, C. N. R., Two-dimensional inorganic analogues of graphene: transition metal dichalcogenides. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2016**, *374* (2076), <http://dx.doi.org/10.1098/rsta.2015.0318>



-
-
41. Rao, C. N. R.; Lingampalli, S. R.; Dey, S.; Roy, A., Solar photochemical and thermochemical splitting of water. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2016**, 374 (2061), <http://dx.doi.org/10.1098/rsta.2015.0088>
 42. Saha, R.; Vasu, K.; Negi, D. S.; Datta, R.; Sundaresan, A.; Rao, C. N. R., Exchange bias at low fields exhibited by the interface between epitaxial layers of ferromagnetic and charge-ordered rare-earth manganites. *Physica Status Solidi-Rapid Research Letters* **2016**, 10 (8), 622-626 <http://dx.doi.org/10.1002/pssr.201600155>
 43. Saha, R.; Vasu, K.; Negi, D. S.; Datta, R.; Sundaresan, A.; Rao, C. N. R., Exchange bias at low fields exhibited by the interface between epitaxial layers of ferromagnetic and charge-ordered rare-earth manganites. *Physica Status Solidi-Rapid Research Letters* **2016**, 10 (8), 622-626 <http://dx.doi.org/10.1002/pssr.201600155>
 44. Shetty, A.; Saha, A.; Makkar, M.; Viswanatha, R., Ligand assisted digestion and formation of monodisperse FeCoS₂ nanocrystals. *Physical Chemistry Chemical Physics* **2016**, 18 (37), 25887-25892 <http://dx.doi.org/10.1039/c6cp04912e>
 45. Narayan, B.; Sorb, Y. A.; Loukya, B.; Samanta, A.; Senyshyn, A.; Datta, R.; Singh, A. K.; Narayana, C.; Ranjan, R., Interferroelectric transition as another manifestation of intrinsic size effect in ferroelectrics. *Physical Review B* **2016**, 94 (10), <http://dx.doi.org/10.1103/PhysRevB.94.104104>
 46. Saha, R.; Sundaresan, A.; Sanyal, M. K.; Rao, C. N. R.; Orlandi, F.; Manuel, P.; Langridge, S., Neutron scattering study of the crystallographic and spin structure in antiferromagnetic EuZrO₃. *Physical Review B* **2016**, 93 (1), <http://dx.doi.org/10.1103/PhysRevB.93.014409>
 47. Gokhale, S.; Ganapathy, R.; Nagamanasa, K. H.; Sood, A. K., Localized Excitations and the Morphology of Cooperatively Rearranging Regions in a Colloidal Glass-Forming Liquid. *Physical Review Letters* **2016**, 116 (6), <http://dx.doi.org/10.1103/PhysRevLett.116.068305>
 48. Mishra, C. K.; Sood, A. K.; Ganapathy, R., Site-specific colloidal crystal nucleation by template-enhanced particle transport. *Proceedings of the National Academy of Sciences of the United States of America* **2016**, 113 (43), 12094-12098 <http://dx.doi.org/10.1073/pnas.1608568113>
 49. Deb, S.; Bhasker, H. P.; Thakur, V.; Shivaprasad, S. M.; Dhar, S., Polarization induced two dimensional confinement of carriers in wedge shaped polar semiconductors. *Scientific Reports* **2016**, 6, <http://dx.doi.org/10.1038/srep26429>
 50. Rao, C. N. R.; Lingampalli, S. R., Generation of Hydrogen by Visible Light-Induced Water Splitting with the Use of Semiconductors and Dyes. *Small* **2016**, 12 (1), 16-23 <http://dx.doi.org/10.1002/smll.201500420>
 51. Roy, A.; Lingampalli, S. R.; Nassar, I. M.; Rao, C. N. R., Effectiveness of NiO in replacing Pt in the photochemical generation of hydrogen by (TiO₂)(1-x)(NiO)(x)/Cd_{0.8}Zn_{0.2}S heterostructures. *Solid State Communications* **2016**, 243, 1-6 <http://dx.doi.org/10.1016/j.ssc.2016.05.018>
 52. Jana, M. K.; Singh, A.; Sampath, A.; Rao, C. N. R.; Waghmare, U. V., Structure and Electron-Transport Properties of Anion-Deficient MoTe₂: A Combined Experimental and Theoretical Study. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2016**, 642 (23), 1386-1396 <http://dx.doi.org/10.1002/zaac.201600314>

Molecular Biology and Genetics Unit (MBGU)

1. Pandey, N.; Xavier, D. F.; Chatterjee, A.; Mani, R. S.; Hiremagalore, R.; Tharakan, A.; Rajashekhar, B.; Anand, A., Functional Analysis of a Novel Connexin30 Mutation in a Large Family with Hearing Loss, Pesplanus, Ichthyosis, Cutaneous Nodules, and Keratoderma. *Annals of Human Genetics* **2016**, *80* (1), 11-19 <http://dx.doi.org/10.1111/ahg.12141>
2. Karnawat, V.; Mehrotra, S.; Balaram, H.; Puranik, M., Exquisite Modulation of the Active Site of Methanocaldococcus jannaschii Adenylosuccinate Synthetase in Forward Reaction Complexes. *Biochemistry* **2016**, *55* (17), 2491-2499 <http://dx.doi.org/10.1021/acs.biochem.5b01386>
3. Datta, A.; Yadav, V.; Ghosh, A.; Choi, J.; Bhattacharyya, D.; Kar, R. K.; Ilyas, H.; Dutta, A.; An, E.; Mukhopadhyay, J.; Lee, D.; Sanyal, K.; Ramamoorthy, A.; Bhunia, A., Mode of Action of a Designed Antimicrobial Peptide: High Potency against Cryptococcus neoformans. *Biophysical Journal* **2016**, *111* (8), 1724-1737 <http://dx.doi.org/10.1016/j.bpj.2016.08.032>
4. Guha, Manti; Srinivasan, Satish; Guja, Kip; Mejia, Edison; Garcia-Diaz, Miguel; Johnson, F Brad; Ruthel, Gordon; Kaufman, Brett A; Rappaport, Eric F; Glineburg, M Rebecca; Fang, Ji-Kang; Szanto, Andres Klein; Nakagawa, Hiroshi; Basha, Jeelan; Kundu, Tapas; Avadhani, Narayan G, HnRNPA2 is a novel histone acetyltransferase that mediates mitochondrial stress-induced nuclear gene expression. *Cell Discovery* **2016**, *2*, <http://dx.doi.org/10.1038/celldisc.2016.45>
5. Pareek, V.; Samanta, M.; Joshi, N. V.; Balaram, H.; Murthy, M. R. N.; Balaram, P., Connecting Active-Site Loop Conformations and Catalysis in Triosephosphate Isomerase: Insights from a Rare Variation at Residue96 in the Plasmodial Enzyme. *Chembiochem* **2016**, *17* (7), 620-629 <http://dx.doi.org/10.1002/cbic.201500532>
6. Karthigeyan, D.; Surabhi, S.; Mizar, P.; Soumik, S.; Banerjee, A.; Sinha, S. H.; Dasgupta, D.; Narayana, C.; Kundu, T. K., A Dual Non-ATP Analogue Inhibitor of Aurora Kinases A and B, Derived from Resorcinol with a Mixed Mode of Inhibition. *Chemical Biology & Drug Design* **2016**, *87* (6), 958-967 <http://dx.doi.org/10.1111/cbdd.12728>
7. Dhanasekaran, K.; Kumari, S.; Boopathi, R.; Shima, H.; Swaminathan, A.; Bachu, M.; Ranga, U.; Igarashi, K.; Kundu, T. K., Multifunctional human transcriptional coactivator protein PC4 is a substrate of Aurora kinases and activates the Aurora enzymes. *FEBS Journal* **2016**, *283* (6), 968-985 <http://dx.doi.org/10.1111/febs.13653>
8. Dhanasekaran, K.; Kumari, S.; Boopathi, R.; Shima, H.; Swaminathan, A.; Bachu, M.; Ranga, U.; Igarashi, K.; Kundu, T. K., Multifunctional human transcriptional coactivator protein PC4 is a substrate of Aurora kinases and activates the Aurora enzymes. *FEBS Journal* **2016**, *283* (6), 968-985 <http://dx.doi.org/10.1111/febs.13653>
9. Swaminathan, A.; Delage, H.; Chatterjee, S.; Belgarbi-Dutron, L.; Cassel, R.; Martinez, N.; Cosquer, B.; Kumari, S.; Mongelard, F.; Lannes, B.; Cassel, J. C.; Boutillier, A. L.; Bouvet, P.; Kundu, T. K., Transcriptional Coactivator and Chromatin Protein PC4 Is Involved in Hippocampal Neurogenesis and Spatial Memory Extinction. *Journal of Biological Chemistry* **2016**, *291* (39), 20303-20314 <http://dx.doi.org/10.1074/jbc.M116.744169>
10. Karmakar, T.; Roy, S.; Balaram, H.; Balasubramanian, S., Structural and dynamical correlations in PfHGXPRT oligomers: A molecular dynamics simulation study. *Journal of Biomolecular Structure & Dynamics* **2016**, *34* (7), 1590-1605 <http://dx.doi.org/10.1080/07391102.2015.1085441>
11. Karmakar, T.; Roy, S.; Balarn, H.; Prakash, M. K.; Balasubramanian, S., Product Release Pathways in



-
-
- Human and Plasmodium falciparum Phosphoribosyltransferase. *Journal of Chemical Information and Modeling* **2016**, 56 (8), 1528-1538 <http://dx.doi.org/10.1021/acs.jcim.6b00203>
12. Bharathy, N.; Suriyamurthy, S.; Rao, V. K.; Ow, J. R.; Lim, H. J.; Chakraborty, P.; Vasudevan, M.; Dhamne, C. A.; Chang, K. T. E.; Min, V. L. K.; Kundu, T. K.; Taneja, R., P/CAF mediates PAX3-FOXO1-dependent oncogenesis in alveolar rhabdomyosarcoma. *Journal of Pathology* **2016**, 240 (3), 269-281 <http://dx.doi.org/10.1002/path.4773>
 13. Verma, A.; Rajagopalan, P.; Lotke, R.; Varghese, R.; Selvam, D.; Kundu, T. K.; Ranga, U., Functional Incompatibility between the Generic NF-kappa B Motif and a Subtype-Specific Sp1III Element Drives the Formation of the HIV-1 Subtype C Viral Promoter. *Journal of Virology* **2016**, 90 (16), 7046-7065 <http://dx.doi.org/10.1128/jvi.00308-16>
 14. Verma, A.; Rajagopalan, P.; Lotke, R.; Varghese, R.; Selvam, D.; Kundu, T. K.; Ranga, U., Functional Incompatibility between the Generic NF-kappa B Motif and a Subtype-Specific Sp1III Element Drives the Formation of the HIV-1 Subtype C Viral Promoter. *Journal of Virology* **2016**, 90 (16), 7046-7065 <http://dx.doi.org/10.1128/jvi.00308-16>
 15. Mitra, Sreyoshi; Rai, Laxmi Shanker; Chatterjee, Gautam; Sanyal, Kaustuv, Chromatin Immunoprecipitation (ChIP) Assay in Candida albicans. *Methods in Molecular Biology* **2016**, 1356, 43-57 http://dx.doi.org/10.1007/978-1-4939-3052-4_4
 16. Hoque, J.; Adhikary, U.; Yadav, V.; Samaddar, S.; Konai, M. M.; Prakash, R. G.; Pararnanandham, K.; Shome, B. R.; Sanyal, K.; Haldar, J., Chitosan Derivatives Active against Multidrug-Resistant Bacteria and Pathogenic Fungi: In Vivo Evaluation as Topical Antimicrobials. *Molecular Pharmaceutics* **2016**, 13 (10), 3578-3589 <http://dx.doi.org/10.1021/acs.molpharmaceut.6b00764>
 17. Kumar, S.; Prakash, S.; Gupta, K.; Dongre, A.; Balaram, P.; Balaram, H., Unexpected functional implication of a stable succinimide in the structural stability of Methanocaldococcus jannaschii glutaminase. *Nature Communications* **2016**, 7, <http://dx.doi.org/10.1038/ncomms12798>
 18. Akhade, V. S.; Dighe, S. N.; Kataruka, S.; Rao, M. R. S., Mechanism of Wnt signaling induced down regulation of mrhl long non-coding RNA in mouse spermatogonial cells. *Nucleic Acids Research* **2016**, 44 (1), 387-401 <http://dx.doi.org/10.1093/nar/gkv1023>
 19. Chatterjee, G.; Sankaranarayanan, S. R.; Guin, K.; Thattikota, Y.; Padmanabhan, S.; Siddharthan, R.; Sanyal, K., Repeat-Associated Fission Yeast-Like Regional Centromeres in the Ascomycetous Budding Yeast Candida tropicalis. *PLoS Genetics* **2016**, 12 (2), <http://dx.doi.org/10.1371/journal.pgen.1005839>
 20. Richard, J. L. C.; Shukla, M. S.; Menoni, H.; Ouararhni, K.; Lone, I. N.; Roulland, Y.; Papin, C.; Ben Simon, E.; Kundu, T.; Hamiche, A.; Angelov, D.; Dimitrov, S., FACT Assists Base Excision Repair by Boosting the Remodeling Activity of RSC. *PLoS Genetics* **2016**, 12 (7), <http://dx.doi.org/10.1371/journal.pgen.1006221>
 21. Roy, S.; Karmakar, T.; Nagappa, L. K.; Rao, V. S. P.; Balasubramanian, S.; Balaram, H., Role of W181 in modulating kinetic properties of Plasmodium falciparum hypoxanthine guanine xanthine phosphoribosyltransferase. *Proteins-Structure Function and Bioinformatics* **2016**, 84 (11), 1658-1669 <http://dx.doi.org/10.1002/prot.25107>
 22. Arunachalam, P. S.; Mishra, R.; Badarinath, K.; Selvam, D.; Payeli, S. K.; Stout, R. R.; Ranga, U., Toll-Like Receptor 9 Activation Rescues Impaired Antibody Response in Needle-free Intradermal DNA Vaccination. *Scientific Reports* **2016**, 6, <http://dx.doi.org/10.1038/srep33564>

-
-
23. Kakade, P.; Sadhale, P.; Sanyal, K.; Nagaraja, V., ZCF32, a fungus specific Zn(II)₂ Cys₆ transcription factor, is a repressor of the biofilm development in the human pathogen *Candida albicans*. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep31124>
 24. Mukhopadhyay, A.; Sehgal, L.; Bose, A.; Gulvady, A.; Senapati, P.; Thorat, R.; Basu, S.; Bhatt, K.; Hosing, A. S.; Balyan, R.; Borde, L.; Kundu, T. K.; Dalal, S. N., 14-3-3 gamma Prevents Centrosome Amplification and Neoplastic Progression. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep26580>
 25. Ranganath, S. H.; Tong, Z. X.; Levy, O.; Martyn, K.; Karp, J. M.; Inamdar, M. S., Controlled Inhibition of the Mesenchymal Stromal Cell Pro-inflammatory Secretome via Microparticle Engineering. *Stem Cell Reports* **2016**, *6* (6), 926-939 <http://dx.doi.org/10.1016/j.stemcr.2016.05.003>
 26. Chinnaswamy, S.; Bhushan, A.; Behera, A. K.; Ghosh, S.; Rampurkar, V.; Chandra, V.; Pandit, B.; Kundu, T. K., Roles for Transcription Factors Sp1, NF-kappa B, IRF3, and IRF7 in Expression of the Human IFNL4 Gene. *Viral Immunology* **2016**, *29* (1), 49-63 <http://dx.doi.org/10.1089/vim.2015.0076>
 27. Negi, N.; Vajpayee, M.; Singh, R.; Sharma, A.; Murugavel, K. G.; Ranga, U.; Thakar, M.; Sreenivas, V.; Das, B. K., Cross-Reactive Potential of HIV-1 Subtype C-Infected Indian Individuals Against Multiple HIV-1 Potential T Cell Epitope Gag Variants. *Viral Immunology* **2016**, *29* (10), 572-582 <http://dx.doi.org/10.1089/vim.2016.0060>

Neuroscience Unit (NSU)

1. Pandey, N.; Xavier, D. F.; Chatterjee, A.; Mani, R. S.; Hiremagalore, R.; Tharakan, A.; Rajashekhar, B.; Anand, A., Functional Analysis of a Novel Connexin30 Mutation in a Large Family with Hearing Loss, Pesplanus, Ichthyosis, Cutaneous Nodules, and Keratoderma. *Annals of Human Genetics* **2016**, *80* (1), 11-19 <http://dx.doi.org/10.1111/ahg.12141>
2. Jeyabalan, N.; Clemente, J. P., SYNGAP1: Mind the Gap. *Frontiers in Cellular Neuroscience* **2016**, *10*, <http://dx.doi.org/10.3389/fncel.2016.00032>
3. Das, A.; Holmes, T. C.; Sheeba, V., dTRPA1 in Non-circadian Neurons Modulates Temperature-dependent Rhythmic Activity in *Drosophila melanogaster*. *Journal of Biological Rhythms* **2016**, *31* (3), 272-288 <http://dx.doi.org/10.1177/0748730415627037>
4. Akhade, V. S.; Dighe, S. N.; Kataruka, S.; Rao, M. R. S., Mechanism of Wnt signaling induced down regulation of mrhl long non-coding RNA in mouse spermatogonial cells. *Nucleic Acids Research* **2016**, *44* (1), 387-401 <http://dx.doi.org/10.1093/nar/gkv1023>

Granted Patent

1. Narayan, K.S.; Gautam, V.; Bag, M *Artificial Retina Device*. 2016.

New Chemistry Unit (NCU)

1. Biswas, K.; Guin, S.N.; Banik, A., Thermolectric Energy Conversion in Layered Metal Chalcogenides. In *2D Inorganic Materials beyond Graphene* Rao, C. N. R., Ed. World Scientific Publisher: Singapore, 2016, 978-1-78634-269-0
2. Avinash, M. B.; Swathi, K.; Narayan, K. S.; Govindaraju, T., Molecular Architectonics of Naphthalenediimides for Efficient Structure-Property Correlation. *ACS Applied Materials & Interfaces* **2016**, *8* (13), 8678-8685 <http://dx.doi.org/10.1021/acsami.6b00011>



-
-
3. Hoque, J.; Akkapeddi, P.; Ghosh, C.; Uppu, Dssm; Haldar, J., A Biodegradable Polycationic Paint that Kills Bacteria in Vitro and in Vivo. *ACS Applied Materials & Interfaces* **2016**, *8* (43), 29298-29309 <http://dx.doi.org/10.1021/acsami.6b09804>
 4. Manchineella, S.; Thrivikraman, G.; Basu, B.; Govindaraju, T., Surface-Functionalized Silk Fibroin Films as a Platform To Guide Neuron-like Differentiation of Human Mesenchymal Stem Cells. *ACS Applied Materials & Interfaces* **2016**, *8* (35), 22849-22859 <http://dx.doi.org/10.1021/acsami.6b06403>
 5. Pandeewar, M.; Senanayak, S. P.; Govindaraju, T., Nanoarchitectonics of Small Molecule and DNA for Ultrasensitive Detection of Mercury. *ACS Applied Materials & Interfaces* **2016**, *8* (44), 30362-30371 <http://dx.doi.org/10.1021/acsami.6b10527>
 6. Vasu, K.; Sreedhara, M. B.; Ghatak, J.; Rao, C. N. R., Atomic Layer Deposition of p-Type Epitaxial Thin Films of Undoped and N-Doped Anatase TiO₂. *ACS Applied Materials & Interfaces* **2016**, *8* (12), 7897-7901 <http://dx.doi.org/10.1021/acsami.6b00628>
 7. Rajasekhar, K.; Madhu, C.; Govindaraju, T., Natural Tripeptide-Based Inhibitor of Multifaceted Amyloid beta Toxicity. *ACS Chemical Neuroscience* **2016**, *7* (9), 1300-+ <http://dx.doi.org/10.1021/acschemneuro.6600175>
 8. Dey, S.; Rao, C. N. R., Splitting of CO₂ by Manganite Perovskites to Generate CO by Solar Isothermal Redox Cycling. *ACS Energy Letters* **2016**, *1* (1), 237-243 <http://dx.doi.org/10.1021/acsenergylett.6b00122>
 9. Ghosh, C.; Manjunath, G. B.; Konai, M. M.; Uppu, Dssm; Paramanandham, K.; Shome, B. R.; Ravikumar, R.; Haldar, J., Aryl-alkyl-lysines: Membrane-Active Small Molecules Active against Murine Model of Burn Infection. *ACS Infectious Diseases* **2016**, *2* (2), 111-122 <http://dx.doi.org/10.1021/acsinfecdis.5b00092>
 10. Avinash, M. B.; Sandeepa, Kulala Vittala; Govindaraju, T., Emergent Behaviors in Kinetically Controlled Dynamic Self-Assembly of Synthetic Molecular Systems. *ACS Omega* **2016**, *1* (3), 378-387 <http://dx.doi.org/10.1021/acsomega.6b00155>
 11. Manchineella, S.; Thrivikraman, G.; Khanum, K. K.; Ramamurthy, P. C.; Basu, B.; Govindaraju, T., Pigmented Silk Nanofibrous Composite for Skeletal Muscle Tissue Engineering. *Advanced Healthcare Materials* **2016**, *5* (10), 1222-1232 <http://dx.doi.org/10.1002/adhm.201501066>
 12. Jana, M. K.; Pal, K.; Waghmare, U. V.; Biswas, K., The Origin of Ultralow Thermal Conductivity in InTe: Lone-Pair-Induced Anharmonic Rattling. *Angewandte Chemie-International Edition* **2016**, *55* (27), 7792-7796 <http://dx.doi.org/10.1002/anie.201511737>
 13. Kumar, R.; Raut, D.; Ramamurty, U.; Rao, C. N. R., Remarkable Improvement in the Mechanical Properties and CO₂ Uptake of MOFs Brought About by Covalent Linking to Graphene. *Angewandte Chemie-International Edition* **2016**, *55* (27), 7857-7861 <http://dx.doi.org/10.1002/anie.201603320>
 14. Yarlagadda, V.; Sarkar, P.; Samaddar, S.; Haldar, J., A Vancomycin Derivative with a Pyrophosphate-Binding Group: A Strategy to Combat Vancomycin-Resistant Bacteria. *Angewandte Chemie-International Edition* **2016**, *55* (27), 7836-7840 <http://dx.doi.org/10.1002/anie.201601621>
 15. Das, S.; Aggarwal, L.; Roychowdhury, S.; Aslam, M.; Gayen, S.; Biswas, K.; Sheet, G., Unexpected superconductivity at nanoscale junctions made on the topological crystalline insulator Pb_{0.6}Sn_{0.4}Te. *Applied Physics Letters* **2016**, *109* (13), <http://dx.doi.org/10.1063/1.4963698>
 16. Rajaji, V.; Malavi, P. S.; Yamijala, Ssrkc; Sorb, Y. A.; Dutta, U.; Guin, S. N.; Joseph, B.; Pati, S. K.; Karmakar, S.; Biswas, K.; Narayana, C., Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe₂. *Applied Physics Letters* **2016**, *109* (17), <http://dx.doi.org/10.1063/1.4966275>

17. Roychowdhury, S.; Shenoy, U. S.; Waghmare, U. V.; Biswas, K., Effect of potassium doping on electronic structure and thermoelectric properties of topological crystalline insulator. *Applied Physics Letters* **2016**, *108* (19), <http://dx.doi.org/10.1063/1.4948969>
18. Uppu, Dssm; Haldar, J., Lipopolysaccharide Neutralization by Cationic-Amphiphilic Polymers through Pseudoaggregate Formation. *Biomacromolecules* **2016**, *17* (3), 862-873 <http://dx.doi.org/10.1021/acs.biomac.5b01567>
19. Uppu, Divakara S. S. M.; Samaddar, Sandip; Hoque, Jiaul; Konai, Mohini M.; Krishnamoorthy, Paramanandham; Shome, Bibek R.; Haldar, Jayanta, Side Chain Degradable Cationic–Amphiphilic Polymers with Tunable Hydrophobicity Show in Vivo Activity. *Biomacromolecules* **2016**, *17* (9), 3094-3102 <http://dx.doi.org/10.1021/acs.biomac.6b01057>
20. Uppu, Dssm; Samaddar, S.; Ghosh, C.; Paramanandham, K.; Shome, B. R.; Haldar, J., Amide side chain amphiphilic polymers disrupt surface established bacterial bio-films and protect mice from chronic *Acinetobacter baumannii* infection. *Biomaterials* **2016**, *74*, 131-143 <http://dx.doi.org/10.1016/j.biomaterials.2015.09.042>
21. Sandoval, S.; Kumar, N.; Oro-Sole, J.; Sundaresan, A.; Rao, C. N. R.; Fuertes, A.; Tobias, G., Tuning the nature of nitrogen atoms in N-containing reduced graphene oxide. *Carbon* **2016**, *96*, 594-602 <http://dx.doi.org/10.1016/j.carbon.2015.09.085>
22. Santhosh, V.; Voggu, R.; Chaturbedy, P.; Ganapathy, R.; Rao, C. N. R., Mechanical properties of C-60 thin films at the air-water interface. *Carbon* **2016**, *96*, 1-5 <http://dx.doi.org/10.1016/j.carbon.2015.08.098>
23. Suseela, Y. V.; Das, S.; Pati, S. K.; Govindaraju, T., Imidazolyl-Naphthalenediimide-Based Threading Intercalators of DNA. *ChemBiochem* **2016**, *17* (22), 2162-2171 <http://dx.doi.org/10.1002/cbic.201600478>
24. Chhetri, M.; U. Gupta, L. Yadgarov; Rosentsveig, R.; Tenne, R.; Rao, C.N.R., Noteworthy effects of p- and n-type doping in IF-MoS on the hydrogen evolution reaction. *ChemElectroChem* **2016**, *3* (11), <http://dx.doi.org/10.1002/celec.201600291>
25. Narayanaswamy, N.; Nair, R. R.; Suseela, Y. V.; Saini, D. K.; Govindaraju, T., A molecular beacon-based DNA switch for reversible pH sensing in vesicles and live cells. *Chemical Communications* **2016**, *52* (56), 8741-8744 <http://dx.doi.org/10.1039/c6cc02705a>
26. Rubio-Magnieto, J.; Kumar, M.; Brocorens, P.; Ide, J.; George, S. J.; Lazzaroni, R.; Surin, M., Chiral supramolecular organization and cooperativity in DNA-templated assemblies of Zn-II-chromophore complexes. *Chemical Communications* **2016**, *52* (96), 13873-13876 <http://dx.doi.org/10.1039/c6cc07414f>
27. Uppu, Dssm; Bhowmik, M.; Samaddar, S.; Haldar, J., Cyclization and unsaturation rather than isomerisation of side chains govern the selective antibacterial activity of cationic-amphiphilic polymers. *Chemical Communications* **2016**, *52* (25), 4644-4647 <http://dx.doi.org/10.1039/c5cc09930g>
28. Shenoy, U. S.; Gupta, U.; Narang, D. S.; Late, D. J.; Waghmare, U. V.; Rao, C. N. R., Electronic structure and properties of layered gallium telluride. *Chemical Physics Letters* **2016**, *651*, 148-154 <http://dx.doi.org/10.1016/j.cplett.2016.03.045>
29. Sreedhara, M. B.; Gopalakrishnan, K.; Bharath, B.; Kumar, R.; Kulkarni, G. U.; Rao, C. N. R., Properties of nanosheets of 2D-borocarbonitrides related to energy devices, transistors and other areas. *Chemical Physics Letters* **2016**, *657*, 124-130 <http://dx.doi.org/10.1016/j.cplett.2016.05.064>
30. Guin, S. N.; Sanyal, D.; Biswas, K., The effect of order-disorder phase transitions and band gap evolution on the thermoelectric properties of AgCuS nanocrystals. *Chemical Science* **2016**, *7* (1), 534-543 <http://dx.doi.org/10.1039/c5sc02966j>



-
-
31. Narayanaswamy, N.; Narra, S.; Nair, R. R.; Saini, D. K.; Kondaiah, P.; Govindaraju, T., Stimuli-responsive colorimetric and NIR fluorescence combination probe for selective reporting of cellular hydrogen peroxide. *Chemical Science* **2016**, *7* (4), 2832-2841 <http://dx.doi.org/10.1039/c5sc03488d>
 32. Uppu, Dssm; Konai, M. M.; Baul, U.; Singh, P.; Siersma, T. K.; Samaddar, S.; Vemparala, S.; Hamoen, L. W.; Narayana, C.; Haldar, J., Isosteric substitution in cationic-amphiphilic polymers reveals an important role for hydrogen bonding in bacterial membrane interactions. *Chemical Science* **2016**, *7* (7), 4613-4623 <http://dx.doi.org/10.1039/c6sc00615a>
 33. Saha, S.; Banik, A.; Biswas, K., Few-Layer Nanosheets of n-Type SnSe₂. *Chemistry-a European Journal* **2016**, *22* (44), 15634-15638 <http://dx.doi.org/10.1002/chem.201604161>
 34. Ghosh, C.; Konai, M. M.; Sarkar, P.; Samaddar, S.; Haldar, J., Designing Simple Lipidated Lysines: Bifurcation Imparts Selective Antibacterial Activity. *Chemmedchem* **2016**, *11* (21), 2367-2371 <http://dx.doi.org/10.1002/cmdc.201600400>
 35. Jana, R.; Bhim, A.; Bothra, P.; Pati, S. K.; Peter, S. C., Electrochemical Dealloying of PdCu₃ Nanoparticles to Achieve Pt-like Activity for the Hydrogen Evolution Reaction. *Chemsuschem* **2016**, *9* (20), 2922-2927 <http://dx.doi.org/10.1002/cssc.201601081>
 36. Dey, S.; Naidu, B. S.; Rao, C. N. R., Beneficial effects of substituting trivalent ions in the B-site of La(0.5)Sr(0.5)Mn(1-x)A(x)O(3) (A = Al, Ga, Sc) on the thermochemical generation of CO and H₂ from CO₂ and H₂O. *Dalton Transactions* **2016**, *45* (6), 2430-2435 <http://dx.doi.org/10.1039/c5dt04822b>
 37. Jana, M. K.; Gupta, U.; Rao, C. N. R., Hydrazine as a hydrogen carrier in the photocatalytic generation of H₂ using CdS quantum dots. *Dalton Transactions* **2016**, *45* (38), 15137-15141 <http://dx.doi.org/10.1039/c6dt02505f>
 38. Pramoda, K.; Kaur, M.; Gupta, U.; Rao, C. N. R., Nanocomposites of 2D-MoS₂ nanosheets with the metal-organic framework, ZIF-8. *Dalton Transactions* **2016**, *45* (35), 13810-13816 <http://dx.doi.org/10.1039/c6dt02667b>
 39. Banik, A.; Vishal, B.; Perumal, S.; Datta, R.; Biswas, K., The origin of low thermal conductivity in Sn_{1-x}Sb_xTe: phonon scattering via layered intergrowth nanostructures. *Energy & Environmental Science* **2016**, *9* (6), 2011-2019 <http://dx.doi.org/10.1039/c6ee00728g>
 40. Chhetri, M.; Maitra, S.; Chakraborty, H.; Waghmare, U. V.; Rao, C. N. R., Superior performance of borocarbonitrides, B_xC_yN_z, as stable, low-cost metal-free electrocatalysts for the hydrogen evolution reaction. *Energy & Environmental Science* **2016**, *9* (1), 95-101 <http://dx.doi.org/10.1039/c5ee02521d>
 41. Guin, S. N.; Banerjee, S.; Sanyal, D.; Pati, S. K.; Biswas, K., Origin of the Order-Disorder Transition and the Associated Anomalous Change of Thermopower in AgBiS₂ Nanocrystals: A Combined Experimental and Theoretical Study. *Inorganic Chemistry* **2016**, *55* (12), 6323-6331 <http://dx.doi.org/10.1021/acs.inorgchem.6b00997>
 42. Roy, S.; Sarkar, S.; Pan, J.; Waghmare, U. V.; Dhanya, R.; Narayana, C.; Peter, S. C., Crystal Structure and Band Gap Engineering in Polyoxometalate-Based Inorganic-Organic Hybrids. *Inorganic Chemistry* **2016**, *55* (7), 3364-3377 <http://dx.doi.org/10.1021/acs.inorgchem.5b02718>
 43. Subbarao, U.; Rayaprol, S.; Dally, R.; Graf, M. J.; Peter, S. C., Swinging Symmetry, Multiple Structural Phase Transitions, and Versatile Physical Properties in RECuGa₃ (RE = La-Nd, Sm-Gd). *Inorganic Chemistry* **2016**, *55* (2), 666-675 <http://dx.doi.org/10.1021/acs.inorg-chem.5b02023>

-
-
44. Subbarao, U.; Roy, S.; Sarma, S. C.; Sarkar, S.; Mishra, V.; Khulbe, Y.; Peter, S. C., Metal Flux Growth, Structural Relations, and Physical Properties of EuCu_2Ge_2 and $\text{Eu}_3\text{T}_2\text{In}_9$ (T = Cu and Ag). *Inorganic Chemistry* **2016**, *55* (20), 10351-10360 <http://dx.doi.org/10.1021/acs.inorgchem.6b01598>
 45. Subbarao, U.; Sarkar, S.; Jana, R.; Bera, S. S.; Peter, S. C., Enhanced Air Stability in REPb_3 (RE = Rare Earths) by Dimensional Reduction Mediated Valence Transition. *Inorganic Chemistry* **2016**, *55* (11), 5603-5611 <http://dx.doi.org/10.1021/acs.inorgchem.6b00676>
 46. Perumal, S.; Roychowdhury, S.; Biswas, K., Reduction of thermal conductivity through nanostructuring enhances the thermoelectric figure of merit in $\text{Ge}_{1-x}\text{Bi}_x\text{Te}$. *Inorganic Chemistry Frontiers* **2016**, *3* (1), 125-132 <http://dx.doi.org/10.1039/c5qi00230c>
 47. Subbarao, U.; Sarkar, S.; Joseph, B.; Peter, S. C., Magnetic and X-ray absorption studies on the $\text{RE}_5\text{X}_2\text{Sb}_6$ (RE = Eu, Yb; X = Al, Ga, In) compounds. *Journal of Alloys and Compounds* **2016**, *658*, 395-401 <http://dx.doi.org/10.1016/j.jallcom.2015.10.232>
 48. Dileep, K.; Sahu, R.; Sarkar, S.; Peter, S. C.; Datta, R., Layer specific optical band gap measurement at nanoscale in MoS_2 and ReS_2 van der Waals compounds by high resolution electron energy loss spectroscopy. *Journal of Applied Physics* **2016**, *119* (11), <http://dx.doi.org/10.1063/1.4944431>
 49. Dey, S.; Rajesh, S.; Rao, C. N. R., Significant reduction in the operating temperature of the Mn(II)/Mn(III) oxide-based thermochemical water splitting cycle brought about by the use of nanoparticles. *Journal of Materials Chemistry A* **2016**, *4* (43), 16830-16833 <http://dx.doi.org/10.1039/c6ta06271g>
 50. Pramoda, K.; Gupta, U.; Ahmad, I.; Kumar, R.; Rao, C. N. R., Assemblies of covalently cross-linked nanosheets of MoS_2 and of MoS_2 -RGO: synthesis and novel properties. *Journal of Materials Chemistry A* **2016**, *4* (23), 8989-8994 <http://dx.doi.org/10.1039/c6ta00645k>
 51. Sreedhara, M. B.; Santhosha, A. L.; Bhattacharyya, A. J.; Rao, C. N. R., Composite of few-layer MoO_3 nanosheets with graphene as a high performance anode for sodium-ion batteries. *Journal of Materials Chemistry A* **2016**, *4* (24), 9466-9471 <http://dx.doi.org/10.1039/c6ta02561g>
 52. Jain, A.; Achari, A.; Eswaramoorthy, M.; George, S. J., Light induced in situ post-modification of clay-chromophore hybrids for multiple white light emissions. *Journal of Materials Chemistry C* **2016**, *4* (14), 2748-2751 <http://dx.doi.org/10.1039/c5tc03319e>
 53. Perumal, S.; Roychowdhury, S.; Biswas, K., High performance thermoelectric materials and devices based on GeTe . *Journal of Materials Chemistry C* **2016**, *4* (32), 7520-7536 <http://dx.doi.org/10.1039/c6tc02501c>
 54. Roy, S.; Chanu, O. B.; Sarkar, S.; Peter, S. C., Selective colorimetric detection of Cu^{2+} by lanthanide based hybrid complexes associated with a single crystal growth mediated transformation. *Journal of Materials Chemistry C* **2016**, *4* (26), 6256-6269 <http://dx.doi.org/10.1039/c6tc00785f>
 55. Suryawanshi, S. R.; Guin, S. N.; Chatterjee, A.; Kashid, V.; More, M. A.; Late, D. J.; Biswas, K., Low frequency noise and photo-enhanced field emission from ultrathin PbBi_2Se_4 nanosheets. *Journal of Materials Chemistry C* **2016**, *4* (5), 1096-1103 <http://dx.doi.org/10.1039/c5tc02993g>
 56. Aggarwala, Leena; Banikb, Ananya; Anandc, Shashwat; Waghmarec, Umesh V.; Biswasb, Kanishka; Shee, Goutam, Local ferroelectricity in thermoelectric SnTe above room temperature driven by competing phonon instabilities and soft resonant bonding *Journal of Materiomics* **2016**, *2* (2), 196-202 <http://dx.doi.org/http://doi.org/10.1016/j.jmat.2016.04.001>
 57. Hoque, J.; Konai, M. M.; Sequeira, S. S.; Samaddar, S.; Haldar, J., Antibacterial and Antibiofilm Activity of Cationic Small Molecules with Spatial Positioning of Hydrophobicity: An in Vitro and in Vivo



-
- Evaluation. *Journal of Medicinal Chemistry* **2016**, *59* (23), 10750-10762 <http://dx.doi.org/10.1021/acs.jmedchem.6b01435>
58. Reddy, G. R.; Avadhani, A. S.; Rajaram, S., Activation of Benzyl Aryl Carbonates: The Role of Cation- π Interactions. *Journal of Organic Chemistry* **2016**, *81* (10), 4134-4141 <http://dx.doi.org/10.1021/acs.joc.6b00441>
59. Yugandar, S.; Konda, S.; Ila, H., Amine Directed Pd(II)-Catalyzed C-H Activation-Intramolecular Amination of N-Het(aryl)/Acyl Enaminonitriles and Enaminones: An Approach towards Multisubstituted Indoles and Heterofused Pyrroles. *Journal of Organic Chemistry* **2016**, *81* (5), 2035-2052 <http://dx.doi.org/10.1021/acs.joc.5b02902>
60. Yugandar, S.; Konda, S.; Parameshwarappa, G.; Ila, H., One-Pot Synthesis of 2,4,5-Trisubstituted Imidazoles via 2+2+1 Cycloannulation of 1,3-Bis(aryl)-monothio-1,3-diketones, α -Substituted Methylamines and Sodium Nitrite through α -Nitrosation of Enaminones. *Journal of Organic Chemistry* **2016**, *81* (13), 5606-5622 <http://dx.doi.org/10.1021/acs.joc.6b00938>
61. Roy, A.; Shenoy, U. S.; Manjunath, K.; Vishnoi, P.; Waghmare, U. V.; Rao, C. N. R., Structure and Properties of Cd₄P₂Cl₃, an Analogue of CdS. *Journal of Physical Chemistry C* **2016**, *120* (28), 15063-15069 <http://dx.doi.org/10.1021/acs.jpcc.6b04058>
62. Sorb, Y. A.; Rajaji, V.; Malavi, P. S.; Subbarao, U.; Halappa, P.; Peter, S. C.; Karmakar, S.; Narayana, C., Pressure-induced electronic topological transition in Sb₂S₃. *Journal of Physics-Condensed Matter* **2016**, *28* (1), <http://dx.doi.org/10.1088/0953-8984/28/1/015602>
63. Sarkar, S.; Borah, R.; Santhosha, A. L.; Dhanya, R.; Narayana, C.; Bhattacharyya, A. J.; Peter, S. C., Heterostructure composites of rGO/GeO₂/PANI with enhanced performance for Li ion battery anode material. *Journal of Power Sources* **2016**, *306*, 791-800 <http://dx.doi.org/10.1016/j.jpowsour.2015.12.094>
64. Banik, A.; Biswas, K., AgI alloying in SnTe boosts the thermoelectric performance via simultaneous valence band convergence and carrier concentration optimization. *Journal of Solid State Chemistry* **2016**, *242*, 43-49 <http://dx.doi.org/10.1016/j.jssc.2016.02.012>
65. Jana, R.; Peter, S. C., One-pot solvothermal synthesis of ordered intermetallic Pt₂In₃ as stable and efficient electrocatalyst towards direct alcohol fuel cell application. *Journal of Solid State Chemistry* **2016**, *242*, 133-139 <http://dx.doi.org/10.1016/j.jssc.2016.02.016>
66. Mumbaraddi, D.; Sarkar, S.; Peter, S. C., A review on the synthesis, crystal growth, structure and physical properties of rare earth based quaternary intermetallic compounds. *Journal of Solid State Chemistry* **2016**, *236*, 94-115 <http://dx.doi.org/10.1016/j.jssc.2015.10.032>
67. Rao, C. N. R.; Dey, S., Generation of H₂ and CO by solar thermochemical splitting of H₂O and CO₂ by employing metal oxides. *Journal of Solid State Chemistry* **2016**, *242*, 107-115 <http://dx.doi.org/10.1016/j.jssc.2015.12.018>
68. Roychowdhury, S.; Ghara, S.; Guin, S. N.; Sundaresan, A.; Biswas, K., Large linear magnetoresistance in topological crystalline insulator Pb_{0.6}Sn_{0.4}Te. *Journal of Solid State Chemistry* **2016**, *233*, 199-204 <http://dx.doi.org/10.1016/j.jssc.2015.10.029>
69. Subbarao, U.; Marakatti, V. S.; Amshumali, M. K.; Loukya, B.; Singh, D. K.; Datta, R.; Peter, S. C., Size and morphology controlled NiSe nanoparticles as efficient catalyst for the reduction reactions. *Journal of Solid State Chemistry* **2016**, *244*, 84-92 <http://dx.doi.org/10.1016/j.jssc.2016.09.020>
-

-
-
70. Banik, A.; Shenoy, U. S.; Saha, S.; Waghmare, U. V.; Biswas, K., High Power Factor and Enhanced Thermoelectric Performance of SnTe-AgInTe₂: Synergistic Effect of Resonance Level and Valence Band Convergence. *Journal of the American Chemical Society* **2016**, *138* (39), 13068-13075 <http://dx.doi.org/10.1021/jacs.6b08382>
 71. Lingampalli, S. R.; Manjunath, K.; Shenoy, S.; Waghmare, U. V.; Rao, C. N. R., Zn₂NF and Related Analogues of ZnO. *Journal of the American Chemical Society* **2016**, *138* (26), 8228-8234 <http://dx.doi.org/10.1021/jacs.6b04198>
 72. Pandeewar, M.; Senanayak, S. P.; Narayan, K. S.; Govindaraju, T., Multi-Stimuli-Responsive Charge-Transfer Hydrogel for Room-Temperature Organic Ferroelectric Thin-Film Devices. *Journal of the American Chemical Society* **2016**, *138* (26), 8259-8268 <http://dx.doi.org/10.1021/jacs.6b03811>
 73. Rajkumar, Jana; Shikha, Dhiman; Sebastian, C. Peter, Facile solvothermal synthesis of highly active and robust Pd_{1.87}Cu_{0.11}Sn electrocatalyst towards direct ethanol fuel cell applications. *Materials Research Express* **2016**, *3* (8), 084001
 74. Hoque, J.; Adhikary, U.; Yadav, V.; Samaddar, S.; Konai, M. M.; Prakash, R. G.; Pararnanandham, K.; Shome, B. R.; Sanyal, K.; Haldar, J., Chitosan Derivatives Active against Multidrug-Resistant Bacteria and Pathogenic Fungi: In Vivo Evaluation as Topical Antimicrobials. *Molecular Pharmaceutics* **2016**, *13* (10), 3578-3589 <http://dx.doi.org/10.1021/acs.molpharmaceut.6b00764>
 75. Pandeewar, M.; Govindaraju, T., Engineering molecular self-assembly of perylene diimide through pH-responsive chiroptical switching. *Molecular Systems Design & Engineering* **2016**, *1* (2), 202-207 <http://dx.doi.org/10.1039/C6ME00012F>
 76. Jungmann, R.; Avendano, M. S.; Dai, M. J.; Woehrstein, J. B.; Agasti, S. S.; Feiger, Z.; Rodal, A.; Yin, P., Quantitative super-resolution imaging with qPAINT. *Nature Methods* **2016**, *13* (5), 439-+ <http://dx.doi.org/10.1038/nmeth.3804>
 77. Jain, A.; George, S. J., Meshing organic nanowires Photogenerated charge carriers from hundreds of self-assembled nanowires are harnessed to make a functional photovoltaic device. *Nature Nanotechnology* **2016**, *11* (10), 842-843 <http://dx.doi.org/10.1038/nnano.2016.136>
 78. Marakatti, V. S.; Peter, S. C., Nickel-antimony nanoparticles confined in SBA-15 as highly efficient catalysts for the hydrogenation of nitroarenes. *New Journal of Chemistry* **2016**, *40* (6), 5448-5457 <http://dx.doi.org/10.1039/c5nj03479e>
 79. Jana, M. K.; Rao, C. N. R., Two-dimensional inorganic analogues of graphene: transition metal dichalcogenides. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2016**, *374* (2076), <http://dx.doi.org/10.1098/rsta.2015.0318>
 80. Rao, C. N. R.; Lingampalli, S. R.; Dey, S.; Roy, A., Solar photochemical and thermochemical splitting of water. *Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences* **2016**, *374* (2061), <http://dx.doi.org/10.1098/rsta.2015.0088>
 81. Saha, R.; Vasu, K.; Negi, D. S.; Datta, R.; Sundaresan, A.; Rao, C. N. R., Exchange bias at low fields exhibited by the interface between epitaxial layers of ferromagnetic and charge-ordered rare-earth manganites. *Physica Status Solidi-Rapid Research Letters* **2016**, *10* (8), 622-626 <http://dx.doi.org/10.1002/pssr.201600155>
 82. Rao, K. V.; Haldar, R.; Maji, T. K.; George, S. J., Dynamic, conjugated microporous polymers: visible light harvesting via guest-responsive reversible swelling. *Physical Chemistry Chemical Physics* **2016**, *18* (1), 156-163 <http://dx.doi.org/10.1039/c5cp05052a>



-
-
83. Saha, R.; Sundaresan, A.; Sanyal, M. K.; Rao, C. N. R.; Orlandi, F.; Manuel, P.; Langridge, S., Neutron scattering study of the crystallographic and spin structure in antiferromagnetic EuZrO₃. *Physical Review B* **2016**, *93* (1), <http://dx.doi.org/10.1103/PhysRevB.93.014409>
 84. Rajasekhar, K.; Narayanaswamy, N.; Murugan, N. A.; Kuang, G. L.; Agren, H.; Govindaraju, T., A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid beta Aggregates. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep23668>
 85. Rao, C. N. R.; Lingampalli, S. R., Generation of Hydrogen by Visible Light-Induced Water Splitting with the Use of Semiconductors and Dyes. *Small* **2016**, *12* (1), 16-23 <http://dx.doi.org/10.1002/smll.201500420>
 86. Roy, A.; Lingampalli, S. R.; Nassar, I. M.; Rao, C. N. R., Effectiveness of NiO in replacing Pt in the photochemical generation of hydrogen by (TiO₂)(1-x)(NiO)(x)/Cd_{0.8}Zn_{0.2}S heterostructures. *Solid State Communications* **2016**, *243*, 1-6 <http://dx.doi.org/10.1016/j.ssc.2016.05.018>
 87. Dowall, S. D.; Bewley, K.; Watson, R. J.; Vasan, S. S.; Ghosh, C.; Konai, M. M.; Gausdal, G.; Lorens, J. B.; Long, J.; Barclay, W.; Garcia-Dorival, I.; Hiscox, J.; Bosworth, A.; Taylor, I.; Easterbrook, L.; Pitman, J.; Summers, S.; Chan-Pensley, J.; Funnell, S.; Vipond, J.; Charlton, S.; Haldar, J.; Hewson, R.; Carroll, M. W., Antiviral Screening of Multiple Compounds against Ebola Virus. *Viruses-Basel* **2016**, *8* (11), <http://dx.doi.org/10.3390/v8110277>
 88. Jana, M. K.; Singh, A.; Sampath, A.; Rao, C. N. R.; Waghmare, U. V., Structure and Electron-Transport Properties of Anion-Deficient MoTe₂: A Combined Experimental and Theoretical Study. *Zeitschrift Fur Anorganische Und Allgemeine Chemie* **2016**, *642* (23), 1386-1396 <http://dx.doi.org/10.1002/zaac.201600314>

Theoretical Sciences Unit (TSU)

1. Chakraborty, B.; Gupta, S. N.; Singh, A.; Kuiri, M.; Kumar, C.; Muthu, D. V. S.; Das, A.; Waghmare, U. V.; Sood, A. K., Electron-hole asymmetry in the electron-phonon coupling in top-gated phosphorene transistor. *2D Materials* **2016**, *3* (1), <http://dx.doi.org/10.1088/2053-1583/3/1/015008>
2. Chakraborty, B.; Gupta, S. N.; Singh, A.; Kuiri, M.; Kumar, C.; Muthu, D. V. S.; Das, A.; Waghmare, U. V.; Sood, A. K., Electron-hole asymmetry in the electron-phonon coupling in top-gated phosphorene transistor. *2D Materials* **2016**, *3* (1), <http://dx.doi.org/10.1088/2053-1583/3/1/015008>
3. Mukherjee, G.; Bhanot, G.; Raines, K.; Sastry, S.; Doniach, S.; Biehl, M.; Ieee, Predicting recurrence in clear cell Renal Cell Carcinoma. *2016 Ieee Congress on Evolutionary Computation (Cec)* **2016**, 656-661
4. Bothra, P.; Pati, S. K., Activity of Water Oxidation on Pure and (Fe, Ni, and Cu)-Substituted Co₃O₄. *ACS Energy Letters* **2016**, *1* (4), 858-862 <http://dx.doi.org/10.1021/acsenerylett.6b00369>
5. Sharma, D.; Upadhyay, S.; Satsangi, V. R.; Shrivastav, R.; Waghmare, U. V.; Dass, S., Ni-Doped Cu₂O Thin Films for Solar-Hydrogen Generation: Experiments and First-Principles Analysis. *Advanced Science Letters* **2016**, *22* (4), 780-784 <http://dx.doi.org/10.1166/asl.2016.6920>
6. Jana, M. K.; Pal, K.; Waghmare, U. V.; Biswas, K., The Origin of Ultralow Thermal Conductivity in InTe: Lone-Pair-Induced Anharmonic Rattling. *Angewandte Chemie-International Edition* **2016**, *55* (27), 7792-7796 <http://dx.doi.org/10.1002/anie.201511737>
7. Sharma, D.; Upadhyay, S.; Satsangi, V. R.; Shrivastav, R.; Waghmare, U. V.; Dass, S., Nanostructured BaTiO₃/Cu₂O heterojunction with improved photoelectrochemical activity for H₂ evolution: Experimental and first-principles analysis. *Applied Catalysis B-Environmental* **2016**, *189*, 75-85 <http://dx.doi.org/10.1016/j.apcatb.2016.02.037>

-
-
8. Rajaji, V.; Malavi, P. S.; Yamijala, Ssrkc; Sorb, Y. A.; Dutta, U.; Guin, S. N.; Joseph, B.; Pati, S. K.; Karmakar, S.; Biswas, K.; Narayana, C., Pressure induced structural, electronic topological, and semiconductor to metal transition in AgBiSe₂. *Applied Physics Letters* **2016**, *109* (17), <http://dx.doi.org/10.1063/1.4966275>
 9. Roychowdhury, S.; Shenoy, U. S.; Waghmare, U. V.; Biswas, K., Effect of potassium doping on electronic structure and thermoelectric properties of topological crystalline insulator. *Applied Physics Letters* **2016**, *108* (19), <http://dx.doi.org/10.1063/1.4948969>
 10. Bothra, P.; Pandey, M.; Pati, S. K., Size-selective electrocatalytic activity of (Pt)(n)/MoS₂ for oxygen reduction reaction. *Catalysis Science & Technology* **2016**, *6* (16), 6389-6395 <http://dx.doi.org/10.1039/c6cy01050d>
 11. Suseela, Y. V.; Das, S.; Pati, S. K.; Govindaraju, T., Imidazolyl-Naphthalenediimide-Based Threading Intercalators of DNA. *ChemBiochem* **2016**, *17* (22), 2162-2171 <http://dx.doi.org/10.1002/cbic.201600478>
 12. Banerjee, S.; Pati, S. K., Anodic performance of black phosphorus in magnesium-ion batteries: the significance of Mg-P bond-synergy. *Chemical Communications* **2016**, *52* (54), 8381-8384 <http://dx.doi.org/10.1039/c6cc04236h>
 13. Bhattacharjee, S.; Yoo, S. J.; Waghmare, U. V.; Lee, S. C., NH₃ adsorption on PtM (Fe, Co, Ni) surfaces: Cooperating effects of charge transfer, magnetic ordering and lattice strain. *Chemical Physics Letters* **2016**, *648*, <http://dx.doi.org/10.1016/j.cplett.2016.01.031>
 14. Shenoy, U. S.; Gupta, U.; Narang, D. S.; Late, D. J.; Waghmare, U. V.; Rao, C. N. R., Electronic structure and properties of layered gallium telluride. *Chemical Physics Letters* **2016**, *651*, 148-154 <http://dx.doi.org/10.1016/j.cplett.2016.03.045>
 15. Jana, R.; Bhim, A.; Bothra, P.; Pati, S. K.; Peter, S. C., Electrochemical Dealloying of PdCu₃ Nanoparticles to Achieve Pt-like Activity for the Hydrogen Evolution Reaction. *Chemsuschem* **2016**, *9* (20), 2922-2927 <http://dx.doi.org/10.1002/cssc.201601081>
 16. Majhi, Kunjalata; Pal, Koushik; Lohani, Himanshu; Banerjee, Abhishek; Mishra, Pramita; Yadav, Anil K; Ganesan, R; Sekhar, BR; Waghmare, Umesh V; Kumar, PS Anil, Emergence of a weak topological insulator from the BixSey family and the observation of weak anti-localization. *Condensed Matter Material Sciences*. **2016**,
 17. Haldar, R.; Prasad, K.; Samanta, P. K.; Pati, S.; Maji, T. K., Luminescent Metal-Organic Complexes of Pyrene or Anthracene Chromophores: Energy Transfer Assisted Amplified Exciplex Emission and Al³⁺ Sensing. *Crystal Growth & Design* **2016**, *16* (1), 82-91 <http://dx.doi.org/10.1021/acs.cgd.5b01448>
 18. Songkhao, Jittikarn; Banerjee, Rajdeep; Debnath, Saikat; Narasimhan, Shobhana; Wannaprom, Napaporn; Vanalabhpata, Parichatr; Seriani, Nicola; Gebauer, Ralph, Structure-property relationship of π -extended boron-dipyrromethene derivatives towards optoelectronic applications. *Dyes and Pigments* **2016**, *142*, 558-571 <http://dx.doi.org/http://doi.org/10.1016/j.dyepig.2017.03.050>
 19. Chhetri, M.; Maitra, S.; Chakraborty, H.; Waghmare, U. V.; Rao, C. N. R., Superior performance of borocarbonitrides, B_xC_yN_z, as stable, low-cost metal-free electrocatalysts for the hydrogen evolution reaction. *Energy & Environmental Science* **2016**, *9* (1), 95-101 <http://dx.doi.org/10.1039/c5ee02521d>
 20. Basu, S.; Majumder, S.; Sutradhar, S.; Das, S. K.; Paul, R., Phase segregation in a binary fluid confined inside a nanopore. *Europhysics Letters* **2016**, *116* (5), <http://dx.doi.org/10.1209/0295-5075/116/56003>
 21. Priyanka; Jain, K., Critical dynamics of classical systems under slow quench. *Europhysics Letters* **2016**, *116* (2), <http://dx.doi.org/10.1209/0295-5075/116/26003>



-
-
22. Guin, S. N.; Banerjee, S.; Sanyal, D.; Pati, S. K.; Biswas, K., Origin of the Order-Disorder Transition and the Associated Anomalous Change of Thermopower in AgBiS₂ Nanocrystals: A Combined Experimental and Theoretical Study. *Inorganic Chemistry* **2016**, *55* (12), 6323-6331 <http://dx.doi.org/10.1021/acs.inorgchem.6b00997>
 23. Roy, S.; Sarkar, S.; Pan, J.; Waghmare, U. V.; Dhanya, R.; Narayana, C.; Peter, S. C., Crystal Structure and Band Gap Engineering in Polyoxometalate-Based Inorganic-Organic Hybrids. *Inorganic Chemistry* **2016**, *55* (7), 3364-3377 <http://dx.doi.org/10.1021/acs.inorgchem.5b02718>
 24. Sharma, D.; Satsangi, V. R.; Shrivastau, R.; Waghmare, U. V.; Dass, S., Understanding the photoelectrochemical properties of nanostructured CeO₂/Cu₂O heterojunction photoanode for efficient photoelectrochemical water splitting. *International Journal of Hydrogen Energy* **2016**, *41* (41), 18339-18350 <http://dx.doi.org/10.1016/j.ijhydene.2016.08.079>
 25. Pan, J.; Niranjana, M. K.; Waghmare, U. V., Aliovalent cation ordering, coexisting ferroelectric structures, and electric field induced phase transformation in lead-free ferroelectric Na_{0.5}Bi_{0.5}TiO₃. *Journal of Applied Physics* **2016**, *119* (12), <http://dx.doi.org/10.1063/1.4944473>
 26. Karmakar, T.; Roy, S.; Balaran, H.; Prakash, M. K.; Balasubramanian, S., Product Release Pathways in Human and Plasmodium falciparum Phosphoribosyltransferase. *Journal of Chemical Information and Modeling* **2016**, *56* (8), 1528-1538 <http://dx.doi.org/10.1021/acs.jcim.6b00203>
 27. Banerjee, A.; Nandi, M. K.; Sastry, S.; Bhattacharyya, S. M., Effect of total and pair configurational entropy in determining dynamics of supercooled liquids over a range of densities. *Journal of Chemical Physics* **2016**, *145* (3), <http://dx.doi.org/10.1063/1.4958627>
 28. Trefz, B.; Das, S. K.; Egorov, S. A.; Virnau, P.; Binder, K., Activity mediated phase separation: Can we understand phase behavior of the nonequilibrium problem from an equilibrium approach? *Journal of Chemical Physics* **2016**, *144* (14), <http://dx.doi.org/10.1063/1.4945365>
 29. Banerjee, S.; Neihial, S.; Pati, S. K., First-principles design of a borocarbonitride-based anode for superior performance in sodium-ion batteries and capacitors. *Journal of Materials Chemistry A* **2016**, *4* (15), 5517-5527 <http://dx.doi.org/10.1039/c6ta01645f>
 30. Aggarwala, Leena; Banikb, Ananya; Anandc, Shashwat; Waghmarec, Umesh V.; Biswasb, Kanishka; Shee, Goutam, Local ferroelectricity in thermoelectric SnTe above room temperature driven by competing phonon instabilities and soft resonant bonding *Journal of Materiomics* **2016**, *2* (2), 196-202 <http://dx.doi.org/http://doi.org/10.1016/j.jmat.2016.04.001>
 31. Kumawat, N. K.; Tripathi, M. N.; Waghmare, U.; Kabra, D., Structural, Optical, and Electronic Properties of Wide Bandgap Perovskites: Experimental and Theoretical Investigations. *Journal of Physical Chemistry A* **2016**, *120* (22), 3917-3923 <http://dx.doi.org/10.1021/acs.jpca.6b04138>
 32. Biswas, S.; Narasimhan, S., Bromine as a Preferred Etchant for Si Surfaces in the Supersaturation Regime: Insights from Calculations of Atomic Scale Reaction Pathways. *Journal of Physical Chemistry C* **2016**, *120* (28), 15230-15234 <http://dx.doi.org/10.1021/acs.jpcc.6b04450>
 33. Ghosh, D.; Parida, P.; Pati, S. K., Spin-State Switching of Manganese Porphyrin by Conformational Modification. *Journal of Physical Chemistry C* **2016**, *120* (7), 3625-3634 <http://dx.doi.org/10.1021/acs.jpcc.5b11227>
 34. Kumar, P.; Yamijala, Ssrkc; Pati, S. K., Optical Unzipping of Carbon Nanotubes in Liquid Media. *Journal of Physical Chemistry C* **2016**, *120* (30), 16985-16993 <http://dx.doi.org/10.1021/acs.jpcc.6b02524>

-
-
35. Pandey, M.; Bothra, P.; Pati, S. K., Phase Transition of MoS₂ Bilayer Structures. *Journal of Physical Chemistry C* **2016**, *120* (7), 3776-3780 <http://dx.doi.org/10.1021/acs.jpcc.5b10904>
 36. Roy, A.; Shenoy, U. S.; Manjunath, K.; Vishnoi, P.; Waghmare, U. V.; Rao, C. N. R., Structure and Properties of Cd₄P₂Cl₃, an Analogue of CdS. *Journal of Physical Chemistry C* **2016**, *120* (28), 15063-15069 <http://dx.doi.org/10.1021/acs.jpcc.6b04058>
 37. Roy, S.; Hazra, A.; Bandyopadhyay, A.; Raut, D.; Madhuri, P. L.; Rao, D. S. S.; Ramamurty, U.; Pati, S. K.; Prasad, S. K.; Maji, T. K., Reversible Polymorphism, Liquid Crystallinity, and Stimuli-Responsive Luminescence in a Bola-amphiphilic pi-System: Structure-Property Correlations Through Nanoindentation and DFT Calculations. *Journal of Physical Chemistry Letters* **2016**, *7* (20), 4086-4092 <http://dx.doi.org/10.1021/acs.jpcllett.6b01891>
 38. Acharya, S.; Medhi, A.; Vidhyadhiraja, N. S.; Taraphder, A., Feasibility of a metamagnetic transition in correlated systems. *Journal of Physics-Condensed Matter* **2016**, *28* (11), <http://dx.doi.org/10.1088/0953-8984/28/11/116001>
 39. Aslam, M.; Paul, A.; Thakur, G. S.; Gayen, S.; Kumar, R.; Singh, A.; Das, S.; Ganguli, A. K.; Waghmare, U. V.; Sheet, G., Evidence of a pseudogap driven by competing orders of multi-band origin in the ferromagnetic superconductor Sr_{0.5}Ce_{0.5}FbS₂. *Journal of Physics-Condensed Matter* **2016**, *28* (19), <http://dx.doi.org/10.1088/0953-8984/28/19/195701>
 40. Bera, A.; Pal, K.; Muthu, D. V. S.; Waghmare, U. V.; Sood, A. K., Pressure-induced phase transition in Bi₂Se₃ at 3 GPa: electronic topological transition or not? *Journal of Physics-Condensed Matter* **2016**, *28* (10), <http://dx.doi.org/10.1088/0953-8984/28/10/105401>
 41. Pandey, B.; Dutta, S.; Pati, S. K., Breakdown of electron-pairs in the presence of an electric field of a superconducting ring. *Journal of Physics-Condensed Matter* **2016**, *28* (19), <http://dx.doi.org/10.1088/0953-8984/28/19/195601>
 42. Vinutha, H. A.; Sastry, S., Geometric aspects of shear jamming induced by deformation of frictionless sphere packings. *Journal of Statistical Mechanics-Theory and Experiment* **2016**, <http://dx.doi.org/10.1088/1742-5468/2016/09/094002>
 43. Banik, A.; Shenoy, U. S.; Saha, S.; Waghmare, U. V.; Biswas, K., High Power Factor and Enhanced Thermoelectric Performance of SnTe-AgInTe₂: Synergistic Effect of Resonance Level and Valence Band Convergence. *Journal of the American Chemical Society* **2016**, *138* (39), 13068-13075 <http://dx.doi.org/10.1021/jacs.6b08382>
 44. Lingampalli, S. R.; Manjunath, K.; Shenoy, S.; Waghmare, U. V.; Rao, C. N. R., Zn₂NF and Related Analogues of ZnO. *Journal of the American Chemical Society* **2016**, *138* (26), 8228-8234 <http://dx.doi.org/10.1021/jacs.6b04198>
 45. Nishimatsu, T.; Grunebohm, A.; Waghmare, U. V.; Kubo, M., Molecular Dynamics Simulations of Chemically Disordered Ferroelectric (Ba,Sr)TiO₃ with a Semi-Empirical Effective Hamiltonian. *Journal of the Physical Society of Japan* **2016**, *85* (11), <http://dx.doi.org/10.7566/jpsj.85.114714>
 46. Anand, S.; Thekkepat, K.; Waghmare, U. V., Two-Dimensional Rectangular and Honeycomb Lattices of NbN: Emergence of Piezoelectric and Photocatalytic Properties at Nanoscale. *Nano Letters* **2016**, *16* (1), 126-131 <http://dx.doi.org/10.1021/acs.nanolett.5b03275>
 47. Mettela, Gangaiah; Mammen, Nisha; Joardar, Joydip; Narasimhan, Shobhana; Kulkarni, G. U., Non-FCC rich Au crystallites exhibiting unusual catalytic activity. *Nano Research* **2016**, 1-9 <http://dx.doi.org/10.1007/s12274-017-1417-y>



-
-
48. Sun, J. W.; Remsing, R. C.; Zhang, Y. B.; Sun, Z. R.; Ruzsinszky, A.; Peng, H. W.; Yang, Z. H.; Paul, A.; Waghmare, U.; Wu, X. F.; Klein, M. L.; Perdew, J. P., Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. *Nature Chemistry* **2016**, *8* (9), 831-836 <http://dx.doi.org/10.1038/nchem.2535>
 49. Vinutha, H. A.; Sastry, S., Disentangling the role of structure and friction in shear jamming. *Nature Physics* **2016**, *12* (6), 578-+ <http://dx.doi.org/10.1038/nphys3658>
 50. Jung, N.; Bhattacharjee, S.; Gautam, S.; Park, H. Y.; Ryu, J.; Chung, Y. H.; Lee, S. Y.; Jang, I.; Jang, J. H.; Park, S. H.; Chung, D. Y.; Sung, Y. E.; Chae, K. H.; Waghmare, U. V.; Lee, S. C.; Yoo, S. J., Organic-inorganic hybrid PtCo nanoparticle with high electrocatalytic activity and durability for oxygen reduction. *NPG Asia Materials* **2016**, *8*, <http://dx.doi.org/10.1038/am.2015.143>
 51. Bandyopadhyay, A.; Pati, S. K., Role of donor-acceptor macrocycles in sequence specific peptide recognition and their optoelectronic properties: a detailed computational insight. *Physical Chemistry Chemical Physics* **2016**, *18* (30), 20682-20690 <http://dx.doi.org/10.1039/c6cp03181a>
 52. Banerjee, S.; Pati, S. K., Charge-transport anisotropy in black phosphorus: critical dependence on the number of layers. *Physical Chemistry Chemical Physics* **2016**, *18* (24), 16345-16352 <http://dx.doi.org/10.1039/c6cp02129h>
 53. Bhat, S. S.; Li, W.; Cheetham, A. K.; Waghmare, U. V.; Ramamurty, U., A first-principles study of pressure-induced phase transformation in a rare-earth formate framework. *Physical Chemistry Chemical Physics* **2016**, *18* (28), 19032-19036 <http://dx.doi.org/10.1039/c6cp03028a>
 54. Sanyal, S.; Painelli, A.; Pati, S. K.; Terenziani, F.; Sissa, C., Aggregates of quadrupolar dyes for two-photon absorption: the role of intermolecular interactions. *Physical Chemistry Chemical Physics* **2016**, *18* (40), 28198-28208 <http://dx.doi.org/10.1039/c6cp05153g>
 55. Sarkar, T.; Kumar, P.; Bharadwaj, M. D.; Waghmare, U., Structural transformation during Li/Na insertion and theoretical cyclic voltammetry of the delta-NH4V4O10 electrode: a first-principles study. *Physical Chemistry Chemical Physics* **2016**, *18* (14), 9344-9348 <http://dx.doi.org/10.1039/c5cp07782f>
 56. Mukhopadhyay, M.; Pandey, B.; Pati, S. K., Tuning the Optically Bright and Dark States of Doped Graphene Quantum Dots. *Physical Review Applied* **2016**, *6* (4), <http://dx.doi.org/10.1103/PhysRevApplied.6.044014>
 57. Baidya, S.; Waghmare, U. V.; Paramakanti, A.; Saha-Dasgupta, T., High-temperature large-gap quantum anomalous Hall insulating state in ultrathin double perovskite films. *Physical Review B* **2016**, *94* (15), <http://dx.doi.org/10.1103/PhysRevB.94.155405>
 58. Dasari, N.; Yamijala, Srkcs; Jain, M.; Dasgupta, T. S.; Moreno, J.; Jarrell, M.; Vidhyadhiraja, N. S., First-principles investigation of cubic BaRuO3: A Hund's metal. *Physical Review B* **2016**, *94* (8), <http://dx.doi.org/10.1103/PhysRevB.94.085143>
 59. Sen, S.; Terletska, H.; Moreno, J.; Vidhyadhiraja, N. S.; Jarrell, M., Local theory for Mott-Anderson localization. *Physical Review B* **2016**, *94* (23), <http://dx.doi.org/10.1103/PhysRevB.94.235104>
 60. Sen, S.; Vidhyadhiraja, N. S., Quantum critical Mott transitions in a bilayer Kondo insulator-metal model system. *Physical Review B* **2016**, *93* (15), <http://dx.doi.org/10.1103/PhysRevB.93.155136>
 61. Zhang, Y.; Nelson, R.; Siddiqui, E.; Tam, K. M.; Yu, U.; Berlijn, T.; Ku, W.; Vidhyadhiraja, N. S.; Moreno, J.; Jarrell, M., Generalized multiband typical medium dynamical cluster approximation: Application to (Ga, Mn)N. *Physical Review B* **2016**, *94* (22), <http://dx.doi.org/10.1103/PhysRevB.94.224208>

-
-
62. Chakraborty, S.; Das, S. K., Fractality in persistence decay and domain growth during ferromagnetic ordering: Dependence upon initial correlation. *Physical Review E* **2016**, *93* (3), <http://dx.doi.org/10.1103/PhysRevE.93.032139>
 63. Priyanka; Jain, K., Critical dynamics of the jamming transition in one-dimensional nonequilibrium lattice-gas models. *Physical Review E* **2016**, *93* (4), <http://dx.doi.org/10.1103/PhysRevE.93.042104>
 64. Liu, S.; Phillabaum, B.; Carlson, E. W.; Dahmen, K. A.; Vidhyadhiraja, N. S.; Qazilbash, M. M.; Basov, D. N., Random Field Driven Spatial Complexity at the Mott Transition in VO₂. *Physical Review Letters* **2016**, *116* (3), <http://dx.doi.org/10.1103/PhysRevLett.116.036401>
 65. Adalikwu, S. A.; Chakraborty, A.; Hazra, A.; Ghosh, D.; Pati, S. K.; Maji, T. K., 2D coordination polymer composed of 1D {Ni-II(μ -O)(μ -H₂O)Ni-II}(n) ferromagnetic chains: Modulation of magnetic properties based on dehydration and rehydration. *Polyhedron* **2016**, *115*, 276-281 <http://dx.doi.org/10.1016/j.poly.2016.05.011>
 66. Sastry, S., Critically jammed. *Proceedings of the National Academy of Sciences of the United States of America* **2016**, *113* (35), 9673-9675 <http://dx.doi.org/10.1073/pnas.1610804113>
 67. S, Sastry, Scaling concepts in describing continuous phase transitions. *Resonance* **2016**, *21* (10), 875–898 <http://dx.doi.org/10.1007/s12045-016-0398-1>
 68. Bhattacharjee, S.; Waghmare, U. V.; Lee, S. C., An improved d-band model of the catalytic activity of magnetic transition metal surfaces. *Scientific Reports* **2016**, *6*, <http://dx.doi.org/10.1038/srep35916>
 69. Jain, K.; John, S., Deterministic evolution of an asexual population under the action of beneficial and deleterious mutations on additive fitness landscapes. *Theoretical Population Biology* **2016**, *112*, 117-125 <http://dx.doi.org/10.1016/j.tpb.2016.08.009>

RESEARCH PUBLICATIONS OF HONORARY FACULTY/ ENDOWED PROFESSORS

1. Karunakaran, V.; Das, S., Direct Observation of Cascade of Photoinduced Ultrafast Intramolecular Charge Transfer Dynamics in Diphenyl Acetylene Derivatives: Via Solvation and Intramolecular Relaxation. *Journal of Physical Chemistry B* **2016**, *120* (28), 7016-7023 <http://dx.doi.org/10.1021/acs.jpccb.6b05264>
2. Ahmed, F.; Roy, S.; Naskar, K.; Sinha, C.; Alam, S. M.; Kundu, S.; Vittal, J. J.; Mir, M. H., Halogen center dot center dot center dot Halogen Interactions in the Supramolecular Assembly of 2D Coordination Polymers and the CO₂ Sorption Behavior. *Crystal Growth & Design* **2016**, *16* (9), 5514-5519 <http://dx.doi.org/10.1021/acs.cgd.6b00983>
3. Aluri, S.; Sah, S.; Miryala, S.; Varshney, U., Physiological role of F_oD (methylenetetrahydrofolate dehydrogenase), F_{ch}A (methenyltetrahydrofolate cyclohydrolase) and F_{hs} (formyltetrahydrofolate synthetase) from *Clostridium perfringens* in a heterologous model of *Escherichia coli*. *Microbiology-Sgm* **2016**, *162*, 145-155 <http://dx.doi.org/10.1099/mic.0.000209>
4. Ansari, M. I. H.; Hassan, S.; Qurashi, A.; Khanday, F. A., Microfluidic-integrated DNA nanobiosensors. *Biosensors & Bioelectronics* **2016**, *85*, 247-260 <http://dx.doi.org/10.1016/j.bios.2016.05.009>



-
-
5. Baliga, C.; Majhi, S.; Mondal, K.; Bhattacharjee, A.; VijayRaghavan, K.; Varadarajan, R., Rational elicitation of cold-sensitive phenotypes. *Proceedings of the National Academy of Sciences of the United States of America* 2016, 113 (18), E2506-E2515 <http://dx.doi.org/10.1073/pnas.1604190113>
 6. Baliga, C.; Varadarajan, R.; Aghera, N., Homodimeric Escherichia coli Toxin CcdB (Controller of Cell Division or Death B Protein) Folds via Parallel Pathways. *Biochemistry* 2016, 55 (43), 6019-6031 <http://dx.doi.org/10.1021/acsbiochem.6b00726>
 7. Bhattacharyya, S.; Varshney, U., Evolution of initiator tRNAs and selection of methionine as the initiating amino acid. *RNA Biology* 2016, 13 (9), 810-819 <http://dx.doi.org/10.1080/15476286.2016.1195943>
 8. Chakrabarty, S.; Das, R.; Karmakar, S.; Dasgupta, C., Understanding the dynamics of glass-forming liquids with random pinning within the random first order transition theory. *Journal of Chemical Physics* 2016, 145 (3), <http://dx.doi.org/10.1063/1.4958632>
 9. Classen, D.; Kiessling, S.; Mangalam, M.; Kaumanns, W.; Singh, M., Fission-fusion species under restricted living conditions: a comparative study of dyadic interactions and physical proximity in captive bonobos and Bornean orangutans. *Current Science* 2016, 110 (5), 839-850
 10. Datta, S.; Bhattacharya, S., Carbon-Nanotube-Mediated Electrochemical Transition in a Redox-Active Supramolecular Hydrogel Derived from Viologen and an L-Alanine-Based Amphiphile. *Chemistry-a European Journal* 2016, 22 (22), 7524-7532 <http://dx.doi.org/10.1002/chem.201600214>
 11. Erinjery, J. J.; Kumara, H. N.; Kavana, T. S.; Singh, M., Are interspecific associations of primates in the Western Ghats a matter of chance? A case study of the lion-tailed macaque. *Journal of Tropical Ecology* 2016, 32, 41-49 <http://dx.doi.org/10.1017/s0266467415000528>
 12. Freericks, J. K.; Cohn, J. R.; van Dongen, P. G. J.; Krishnamurthy, H. R., Infinite single-particle bandwidth of a Mott-Hubbard insulator. *International Journal of Modern Physics B* 2016, 30 (13), <http://dx.doi.org/10.1142/s0217979216420017>
 13. Ji, U. C.; Sinha, K. B., Quantum stochastic calculus associated with quadratic quantum noises. *Journal of Mathematical Physics* 2016, 57 (2), <http://dx.doi.org/10.1063/1.4939919>
 14. Majumder, R.; Pandit, R.; Panfilov, A. V., Scroll-Wave Dynamics in the Presence of Ionic and Conduction Inhomogeneities in an Anatomically Realistic Mathematical Model for the Pig Heart. *JETP Letters* 2016, 104 (11), 796-799 <http://dx.doi.org/10.1134/s0021364016230041>
 15. Mangalam, M.; Desai, N.; Singh, M., Division of labour: a democratic approach towards understanding manual asymmetries in non-human primates. *Current Science* 2016, 110 (9), 1630-1638 <http://dx.doi.org/10.18520/cs/v110/i9/1630-1638>
 16. Mangalam, M.; Desai, N.; Singh, M., Self-organization of laterally asymmetrical movements as a consequence of space-time optimization. *Journal of Theoretical Biology* 2016, 390, 50-60 <http://dx.doi.org/10.1016/j.jtbi.2015.10.038>
 17. Misra, S. K.; Moitra, P.; Kondaiah, P.; Bhattacharya, S., Co-liposomes having anisamide tagged lipid and cholesteryl tryptophan trigger enhanced gene transfection in sigma receptor positive cells. *Colloids and Surfaces B-Biointerfaces* 2016, 142, 130-140 <http://dx.doi.org/10.1016/j.colsurfb.2016.02.044>

-
-
18. Mukherjee, S.; Pal, B.; Choudhury, D.; Sarkar, I.; Drube, W.; Gorgoi, M.; Karis, O.; Takagi, H.; Matsuno, J.; Sarma, D. D., Origin and distribution of charge carriers in LaAlO₃-SrTiO₃ oxide heterostructures in the high carrier density limit. *Physical Review B* 2016, 93 (24), <http://dx.doi.org/10.1103/PhysRevB.93.245124>
 19. Pal, N.; Perlekar, P.; Gupta, A.; Pandit, R., Binary-fluid turbulence: Signatures of multifractal droplet dynamics and dissipation reduction. *Physical Review E* 2016, 93 (6), <http://dx.doi.org/10.1103/PhysRevE.93.063115>
 20. Sarkar, D.; Shukla, A.; Sarma, D. D., Substrate Integrated Nickel-Iron Ultrabattery with Extraordinarily Enhanced Performances. *ACS Energy Letters* 2016, 1 (1), 82-88 <http://dx.doi.org/10.1021/acsenergylett.6b00067>
 21. Shetty, S.; Varshney, U., An evolutionarily conserved element in initiator tRNAs prompts ultimate steps in ribosome maturation. *Proceedings of the National Academy of Sciences of the United States of America* 2016, 113 (41), E6126-E6134 <http://dx.doi.org/10.1073/pnas.1609550113>
 22. Shukla, V.; Brachet, M.; Pandit, R., Sticking transition in a minimal model for the collisions of active particles in quantum fluids. *Physical Review A* 2016, 94 (4), <http://dx.doi.org/10.1103/PhysRevA.94.041602>
 23. Shukla, V.; Pandit, R., Multiscaling in superfluid turbulence: A shell-model study. *Physical Review E* 2016, 94 (4), <http://dx.doi.org/10.1103/PhysRevE.94.043101>
 24. Tripathi, A.; Gupta, K.; Khare, S.; Jain, P. C.; Patel, S.; Kumar, P.; Pulianmackal, A. J.; Aghera, N.; Varadarajan, R., Molecular Determinants of Mutant Phenotypes, Inferred from Saturation Mutagenesis Data. *Molecular Biology and Evolution* 2016, 33 (11), 2960-2975 <http://dx.doi.org/10.1093/molbev/msw182>
 25. Valdiya, K. S., Geological marvels, hallowed shrines and unification of people of India. *Current Science* 2016, 110 (6), 987-995
 26. Velankar, A. D.; Kumara, H. N.; Pal, A.; Mishra, P. S.; Singh, M., Population Recovery of Nicobar Long-Tailed Macaque *Macaca fascicularis umbrosus* following a Tsunami in the Nicobar Islands, India. *PLoS One* 2016, 11 (2), <http://dx.doi.org/10.1371/journal.pone.0148205>

Books and Book Chapters

1. Singh, M.; Kumara, H. N.; Kavana, T. S.; Erinjery, J. J.; Kumar, S., Demography and reproductive output in langurs of the Western Ghats, India. *Primates* 2016, 57 (4), 501-508 <http://dx.doi.org/10.1007/s10329-016-0550-2>
2. Ranjan, R.; Deshpande, S. M.; Narasimha, R., A High-Resolution Compressible DNS Study of Flow Past a Low-Pressure Gas Turbine Blade. 2016; p 291-301 978-981-4635-16-5; 978-981-4635-15-8.
3. Das, S.; Dutta, S.; Chaudhri, A.; Erinjery, J. J.; Singh, M., Extension of the known range of *Dryocalamus nympha* (DAUDIN, 1803), in India. *Herpetozoa* 2016, 28 (3-4), 206-209
4. Chattopadhyay, A.; Sinha, K. B., A New Proof of the Helton-Howe-Carey-Pincus Trace Formula. 2016; p 56-67 978-3-319-31756-4; 978-3-319-31755-7.



AWARDS / DISTINCTIONS

Prof. C.N.R. Rao

- Hon. Doctorate, Assam Kaziranga University, Jorhat
- Hon. Doctorate, Jamia Hamdard University, New Delhi
- Doctor of Science (Honoris Causa) from Yenepoya University, Mangalore
- Gitam Foundation Annual Award
- Bhaskaracharya Award by Poojya Shree Channaveerswamiji Sarangamath, Sindgi, Vijayapur.

Prof. V. Nagaraja

- G. N. Ramachandran Gold Medal for Excellence in Biological S&T for the year 2016 during CSIR Foundation Day on September 26, 2016.

Prof. Roddam Narasimha

- Felicitation by the Indian Mathematics Consortium (TIMC), for great impact on research, teaching and service to the Indian Mathematical community, on its first Conference at BHU organized in collaboration with the American Mathematical Society on December 15, 2016.

Prof. K. S. Valdiya

- "Pramathanath Bose Memorial Medal" of Asiatic Society for his outstanding contribution in the field of Practical & Theoretical Geology.

Prof. K. S. Narayan

- The National Prize for Research on Energy Materials and Devices given by the C. N. R. Rao Education Foundation, supported by the AVRA Laboratories Pvt. Ltd., Hyderabad.

Prof. Hemalatha Balaram

- Dr. Raja Ramanna State Award 2015-16 from the Department of Information Technology, Biotechnology and Science and Technology, Government of Karnataka.

Prof. S. M. Shivaprasad

- Distinguished Lectureship' Award from the Materials Research Society of India, at its AGM held at IIT-Bombay in February 2017.
- Conferred with Honorary Doctorate (D. Sc.) by the Vijayanagara Sri Krishnadevaraya University, Bellary, Karnataka.

Prof. Umesh Waghmare

- Distinguished Alumnus Award 2017, IIT Bombay.

Prof. Chandrabhas Narayana

- MRSI-ICSC Super Conductivity and Materials Science Senior Award 2017

Prof. A. Sundaresan

- Article chosen as Editors' Choice 2016 of Solid State Communications journal, doi:10.1016/j.ssc.2015.01.002

Dr. T. Govindaraju

- DST SwarnaJayanti Fellowship Award 2015-2016
- Indian Peptide Society-Young Scientist Award 2016-2017;
- MRSI Medal 2016-2017, Materials Research Society of India;
- AVRA Young Scientist Award (2015), AVRA Laboratories;
- CRSI Bronze Medal (2016) of Chemical Research Society of India.

Dr. Subi J. George

- Received 'Author Profile' in Angewandte Chemie journal for publishing his 10th article in this journal in 10 years.

Dr. Sebastian C. Peter

- Selected as Emerging Investigator by the Journal of Materials Chemistry A, Royal Society of Chemistry (RSC) in 2017.
- Selected as Emerging Investigator by Materials Research Express, IOP Science in 2017.
- Selected as the Emerging investigator by Institute of Physics in Material science;

Dr. Ranjani Viswanatha

- DST young career award in Nano Science and Technology for the year 2017
- SERB Womens' Excellence Award

Dr. Sarit Agasti

- The Innovative Young Biotechnologist Award (IYBA) from DBT.

Dr. Jayanta Haldar

- CSIR-CDRI Awards 2017 for Excellence in Drug Research in chemical sciences
- BIRAC-SRISTI-Gandhian Young Technological Innovation (GYTI) award-2016
- BIRAC-SRISTI Appreciation Award-2016

Dr. Kanishka Biswas

- Selected as Emerging Investigator by the Journal of Materials Chemistry C, Royal Society of Chemistry (RSC) in 2017.
- Materials Research Society (MRSI) Medal (2017)
- Young Scientist Medal, Indian National Science Academy (INSA), India (2016) for probing and developing new thermoelectrics for energy harvesting;
- Alkyl Amines and Chemicals Ltd. and ICT Young Scientist Award, (2016).
- Selected for the "IUMRS-MRS Singapore Young Researcher Merit Award", which is jointly instituted by the International Union of Materials Research Societies (IUMRS) and the Materials Research Society (MRS) of Singapore.



Dr. C. P. Rajendran

- C.N.R. Rao Oration Award (2016)

Dr. Rajesh Ganapathy

- DST SwarnaJayanti Fellowship Award 2015-2016.
- N S Satyamurthy Award for Young Scientists (2014) of the Indian Physics Association

The Most Valuable Staff Member prize:

Mrs. Sudha J., Sr. Stenographer Gr. I. has been awarded The Most Valuable Staff Member prize for the year 2016.

Best Ornamental/Vegetable Garden to the Centre

JNCASR received the "Best Maintained Garden Award" by the Mysore Horticultural Society.

The Centre bagged consolidated prize for "Best Ornamental/Vegetable Garden" instituted by the Mysore Horticultural Society, Lalbagh, Bangalore.

AWARDS RECEIVED BY THE STUDENTS

1. N. Nagarjun, Bioorganic Chemistry Laboratory, New Chemistry Unit (Research Guide: Dr. T. Govindaraju, <http://www.jncasr.ac.in/tgraju/>) has won the "2016 Eli Lilly and Company Asia Outstanding Thesis Award".
2. Ms. Ananya Mishra from Dr. Subi J. George's research group (NCU) received the "RISING STAR" award in the CEMSupra 2016 conference held at Tokyo, Japan during 05-06 December 2016.
3. Koushik Pal has received the 2017 Ovshinsky Student Travel Award of the American Physical Society.
4. Mr. Krishnendu Jalani (Research Supervisor: Dr. Subi J. George) received the ACS Omega Best Poster Award in 20th CRSI National Symposium in Chemistry 2017.
5. K. Rajasekhar of NCU (Guide: Prof. T. Govindaraju) received Gandhian Young Technological Innovation (GYTI) Award 2017
6. Y. V Suseela of NCU (Guide: Prof. T Govindaraju) received one of the Best Oral Presentations Awards in International Conference on Emerging Trends in Nanoworld (ICETN) on February 27-28, 2017.

AWARDS RECEIVED BY HONORARY FACULTY MEMBERS**Dr. N. Sathyamurthy**

- SASTRA-CNR Rao Award for Chemistry and Material Science 2016, Sastra University, Thanjavur, Tamilnadu
- Sir C V Raman Medal, Indian National Science Academy, New Delhi, 2016

Prof. Umesh Varshney

- Outstanding alumnus of College of Basic Science and Humanities, G. B. Pant University of Agriculture and Technology, Pantnagar, 2016.
- Prof. J. V. Bhat Endowment Oration 2016, Manipal University, Manipal.

Prof. Raghavan Varadarajan

- IISc Alumni award for excellence in research (2017)

Prof. Dipankar Chatterji

- Distinguished Alumni award from Jadavpur University Kolkata, 2017.

FELLOWSHIPS

Mrs. Indumati Rao

- Fellow of the National Academy of Sciences, Allahabad.

Prof. G. U. Kulkarni

- Fellow of International Senior Fellowship of University of Bayreuth 2016
- Fellow of the Asia Pacific Academy of Materials (APAM)

Prof. Chandrabhas Narayana

- Fellow of the Royal Society of Chemistry.
- Sheikh Saqr RAK-CAM Senior Fellowships.

Prof. Srikanth Sastry

- Sheikh Saqr RAK-CAM Senior Fellowships.

Prof. Maneesha S. Inamdar

- Fellow of the Indian Academy of Science, Bangalore

Dr. Kaustuv Sanyal

- Fellow of the National Academy of Sciences India (NASI), Allahabad (year of election 2014)
- Fellow of the Indian Academy of Sciences, Bangalore (year of election 2017).

Dr. Rajesh Ganapathy

- Sheikh Saqr Career Award Fellowships

Dr. Ranjani Viswanatha

- Sheikh Saqr Career Award Fellowships

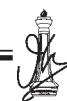
Dr. Sarit Agasti

- The Wellcome Trust/DBT India Alliance Intermediate Fellowship;

FELLOWSHIP RECEIVED BY HONORARY FACULTY MEMBER

Prof. Rahul Pandit

- Fellowship of TWAS (Ceremony in Kigali Rwanda in November 2016).



MEMBERSHIPS / APPOINTMENTS

Prof. C.N.R. Rao

- Distinguished Adjunct Professor, Temple University, Philadelphia

Prof. V. Nagaraja

- Convenor, Sectional Committee-Microbiology & Immunology, INSA

Prof. Amitabh Joshi

- Elected as Convenor, Sectional Committee on Animal Sciences, Indian National Science Academy, New Delhi, for 2017.

Prof. G. U. Kulkarni

- Adjunct Member of the faculty for Science and Technology, Gulbarga University, Gulbarga

Prof. Tapas Kumar Kundu

- Vice President of Society of Biological Chemists (India).
- Visiting Professor in the Department of Biological Science, Indian Institute of Science Education and Research, Kolkata, 2015.
- Lifetime Distinguished Professor, conferred by University of Mysore, Mysore, Karnataka. (2016 onwards)

Prof. Shobhana Narasimhan

- Nominated to the Board of Governors of IIT Gandhinagar, NIT, Rourkela, Central University of Madhya Pradesh

Prof. Maneesha S. Inamdar

- Member, JAX Regional Council of the Jackson Laboratories, Bar Harbor, Maine, USA.

Prof. S Ganesh Subramanian

- Invited visiting professor IMFT (Institut de Mécanique des Fluides de Toulouse), Toulouse, France.

Dr. T. Govindaraju

- Member of Board of Scientific Advisors of Bioorganics & Applied Materials Private Limited.
- Secretary, Chemical Research Society of India (CRSI)

Dr. Sebastian C. Peter

- Elected as member of the Royal Society of Chemistry.
- Member of Indian National Young Academy of Science.
- Executive Committee member in the Catalysis Research of India, Bangalore Chapter, India.

-
-
- Doctoral Advisory Committee (DAC) member of Poornaprajna Institute of Scientific Research (PPISR), Bengaluru, India.
 - Expert member of the Selection Committee of Technology Mission Division of Department of Science and Technology, India.

Dr. Kanishka Biswas

- INYAS membership (2017-2021)

Dr. James P.C. Chelliah

- Life member of Indian Academy of Neuroscience.

Dr. C. P. Rajendran

- Inducted as GB Member of Karnataka State Natural Disaster Monitoring Centre.

Dr. Diwakar S. Venkatesan

- Visiting Scientist, French space agency, CNES, to carry out micro-gravity experiments in the parabolic flight campaign.

Dr. Sarit Agasti

- Selected as member of early career researcher Board of @ MaterHoriz, RSC.

Dr. Jayanta Haldar

- Editorial advisory board member of the journal “Biomacromolecules” of American Chemical Society-2017.
- Editorial advisory board member of the journal “ACS Infectious Diseases” of American Chemical Society-2017.

EDITORIAL BOARDS

Prof. V. Nagaraja

- Editorial Board: Nucleic Acids Research

Prof. Amitabh Joshi

- Editor of Publications, Indian Academy of Sciences, Bengaluru



FINANCIAL STATEMENT

Name : JAWAHARLAL NEHRU CENTRE FOR
ADVANCED SCIENTIFIC RESEARCH

Address : Jakkur Post, Bangalore - 560 064

Year Ended : 31st March 2017

Assessment Year : 2017-18



AUDITOR'S REPORT

**TO THE MEMBERS OF THE GOVERNING BODY OF JAWAHARLAL NEHRU CENTRE FOR ADVANCED
SCIENTIFIC RESEARCH, BANGALORE**

Report on the Financial Statements

We have audited the financial statements of "Jawaharlal Nehru Centre For Advanced Scientific Research" Jakkur, Bangalore 560 064, which comprise the Balance Sheet as at 31st March 2017, the Statement of Income & Expenditure Account, Receipts and Payments for the year then ended and a summary of significant accounting policies and other explanatory information.

Management's Responsibility for the Financial Statements

Management is responsible for the preparation of the financial statements. This responsibility includes the design, implementation and maintenance of internal control relevant to the preparation of the financial statements that are free from material misstatement, whether due to fraud or error.

Auditor's Responsibility

Our responsibility is to express an opinion on these financial statements based on our audit. We conducted our audit in accordance with the Standards on Auditing issued by the Institute of Chartered Accountants of India. Those Standards require that we comply with ethical requirements and plan and perform the audit to obtain reasonable assurance about whether the financial statements are free from material misstatement.

An audit involves performing procedures to obtain audit evidence about the amounts and disclosures in the financial statements. The procedures selected depend on the auditor's judgment, including the assessment of the risks of material misstatement of the financial statements, whether due to fraud or error. In making those risk assessments, the auditor considers internal control relevant to the preparation and fair presentation of the financial statements in order to design audit procedures that are appropriate in the circumstances. An audit also includes evaluating the appropriateness of the accounting policies used and the reasonableness of the accounting estimates made by management, as well as evaluating the overall presentation of the financial statements.

We believe that the audit evidence we have obtained is sufficient and appropriate to provide a basis for our audit opinion on the financial statement.



Opinion

In our opinion and to the best of our information and according to the explanations given to us, the said accounts give the information required & give a true and fair view in conformity with the accounting principles in India.

- 1) In the case of the Balance Sheet, of the state of affairs of Jawaharlal Nehru Centre for Advanced Scientific Research, as at 31st March 2017.
- 2) In the case of Income & Expenditure Account, of the Excess of Income over expenditure for the year ended on that date.

We further report that:

- a) The Balance Sheet & Income & Expenditure Account dealt with by this report, are in agreement with the books of Accounts.
- b) In our opinion, proper books of accounts as required have been kept by the Centre, so far as appears from our examination of those books.
- c) 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 conformity with the Accounting Standard 15 (Accounting for retirement benefits in the financial statements of Employees) issued by the Institute of Chartered Accountants of India.
 - ii) All capital expenditure incurred during the year for purchase of Fixed Assets is charged to Income and Expenditure account, under the head "Fixed assets acquired during the year (net)" and the corresponding credit is added to Capital Fund account. This is not in conformity with the Accounting Standard – 10 issued by the Institute of Chartered Accountants of India. It has been explained that this format has been consistently followed by the Centre.
 - iii) The Institute has to regularize the contributions / grants received during the year from foreign funding agencies, as the registration granted to the institution under the provisions of Foreign Contribution Regulation Act, 2010 has been withdrawn w.e.f 19th June, 2015. The Foreign contributions received thereafter require approval from the authorities concerned.

Place: Bangalore
Date : 18.08.2017



For B R V GOUD & CO.,
Chartered Accountants
F R N. 000992S

(A B SHIVA SUBRAMANYAM)
PARTNER
M. No. 201108

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
BALANCE SHEET AS AT 31ST MARCH 2017**

Amount in Rs.

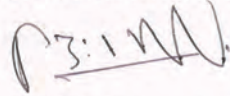
Description	Schedule No.	Current year	Previous year
		2016-17	2015-16
LIABILITIES			
Corpus/capital fund	1	1,61,22,89,974	1,56,74,11,558
Reserves & surpluses	2	7,51,02,333	18,72,373
Earmarked and endowment funds	3	30,97,14,007	27,59,27,184
Secured loans and borrowings	4	0	0
Unsecured loans and borrowings	5	0	0
Deferred credit liabilities	6	0	0
Current liabilities and provisions	7	9,48,29,252	2,04,27,968
Other funds-cluster studies		0	39,541
Scheme balances		87,23,67,255	54,57,69,289
Total		2,96,43,02,820	2,41,14,47,913
ASSETS			
Fixed assets (Gross)	8	1,61,22,89,974	1,56,74,11,558
Investments-Endowment funds	9	28,63,45,283	25,35,59,102
Investment - Others	10	7,25,00,000	0
Current Assets, loans, advances etc.	11	99,31,67,564	59,04,77,253
Total		2,96,43,02,820	2,41,14,47,913
Significant accounting policies	24		
Contingent liabilities & notes on accounts	25		

Schedules 1 to 25 are integral part of accounts

Vide our report of even date,

**For Jawaharlal Nehru Centre for
Advanced Scientific Research**

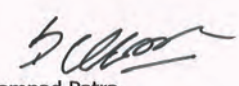
For B.R.V. Goud & Co.
Chartered Accountants, FRN : 000992S

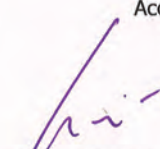


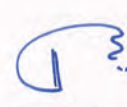
[A.B. Shiva Subramanyam]
Partner

Membership No. 201108
Place : Bangalore, Date : 18/08/2017.




Sampad Patra
Accounts Officer


Prof. V. Nagaraja
President


A. N. Jayachandra
Sr. Administrative Officer



**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
INCOME AND EXPENDITURE ACCOUNT FOR THE YEAR ENDED 31ST MARCH 2017**

Amount in Rs.

Description	Schedule No.	Current year 2016-17	Previous year 2015-16
Income			
Income from services	12	0	0
Grants/subsidies received	13	73,98,00,000	60,00,00,000
		73,98,00,000	60,00,00,000
Less: Fixed assets acquired during the year (net)		14,51,97,219	5,84,94,339
		59,46,02,781	54,15,05,661
Income from fees/subscriptions etc	14	32,81,876	22,88,005
Income from investments	15	0	0
Royalty income, publication, licence fee etc	16	2,96,760	1,10,949
Interest earned	17	96,94,181	26,24,252
Other income	18	2,22,76,901	2,78,38,101
Increase/decrease in stocks	19	0	0
Total		63,01,52,499	57,43,66,968
Expenditure			
Establishment expenses	20	32,00,05,896	30,86,52,566
Other administrative expenses	21	23,54,99,813	21,36,58,488
Expenditure on grants, subsidies etc	22	0	0
Interest & bank charges	23	16,592	35,255
Total		55,55,22,301	52,23,46,310
Excess of income over expenditure		7,46,30,198	5,20,20,658
- Prior period expenses		14,00,237	1,34,249
Balance brought forward		18,72,373	-5,00,14,036
Balance carried to balance sheet		7,51,02,333	18,72,373
Significant accounting policies	24		
Contingent liabilities & notes on accounts	25		

Schedules 1 to 25 are integral part of Accounts

Vide our report of even date,

**For Jawaharlal Nehru Centre for
Advanced Scientific Research**

For B.R.V. Goud & Co.
Chartered Accountants, FRN : 000992S

[A.B. Shiva Subramanyam]
Partner

Membership No. 201108

Place : Bangalore, Date : 18/08/2017.



Sampad Patra
Accounts Officer

Prof. M. Nagaraja
President

A. N. Jayachandra
Sr. Administrative Officer

Note : The amount of Rs.7,46,30,198/- indicated Income and Expenditure Account as Excess of income over expenditure includes Rs.3,75,00,000/- towards infrastructural support for which specific grants have been released during the end of the financial year. Further, the Centre holds a commitment of Rs.9,07,22,826/- as of 31st March 2017 (Rs.8,22,83,899/- towards capital assets and Rs.84,38,927/- towards consumables/pendables) which has not been included as expenditure.

**JAWAHARLAL CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
RECEIPTS AND PAYMENT ACCOUNT FOR THE YEAR ENDED 31ST MARCH 2017**

	2016-17	2015-16	2016-17	2015-16
OPENING BALANCES & RECEIPTS			PAYMENTS & CLOSING BALANCES	
I. Opening Balances:			I. Expenses:	
- Cash in hand & imprest at Centre	1,60,650	3,67,733	- Establishment Expenses	32,89,85,741
Bank balances:			- Administrative Expenses	20,40,49,076
<i>In savings bank Accounts:</i>			- Expenditure out of Endowments	37,86,069
- Canara bank	2,83,86,549	2,37,14,948	Sub Total :	51,52,63,890
- Union Bank of India	1,89,537	1,82,177		
- SBI	4,95,435	2,20,082	II. Expenditure on Fixed assets and Capital Work-in-progress:	
<i>In Deposit accounts:</i>			- Purchase of fixed assets	13,24,39,902
- At Canara Bank	5,69,67,000	5,69,67,000		
- At SBI	7,72,66,669	6,15,00,000	III. Refund of surplus money/loans	0
- At HDFC Trust	10,67,05,500	8,67,05,500	IV. Finance charges(Bank charges)	0
Sub Total :	27,01,71,440	22,96,57,440		36,312
II. Grants Received:			V. Other payments:	
- From DST-Grant in aid	73,98,00,000	60,00,00,000	- Earnest money deposit returned	0
- On behalf of endowments/corpus	62,40,049	27,79,168	- Staff advances (Festival adv. etc.)	36,10,567
	74,60,40,049	60,27,79,168	- Refund to projects	0
III. Income on Investments:			- Other advances	86,72,889
<i>Interest on FD's:</i>			- Security deposit returned	7,45,265
- From earmarked/endowment funds	1,99,59,012	36,34,816	- TDS payments	2,71,06,185
- From own funds	72,88,266	2,15,13,250	- Professional tax	6,73,400
Sub Total :	2,72,47,278	2,51,48,066	- Provident fund	2,19,45,946
			- Advances to faculty	29,78,116
IV. Interest received on SB accounts:			- Payment to sundry creditors	1,48,72,616
- From grant in aid	24,05,915	26,24,252	Sub Total :	8,06,04,984
- From own funds	3,01,137	6,48,677		
Sub Total :	27,07,052	32,72,929	VI. Closing Balances:	
			- Cash in hand & imprest at centre	51,435
V. Other Income:			- Bank balances:	
- Collections from visitors, guest room etc	35,56,586	22,70,417	<i>In savings bank accounts at:</i>	
- From fee, subscription etc	19,56,777	6,64,075	- Canara Bank	6,21,29,290
- CSIR fellowships,UGC, DBT, SRFP	1,67,93,010	1,96,91,074	- Union Bank of India	0
- Overhead recoveries	1,00,13,500	0	- State Bank Of India	28,33,039
- From others	7,56,23,083	30,18,093	- HDFC BANK	37,018
Sub total :	10,81,42,956	2,58,43,659	Sub Total :	6,50,50,783
Balance carried forward	1,15,43,08,775	88,67,01,261	Balance carried forward	81,49,16,555
				65,55,37,299



**JAWAHARLAL CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
RECEIPTS AND PAYMENT ACCOUNT FOR THE YEAR ENDED 31ST MARCH 2017 (Contd...)**

	PAYMENTS & CLOSING BALANCES		Amount in Rs.	
OPENING BALANCES & RECEIPTS	2016-17	2015-16	2016-17	2015-16
Balance Brought Forward	1,15,43,08,775	88,67,01,261	81,49,16,555	65,55,37,299
VI. Other receipts:				
Income tax refunds	0	13,52,978	5,34,67,000	5,69,67,000
From Sundry Creditors	0	0	7,72,66,669	7,72,66,669
Staff advances recovered	2,810	3,882	8,77,05,500	10,67,05,500
Settlement of advance to faculty	2,12,634	2,91,439	1,75,00,000	0
Earnest money received	0	0	3,80,00,000	0
Project funding received	0	0	7,25,00,000	0
GSLI receipt	1,24,453	0	34,64,39,169	24,09,39,169
Support to meetings	67,07,052	81,26,908		
Sub Total :	70,46,949	97,75,207		
TOTAL	1,16,13,55,724	89,64,76,468	1,16,13,55,724	89,64,76,468

Vide our report of even date,

For B.R.V. Goud & Co.
Chartered Accountants, FRN : 0009925



(Signature)

[A.B. Shiva Subramanyam]
Partner

Membership No. 201108
Place : Bangalore, Date : 18/08/2017.

For Jawaharlal Nehru Centre for Advanced Scientific Research

(Signature)

Prof. V. Nagaraja
President

(Signature)

A. N. Jayachandra
Sr. Administrative Officer

(Signature)

Sampad Patra
Accounts Officer

**JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
CPF & NPS FUND STATEMENT OF AFFAIRS FOR THE YEAR ENDED 31ST MARCH 2017**

Particulars	Amount in Rs.	Amount in Rs.	Particulars	Amount in Rs.	Amount in Rs.
Contributory provident fund			Investment of funds:		
Subscription:			Government of India 8 % Bonds (SHCIL)		4,25,00,000
Opening balance	7,77,61,106		Fixed Deposits at PNB housing finance		3,75,00,000
Add : Subscriptions received during the year	81,29,222		Fixed Deposits at Canara bank		3,03,18,897
Advances repayments	22,89,285		Fixed Deposit at HDFC		3,05,00,000
Interest on subscriptions	64,83,915				14,08,18,897
Sub total	9,46,63,528				
Less : Advances / part finals granted	29,38,295		Cash at Bank:		
Less : Final settlement/adjustment	7,40,934		Canara Bank, SB A/C No. 0683101017513	41,776	41,776
Sub total	36,79,229				
Closing balance		9,09,84,299	TDS receivable:		
			Gol Bonds (2013-14) receivable	1,48,000	
Contribution:			Gol Bonds (2014-15) receivable	1,48,000	
Opening balance	5,12,59,050		Gol Bonds (2015-16) receivable	1,49,400	
Add : Contribution during the year	30,38,368		Gol Bonds (2016-17) receivable	63,245	5,08,645
Interest on total contributions	40,92,377				
Sub total	5,83,89,795		Accrued interest:		
Less : Final settlement/adjustment	4,37,928		Accrued interest on deposits in Gol 8 % Bonds (SHCIL)	4,21,597	
Closing balance		5,79,51,867	Accrued interest on Deposits in PNB housing finance	11,32,925	
			Accrued interest on Deposits in Canara bank	23,69,779	
New pension scheme			Accrued interest on Deposits in HDFC	40,96,537	80,20,838
Subscription:					
Opening balance	80,551				
Less : Adjustment during the year	80,551				
Closing balance		0			
Contribution:					
Opening balance	74,482				
Less : Adjustment during the year	74,482				
Closing balance		0			
Payable to Centre		2,14,305			
Payable to canteen		1,390			
Payable to endowment		1,32,000			
Balance surplus		1,06,296			
Total		14,93,90,157	Total		14,93,90,157

For Jawaharlal Nehru Centre for Advanced Scientific Research

For B.R.V. Goud & Co.
Chartered Accountants, FRN : 0009925



[Signature]
[A.B. Shiva Subramanyam]
Partner

Membership No. 201108
Place : Bangalore, Date : 18/08/2017.

[Signature]

A. N. Jayachandra
Sr. Administrative Officer

[Signature]
Sampad Patra
Accounts Officer



JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

Description	2016-17	2015-16
	Amount in Rs.	Amount in Rs.
SCHEDULE 1- Capital fund:		
Balance as at the beginning of the year	1,56,74,11,558	1,59,98,91,861
Add : Fixed assets acquired during the year (net)	14,51,97,219	5,84,94,339
	1,71,26,08,778	1,65,83,86,200
Less : Depreciation for the current year	10,03,18,804	9,09,74,642
TOTAL	1,61,22,89,974	1,56,74,11,558
SCHEDULE 2- Reserves and surpluses:		
General reserve:		
Surplus/deficit in income and expenditure account	7,51,02,333	18,72,373
SCHEDULE 3- Earmarked / endowment funds:		
A : Infrastructure corpus fund		
Opening balance	19,93,71,034	17,22,35,150
Additions during the year	1,23,83,639	1,03,88,009
Funds-Income from investments made	1,60,94,996	1,60,99,198
Interest from savings bank - Endowment account	3,01,137	6,48,677
Sub total	22,81,50,806	19,93,71,034
Less : Funds-utilisation/expenditure incurred	471	0
Total : Infrastructure corpus fund	22,81,50,335	19,93,71,034
B : Other funds		
Opening balance of the Funds	7,65,56,150	7,32,32,418
Add : Additions :		
Funds/donations/grants/royalties	46,00,000	23,94,734
Funds-Income from investments made	43,55,327	44,45,774
	8,55,11,478	8,00,72,926
Less : Funds-utilisation/expenditure incurred	39,47,806	35,16,776
Total : Other funds	8,15,63,672	7,65,56,150
Grand Total - Infrastructure corpus and other funds	30,97,14,007	27,59,27,184
SCHEDULE 4- Secured loans and borrowings:	0	0
SCHEDULE 5- Unsecured loans and borrowings:	0	0
SCHEDULE 6- Deferred credit liabilities:	0	0
SCHEDULE 7- Current liabilities and provisions		
Sundry creditors EMD/security deposits	29,15,829	57,91,246
Grant - Payable to endowment account	65,12,420	0
Grant - Payable to scheme account	1,48,42,872	0
Sundry creditors for others	6,76,70,872	1,44,23,504
Unpaid stipend/salary	28,87,259	2,13,218
TOTAL	9,48,29,252	2,04,27,968



Sampad Patra
Sampad Patra
Accounts Officer

JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

Description	2016-17	2015-16
	Amount in Rs.	Amount in Rs.
SCHEDULE 8- Fixed assets		
Land - Free hold	1,77,15,351	1,77,15,351
Buildings :		
General	8,78,33,491	8,78,33,491
Hostel building	1,56,60,055	1,56,60,055
New lab building - AMRL	2,59,30,339	2,59,30,339
Animal house	67,88,701	67,88,701
Staff housing	43,19,353	43,19,353
ETU building	30,91,348	30,91,348
Engineering & mechanical unit block	74,26,272	74,26,272
Other buildings like extn. to hostel, College etc.,	1,18,83,626	1,18,83,626
Nano science block	70,42,909	70,42,909
Extention to pauling building - Biology block	47,66,109	47,66,109
Dining hall & kitchen block	1,24,04,330	1,24,04,330
Radio active lab	2,03,233	2,03,233
International centre for material science	5,01,48,316	5,01,48,316
Lecture hall & academic block	96,36,712	96,36,712
Hostel phase II	1,95,52,377	1,95,52,377
STP building	2,91,699	2,91,699
Hostel phase III	2,75,01,103	2,75,01,103
International house	2,31,42,418	2,31,42,418
CNR Rao hall of science	1,03,33,669	1,03,33,669
Extention to HIV lab	10,16,085	10,16,085
Security office block	7,42,632	7,42,632
Animal house - Additional block	82,92,632	82,92,632
Residential quarters (Sr. AO)	36,59,034	36,59,034
Child care centre	7,28,827	7,28,827
Hostel phase -IV	2,59,34,842	2,59,34,842
Extention to biology lab	1,94,24,005	1,94,24,005
SCADA - DG room	2,40,660	2,40,660
President's residence	77,88,054	77,88,054
Visiting students hostel	3,39,82,070	3,39,82,070
Health centre	32,43,422	32,43,422
Nano institute shivanapura	37,09,242	37,09,242
EOBU lab block	2,09,11,646	2,09,11,646
Post-Doc housing-Srirampuram	1,54,86,086	1,54,86,086
Material science lab block	5,54,31,961	5,54,31,961
New auditorium	2,20,24,759	2,20,24,759
New auditorium Phase II	1,03,500	0
Radio active lab-Type II	28,32,158	28,32,158
Sub Total	55,35,07,676	55,34,04,176
Infrastructure facilities:		
Roads, streetlights, drianages, partitions etc	9,88,28,587	9,60,86,502
Tubewells and water supply	2,48,912	2,48,912
Sub Total	9,90,77,499	9,63,35,414
Plant/machinery/equipment:		
Scientific equipments/plant/machinery	93,01,65,128	85,69,65,733
ICMS - Laboratory equipments & facilities	28,28,83,804	25,55,39,691
Equipments - Chemistry & physics of materials	7,40,41,456	7,40,41,456
Sub Total	1,28,70,90,388	1,18,65,46,880
Others :		
Vehicles	46,54,458	38,12,510
Furniture and fixtures	8,69,23,596	7,60,00,106
Office equipment	2,11,13,679	2,00,56,041
Computer/peripherals	7,93,75,185	7,47,66,175
Electrical installations	11,27,38,560	11,27,38,560
Library books	2,89,62,165	2,86,10,377
Library journals	18,76,47,997	17,08,36,276
Sub Total	52,14,15,641	48,68,20,046
Intangible Assets: Softwares		
	2,36,77,272	1,64,64,741
TOTAL	2,50,24,83,827	2,35,72,86,607
Less - Depreciation up to the end of previous year	78,98,75,049	69,89,00,407
Depreciation for the current year	10,03,18,804	9,09,74,642
Written down value of the assets as at the year end	1,61,22,89,974	1,56,74,11,558



Sampad Patra
Sampad Patra
Accounts Officer



JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

Description	2016-17 Amount in Rs.	2015-16 Amount in Rs.
SCHEDULE 9- Investments - Earmarked/endowment funds		
Long term deposits		
Fixed deposits with HDFC (Trust deposits)	8,77,05,500	10,67,05,500
Fixed deposits with Canara Bank	5,34,67,000	5,69,67,000
Fixed deposit with SBI	7,72,66,669	7,72,66,669
Fixed deposit with PNB	1,75,00,000	0
Fixed deposit with Stock Holding Corporation of India	3,80,00,000	0
Interest accrued on fixed deposits with banks / HDFC	1,24,06,114	1,26,19,933
TOTAL	28,63,45,283	25,35,59,102
SCHEDULE 10- Investments - Others		
Short Term Deposits		
	7,25,00,000	0
TOTAL	7,25,00,000	0
Schedule 11- Current Assets, loans, advances etc.,		
Cash & bank balances (Schemes)		
Cash in hand - Schemes account	0	63,211
Cash at bank - Schemes - Canara Bank	47,53,917	92,28,655
Fixed deposit with Canara Bank (Schemes)	28,80,75,432	47,42,00,000
Fixed deposit with SBI (Schemes)	19,59,991	18,71,395
Fixed deposit with PNB	29,25,00,000	0
Fixed deposit with Stock Holding Corporation of India	20,00,00,000	0
Sub total	78,72,89,340	48,53,63,261
Loans and advances (Schemes)		
Interest accrued on fixed deposits with banks	2,34,18,513	1,37,82,162
TDS receivable	8,61,641	4,58,463
Receivables from Centre	1,48,42,872	0
Receivables from various funding agencies	4,59,54,889	4,61,65,403
Sub total	8,50,77,914	6,04,06,028
Total of Schemes	87,23,67,255	54,57,69,289
Cash & bank balances		
Cash in hand grant account	12,425	1,40,320
Cash in hand endowment account	0	20,330
Cash at bank - Canara Bank - Grants	5,59,91,316	2,20,11,845
Cash at bank - Canara Bank - Endowments	61,37,974	63,74,805
Cash at bank - Union Bank	0	1,89,537
Cash at bank - SBI	28,33,039	4,95,435
Cash at bank - HDFC	37,018	0
Sub total	6,50,11,773	2,92,32,271
Loans and advances		
Advances to staff	17,16,521	9,78,882
Deposits	6,87,259	0
Other advances & receivables	1,52,82,840	14,29,777
Receivables- CSIR, UGC, DBT, DST	1,83,09,720	0
Endowment Account - Receivable from Scheme Account	1,00,00,000	1,00,00,000
SRFP - Receivables	0	6,38,405
Endowment Account - Advance to Supplier	25,600	0
Endowment Account - Receivable from CPF Account	1,32,000	0
Endowment Account - Receivable from Grant Account	65,12,420	0
TDS receivable - Grant Account	25,22,436	23,95,770
TDS receivable - Endowment Account	5,60,731	0
Imprest balance	39,010	32,859
Sub total	5,57,88,536	1,54,75,693
Total of other than Schemes	12,08,00,309	4,47,07,964
TOTAL	99,31,67,564	59,04,77,253



Sampad Patra
Sampad Patra
Accounts Officer

JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

Description	2016-17	2015-16
	Amount in Rs.	Amount in Rs.
SCHEDULE 12- Income from sales / services	0	0
SCHEDULE 13- Grants/subsidies :		
Grants - DST	73,98,00,000	60,00,00,000
Grants - From Government agencies/travel grants etc.	0	0
Grants - From other Institutes	0	0
Grants - Other international agencies	0	0
TOTAL	73,98,00,000	60,00,00,000
SCHEDULE 14- Income from fee/subscriptions etc :		
Income from fee, subscriptions, medical contribution etc.,	32,81,876	22,88,005
TOTAL	32,81,876	22,88,005
SCHEDULE 15- Income from investments;	0	0
SCHEDULE 16- Royalty income, publication, licence fee etc :		
From royalty	0	0
Licence fee	2,96,760	1,10,949
TOTAL	2,96,760	1,10,949
SCHEDULE 17- Interest earned:		
From term deposits	72,88,266	0
From SB accounts with nationalised banks	24,05,915	26,24,252
TOTAL	96,94,181	26,24,252
SCHEDULE 18- Other income:		
From Visitors house, Guest rooms, Students residence etc,	70,85,058	45,52,850
CSIR Fellowships, ICMS, SRFP reimbursement etc.,	98,58,982	1,58,52,986
Prior Year Receipts	33,36,937	40,38,088
Other funds-cluster studies	39,541	0
Support from JNC Corpus	0	0
Miscellaneous income	6,07,860	1,16,675
From others (tender fee & other fee collected)	0	32,77,502
Other Receipts (Uncashed Cheques reversed)	13,48,523	0
TOTAL	2,22,76,901	2,78,38,101
SCHEDULE 19- Increase / decrease in stock:	0	0



Sampad Patra
Sampad Patra
Accounts Officer



JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

Description	2016-17	2015-16
	Amount in Rs.	Amount in Rs.
SCHEDULE 20- Establishment expenses:		
Salaries & scholarship to students	23,43,09,167	22,63,32,391
Wages	5,61,05,877	6,19,07,509
Allowances (Medical reimbursements etc.,)	76,55,179	63,84,799
Bonus	7,87,512	3,09,708
Contribution to CPF	82,26,370	47,88,803
Contribution to new pension scheme	63,84,216	48,40,482
Contribution to group gratuity scheme	41,21,110	23,19,171
Leave encashment benefits	8,58,443	5,96,231
LTC	15,58,022	11,73,472
TOTAL	32,00,05,896	30,86,52,566
SCHEDULE 21- Other Administrative expenses		
Electricity & power	5,80,68,150	4,97,04,585
Water charges	60,37,638	59,60,871
Insurance	7,95,329	8,33,263
Repairs & maintenance	5,82,36,443	3,71,85,964
Rents, rates & taxes	12,69,232	6,63,283
Vehicles running & maintenance	65,07,546	65,78,250
Postage, telephone & communication	36,31,828	74,40,320
Printing, stationery, books	51,38,661	76,69,264
Travelling and conveyance	45,72,817	61,68,955
Expnses on seminars/workshops/discussion meetings	55,48,880	58,83,684
Membership & subscriptions	14,18,794	1,54,330
Professional charges	74,45,976	67,93,304
Laboratory consumables	4,17,54,638	4,88,48,872
Frieght inwards	0	4,62,250
Advertisement & publicity	14,13,375	27,25,721
Student residence, guest house, I house, etc	43,90,305	29,53,420
Statutory audit fee	70,000	70,000
POBE & POCE prgramme	9,51,859	5,30,064
Summer research fellowship & student programme	22,96,021	44,81,154
ICMS - Workshops, Schools etc.,	15,84,567	14,13,435
ICMS - Visitor programmes (National & international)	1,50,583	1,99,492
ICMS - Recurring expenses	1,18,58,171	81,69,029
ICMS - Scientists & supporting staff	1,23,59,000	86,88,778
Commonwealth meeting	0	80,200
TOTAL	23,54,99,813	21,36,58,488
SCHEDULE 22- Expenditure on grants, subsidies etc:	0	0
SCHEDULE 23- Interest and bank charges:	16,592	35,255



Sampad Patra
Sampad Patra
Accounts Officer

JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017
SCHEDULE NO. 24 : Significant accounting policies

OVERVIEW :

Jawaharlal Nehru Centre For Advanced Scientific Research is registered as a society under the Karnataka Societies Registration Act, 1960 and also registered under Section 35(1)(ii) of the Income Tax Act, 1961. It is an autonomous institution recognised and substantially funded by the Department of Science and Technology, Government of India.

The main objects of the Centre are establish & conduct world-class research in science & engineering, foster interdisciplinary & collaborative research, establish state-of-the-art laboratories, computational & infrastructural facilities for conduct of scientific research, generate human capital through high-quality Ph.Ds in science & engineering, increase awareness about science & research among school & college students through science outreach & extension activities and take research from laboratory to society.

SIGNIFICANT ACCOUNTING POLICIES :

1. **Accounting Conventions :** The financial statements are drawn up in accordance with historical accounting conventions and on the going concern concept. Accrual method of accounting is followed to record Income and Expenditure.

The guidelines as per the Uniform Format of Accounts for Central Autonomous Institutions, as applicable and to the extent practicable, are followed in the presentation of the financial statements of the Centre.

2. **Investments :** Investments are stated at cost and Interest from Investments are accounted on accrual basis.

3. **Fixed Assets :** Fixed assets are stated at written down value and are accounted at cost of acquisition, inclusive of inward freight, duties, taxes and incidental expenses related to acquisition.

4. **Depreciation :** Depreciation on Fixed assets has been provided on Written Down Value Method.

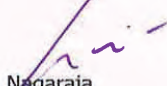
5. **Government Grants / Other Grants :** The Grants received are recognized in the accounts on realisation basis. Grants received and utilized for procurement of Fixed Assets have been reduced from the total grants received in the Income and Expenditure Account and the same have been included under the Capital Fund Account.

6. **Retirement Benefits :** The Centre has obtained group gratuity policy from the Life Insurance Corporation of India in respect of gratuity and accordingly, premium has been paid annually. No provision has been made in respect of the Leave Encashment as required by AS 15. However, the same is accounted on cash basis as and when the liability is discharged.


7. **Allocation / Transfer to Schemes :** The Centre has a policy to allocate / transfer interest earned on investments relating to certain schemes.

8. **Foreign Currency and its Fluctuations :** The Foreign currency transactions are translated at the rates prevailing on the date of transaction. Fluctuations in foreign currency on account of procurement of fixed assets are capitalized with the respective fixed assets.


Sampad Patra
Accounts Officer

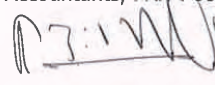

Prof. V. Nagaraja
President

Place : Bangalore
Date : 18/08/2017.


A. N. Jayachandra
Sr. Administrative Officer



For B.R.V. Goud & Co.
Chartered Accountants, FRN : 000992S


[A.B. Shiva Subramanyam]
Partner
Membership No. 201108



JAWAHARLAL NEHRU CENTRE FOR ADVANCED SCIENTIFIC RESEARCH
Schedules forming part of the accounts for the year ended 31st march 2017

SCHEDULE 25 : Contingent liabilities and notes on accounts

A. Contingent liabilities :	2016-17	2015-16
	Amount in Rs.	Amount in Rs.
1. Claims against the entity not acknowledged as debts	NIL	NIL
2. Letter of credit outstanding	NIL	NIL

B. Notes on accounts :

1. The amount of Rs.7,46,30,198/- indicated Income and Expenditure Account as Excess of income over expenditure includes Rs.3,75,00,000/- towards infrastructural support for which specific grants have been released during the end of the financial year. Further, the Centre holds a commitment of Rs.9,07,22,826/- as of 31st March 2017 (Rs.8,22,83,899/- towards capital assets and Rs. 84,38,927/- towards consumables/expendables) which has not been included as expenditure.


2. Figures are rounded off to the nearest rupee and figures of previous year have been regrouped and reclassified to conform to that of the current year.

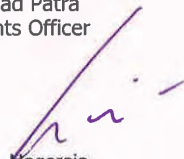
3. Depreciation on fixed assets amounting to Rs.10,03,18,804/- calculated for the year is debited to the Capital Fund.

4. Income Tax : The Centre is registered under Section 35(1)(ii) of the Income Tax Act, 1961 and is eligible for exemption from tax and hence no provision has been made towards Income Tax.

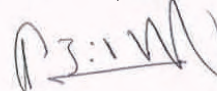
5. Schedules 1 to 25 are annexed to and form an integral part of the Balance Sheet as at 31st March 2017 and the Income and Expenditure Account for the year ended on that date.


Sampad Patra
Accounts Officer


A. N. Jayachandra
Sr. Administrative Officer


Prof. V. Nagaraja
President

For B.R.V. Goud & Co.
Chartered Accountants, FRN : 0009925


[A.B. Shiva Subramanyam]
Partner

Membership No. 201108
Place : Bangalore, Date : 18/08/2017.



