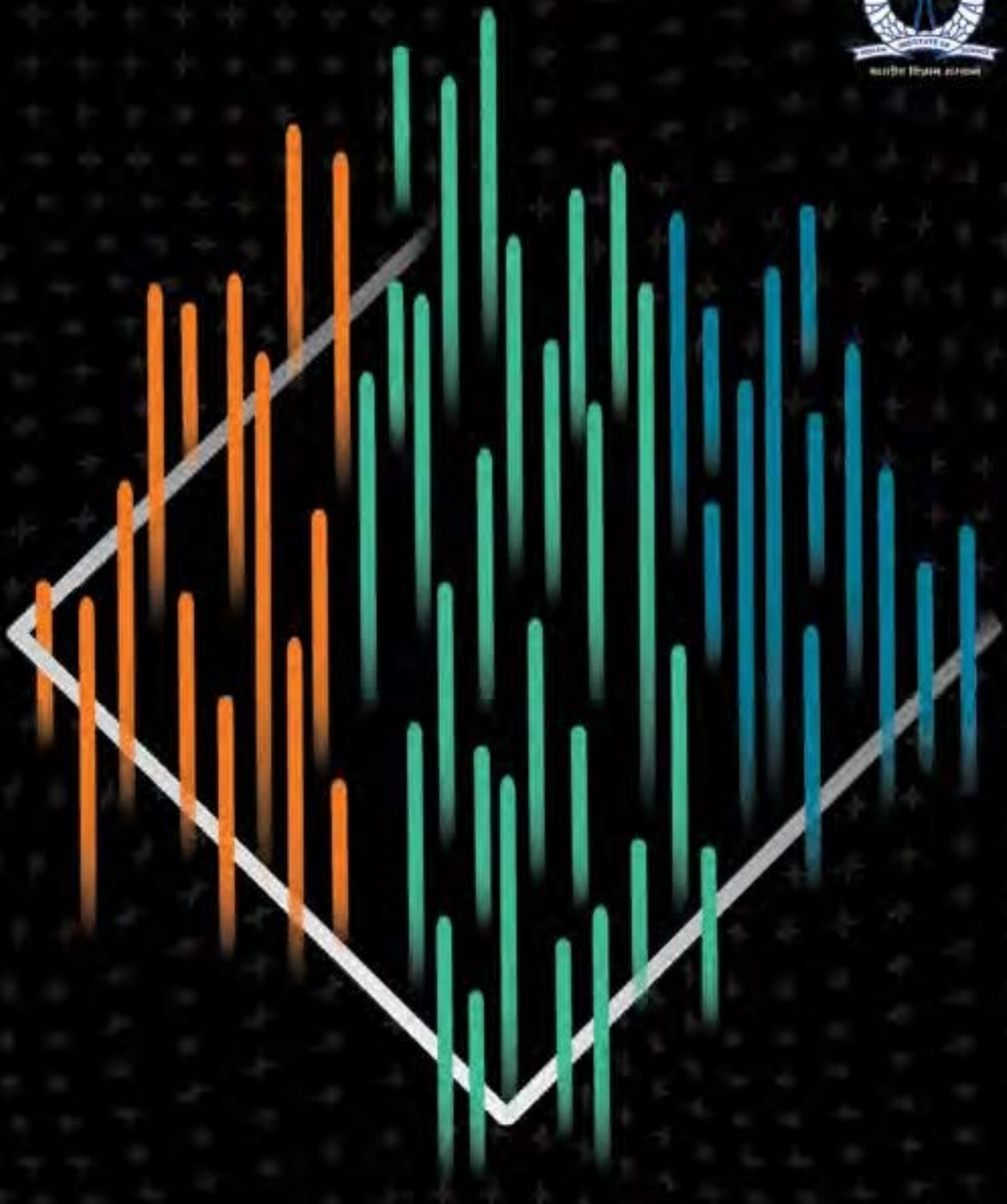
ANNUAL REPORT

IISc 2018-19



VISITOR
The President of India

PRESIDENT OF THE COURT
N Chandrasekaran

CHAIRMAN OF THE COUNCIL
P Rama Rao

DIRECTOR
Anurag Kumar

DEANS
SCIENCE: Biman Bagchi
ENGINEERING: K Kesava Rao
UG PROGRAMME: P S Anil Kumar

REGISTRAR
V Rajarajan

IISc RANKED INDIA'S TOP UNIVERSITY

In 2016, 2017, 2018 IISc was ranked Number 1 among universities by the National Institutional Ranking Framework (NIRF) under the auspices of the Ministry of Human Resource Development. Again in 2019 IISc was ranked Number 1 among universities and second in the overall category by NIRF. This year IISc ranked fourth under the category of Government funded institutions by Atal Ranking of Institutions on Innovation Achievements (ARIIA).

Contents

Foreword

The Indian Institute of Science (IISc, or just "The Institute") was established in 1909 by a visionary partnership between the industrialist Jamsetji Nusserwanji Tata, the Maharaja of Mysore, and the Government of India. Over the last 110 years, IISc has become a premier institute for advanced scientific and technological research and education in India. As stated in the "Scheme" under which the Institute operates, the primary "Object" of the Institute is "to provide for advanced instruction and to conduct original investigations in all branches of knowledge and, in particular, in such branches of knowledge as are likely to promote the material and industrial welfare of India." In keeping with this guiding principle, the Institute has strived to foster a balance between pursuit of basic knowledge and applying its research for industrial and social benefit. In the recent years, the Institute has initiated the practice of undergoing international peer reviews by eminent scientists and engineers from both academia and the industry, in a conscious effort to keep its research activities relevant to the demands of contemporary science and technology.

During 2018-19, several events of notable import occurred in the institute. The most significant is that IISc acquired the Institute of Eminence (IoE) tag. The Institute was one of the first to achieve this distinction. The IoE tag will enable the Institute to gain access to enhanced MHRD funding and to have greater autonomy in governing itself. It must be noted that the additional MHRD support under IoE will have to be matched by the Institute, with funds raised from other sources. The Institute has initiated many new programmes under IoE. It was long felt that a research university of the stature of the Institute must have a strong post-doctoral programme which would give the necessary support to the formation of large research teams under individual or groups of faculty. With this in mind, the Raman Post Doctoral program, a highly selective program with 50 positions, carrying an enhanced salary of INR 1 Lakh per month and an annual research grant of INR 8 Lakh, has been introduced to attract intensely motivated individuals with an established record of high quality research. In the first year of its inception, about 14 Raman Post Docs have accepted the offers made to them after an intensive selection process. In the same spirit, to foster collaborative research, the Institute has internally funded research proposals, which were selected by a competitive process. In order to ensure that major common research facilities

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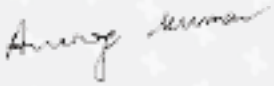
are well supported, the Institute has provided funding for spares, consumables, and maintenance to several large facilities such as the Centre for Nanoscience and the Supercomputer Education and Research Centre that cater to a large group of faculty members across the institute. A research institute must strengthen ties with its peers around the world and the best way to do so is to facilitate interaction with distinguished scientists abroad through visiting programs. Under the IoE program, the Institute has initiated the Satish Dhawan visiting positions for distinguished researchers from abroad and has until date made 12 such offers. The Institute has also deployed matching grants to support faculty travel to conferences and for collaboration, and to start construction of a new building for Centre for Product Design and Manufacturing. CSR funding from industry is being used to start new research facilities and enhance existing ones. There is also an in-principle commitment from the TCS Foundation to support the new building for interdisciplinary research, to be called the TCS Smart-X Hub.

To facilitate gender equality among the student population, a new women's hostel has started construction. The Chemical Sciences building complex that will now house all the different departments of chemistry in the Institute under one roof has now been completed and the departments are likely to start operating from the new buildings shortly. Among the new academic programmes, the PhD/MTech programmes under climate science and manufacturing disciplines are worth noting. The new MTech Programme in Artificial Intelligence by the Division of EECS has been conceived of and is intended to serve the purpose of producing high quality manpower in this cutting edge area. Safety is a matter of concern in a large institute such as IISc, with a large diversity of experimental research. An Office of Laboratory Safety and Environmental Health was created in 2018, and has been staffed with three experienced officers. A Safety Policy has been developed, and a process of safety audits has been started. The level of safety consciousness has been raised and soon IISc expects to have world-class safety practices in all its laboratories.

I am happy to report that the institute continues to receive support for its research activities from various governmental and private industry sources in the form of research grants and consultancy. In return, the Institute has been serving the nation and the society at large by producing high quality scientific manpower and research output in the form of publications in top scientific journals, making new discoveries, and bridging the gap between fundamental research and applications. Recent discoveries in the field of superconductivity by a group of researchers in the Institute have attracted considerable attention of the scientific community and are likely to lead to potentially path-breaking research in this area.

I am honoured to present the IISc Annual Report recording the academic output and achievements during the period 2018-19. It stands witness to the intellectual activities of the faculty members and the students, with the support of the technical and administrative personnel, and financial support from various funding agencies. As I complete my fifth year as Director of this unique institution, I place on record my personal gratitude to the Chair and the Members of the Council of the Institute for their valuable support and guidance.



Anurag Kumar
Director
September 2019

IISc at a glance
2018-19

Academic Structure

Division of Biological Sciences	BC	Biochemistry
	CAF	Central Animal Facility
	CES	Centre for Ecological Sciences
	CIDR	Centre for Infectious Disease Research
	CNS	Centre for Neuroscience
	MCB	Microbiology and Cell Biology
	MBU	Molecular Biophysics Unit
	MRDG	Molecular Reproduction, Development and Genetics
Division of Chemical Sciences	IPC	Inorganic and Physical Chemistry
	MRC	Materials Research Centre
	NRC	NMR Research Centre
	OC	Organic Chemistry
	SSCU	Solid State and Structural Chemistry Unit
Division of Electrical, Electronics, and Computer Science	CSA	Computer Science and Automation
	ECE	Electrical Communication Engineering
	EE	Electrical Engineering
	ESE	Electronic Systems Engineering
Division of Interdisciplinary Research	BSSE	Centre for BioSystems Science and Engineering
	CSP	Centre for Society and Policy
	CISTUP	Centre for Infrastructure, Sustainable Transportation and Urban Planning
	CENSE	Centre for Nano Science and Engineering
	CDS	Computational and Data Sciences
	MS	Management Studies
	ICER	Interdisciplinary Centre for Energy Research
	ICWAR	Interdisciplinary Centre for Water Research
	RBCCPS	Robert Bosch Centre for Cyber Physical Systems
	SERC	Supercomputer Education and Research Centre

Division of Mechanical Sciences

AE	Aerospace Engineering
CPDM	Centre for Product Design and Manufacturing
CE	Chemical Engineering
MT	Materials Engineering
ME	Mechanical Engineering
CIE	Civil Engineering
CEAS	Centre for Earth Sciences
CAOS	Centre for Atmospheric and Oceanic Sciences
CST	Centre for Sustainable Technologies
DCCC	Divecha Centre for Climate Change

Division of Physical and Mathematical Sciences

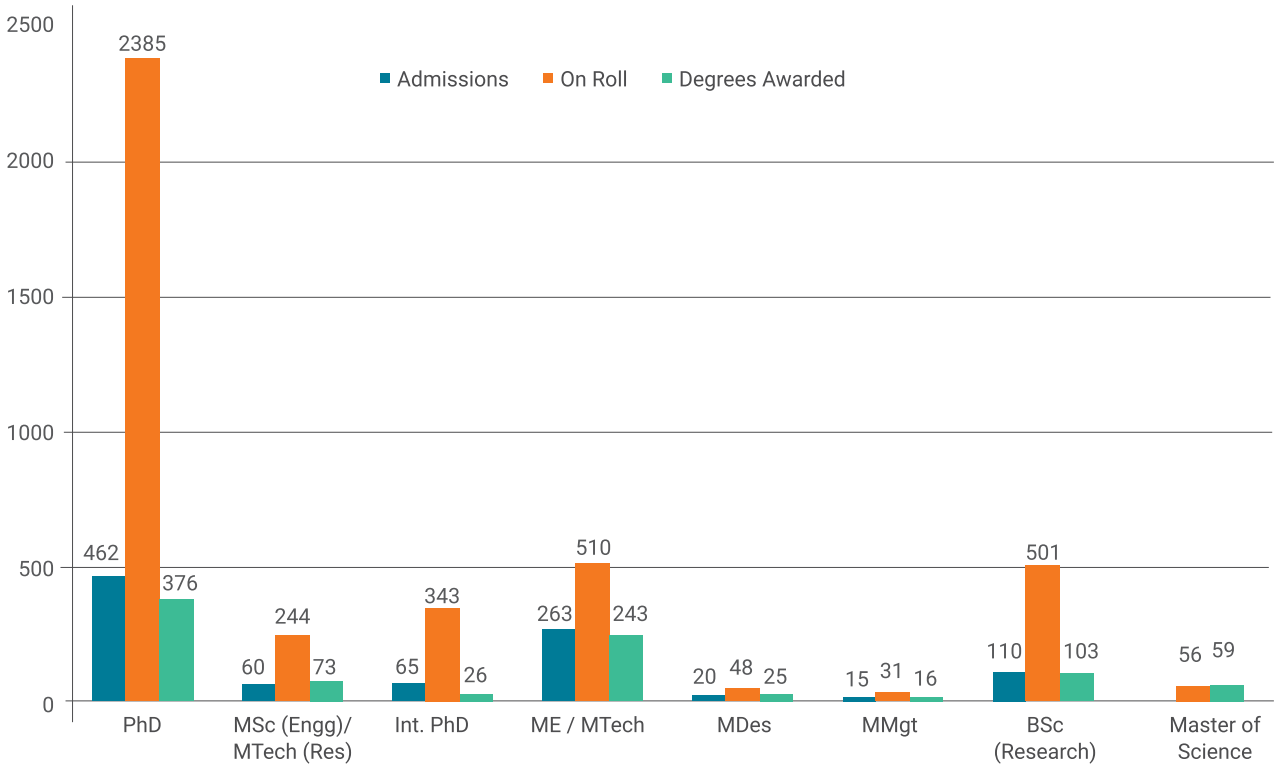
CCT	Centre for Cryogenic Technology
CHEP	Centre for High Energy Physics
IAP	Instrumentation and Applied Physics
MA	Mathematics
PHY	Physics

Centres under the Director

LIB	JRD Tata Memorial Library
OOC	Office of Communications
OIR	Office of International Relations
CCE	Centre for Continuing Education
CSSP	Centre for Sponsored Schemes & Projects
ODAA	Office of Development and Alumni Affairs
IPTEL	Office of Intellectual Property and Technology Licensing
CC	Challakere Campus
CSIC	Centre for Scientific and Industrial Consultancy
DIGITS	Digital Campus and IT Services Office
SID	Society for Innovation and Development
CBR	Centre for Brain Research
KVPY	Kishore Vaigyanik Protsahan Yojana
KSCST	Karnataka State Council for Science and Technology
IISCAA	IISc Alumni Association
OCCAP	Office of career Counselling and Placement

Students

Students – Admissions, On Roll and Degrees Awarded 2017-18



Hostels	(3469)
Men	2542
Women	954
Messes	(4)

Continuing Education	(1,450)
QIP Degree program	22
QIP Short Term Courses	534
CCE Proficience	559
Industry sponsored courses	335

Scholarships/Fellowships	(3,519)
IISc	3322
Others	197

Faculty 2018-19

Staff (900)

	SC/ST	OBC	GN
Academic, Scientific & Technical (546)			
Academic	12	9	420
Scientific	27	3	44
Technical	15	0	16
Support (354)			
Officers	10	5	18
Administrative	57	8	70
Technical	18	2	26
Maintenance	53	4	80
Others	1	0	2

Interactions

On Campus	
Institute Lectures	15
Conferences	236
Visitors	384
Delegations	86
Staff	
Visits	416
Conferences	409
Lectures delivered	680
Assistance in Other Institutions	779

Publication (2763)

Biological Sciences	362
Chemical Sciences	391
Electrical, Electronics, and Computer Sciences	517
Mechanical Sciences	613
Physical & Mathematical Sciences	290
Interdisciplinary Research	590

Awards and Distinctions (289)

Fellows	
National Science and Engineering Academies	15
Other Science and Engineering Academies	49
Shanti Swarup Bhatnagar Award	2
Padma Shri	1
C. V. Raman state award (2005: young scientist award by Karnataka State Govt)	1
Prof. Satish Dhawan Award from the Government of Karnataka	1
CNR Rao Award for Nanoscience	1
SASTRA-CNR Rao Award	1
Young investigator Award, European molecular biology organization	1
INAE Young Engineering Award	1
NASI Young Scientist Platinum Jubilee Award 2018	1
Infosys Prize, 2018	1
Awards and Honours	**219**

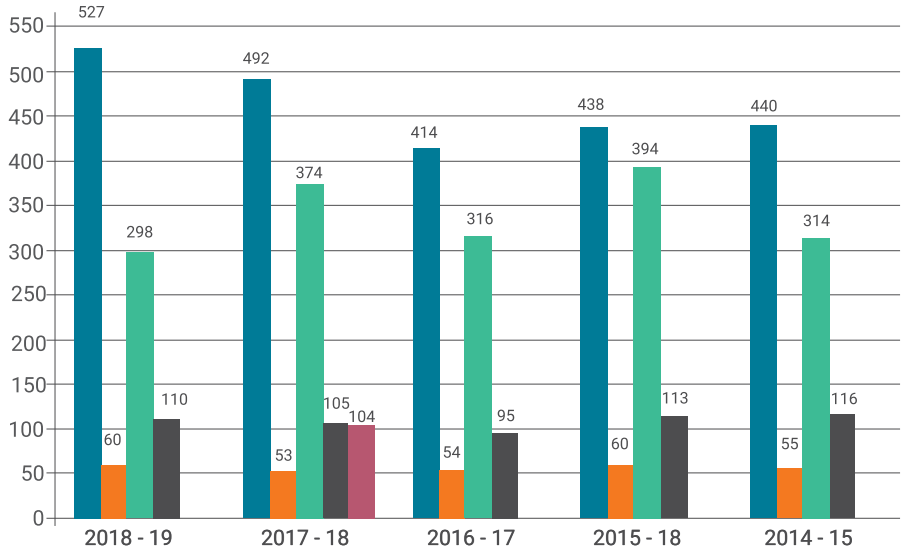
Academic Divisions: 6 Departments: 42

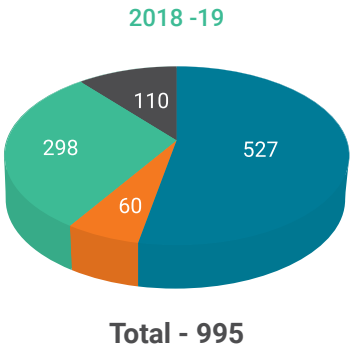
Biological Sciences	8
Chemical Sciences	5
Electrical Sciences	4
Mechanical Sciences	10
Physical & Mathematical Sciences	5
Interdisciplinary Research	10

Students

ADMISSIONS, CONFERMENT, ON ROLL

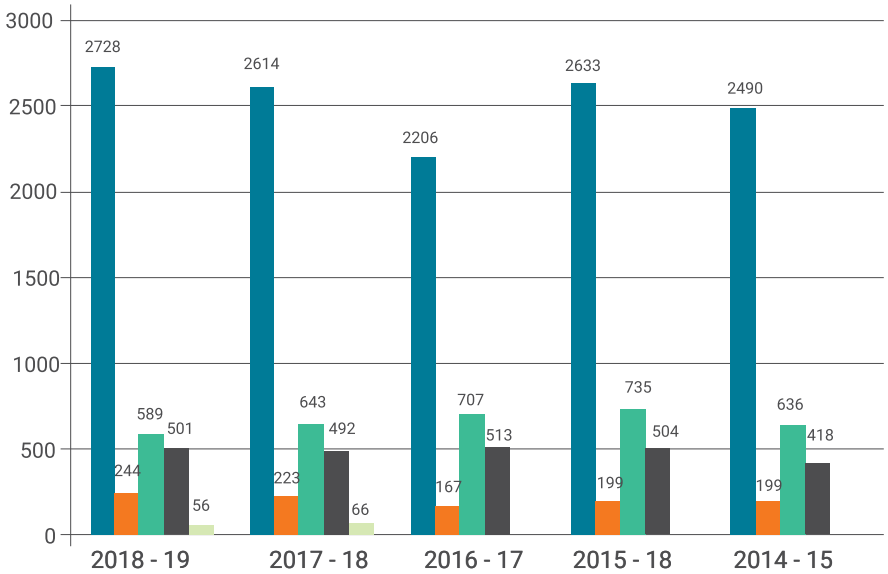
Students Admissions from 2014 to 2019

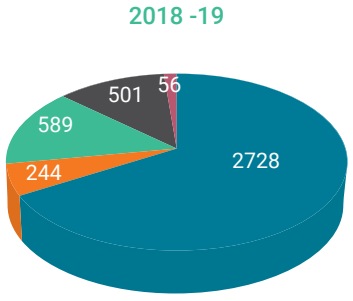




Total - 995

On Roll from 2014 to 2019

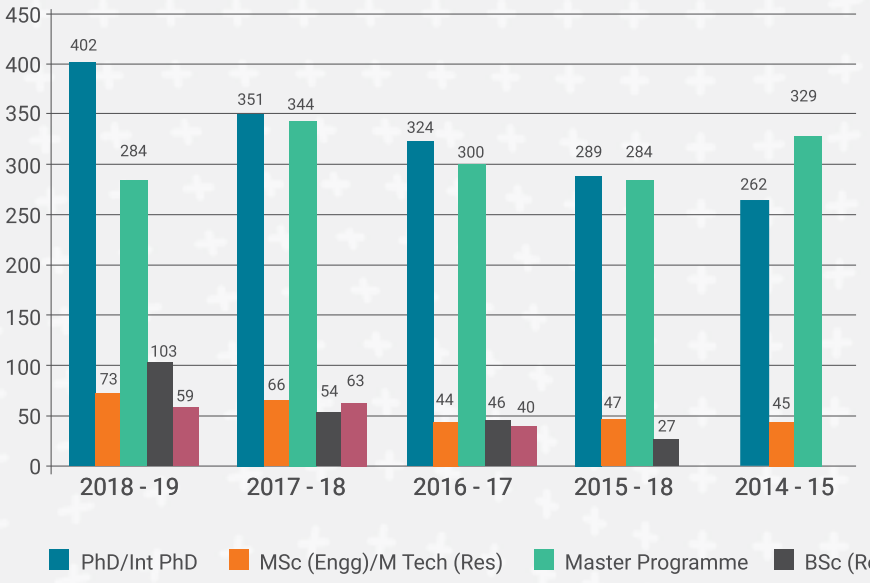


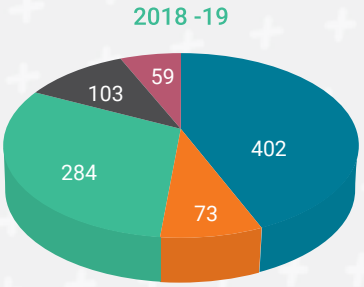


Total - 4118

PhD/Int PhD | MSc (Engg)/M Tech (Res) | Master Programme | BSc (Research) | Master of Science

Conferments from 2014 to 2019

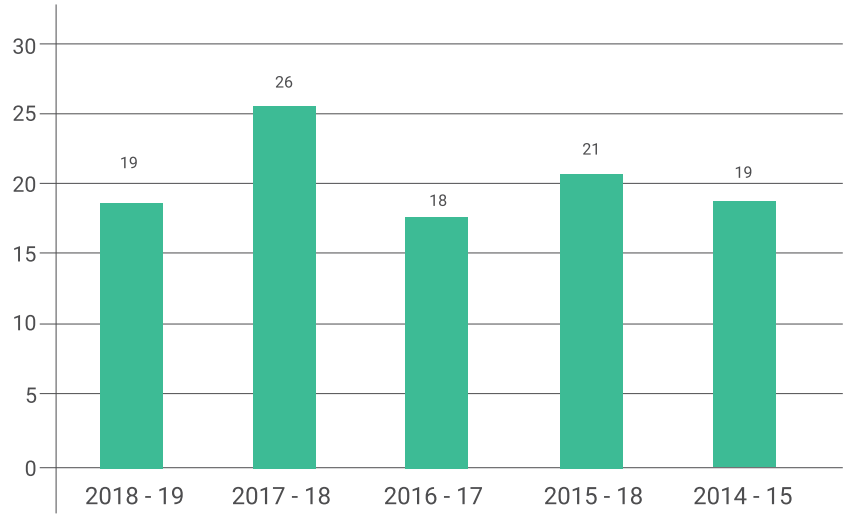




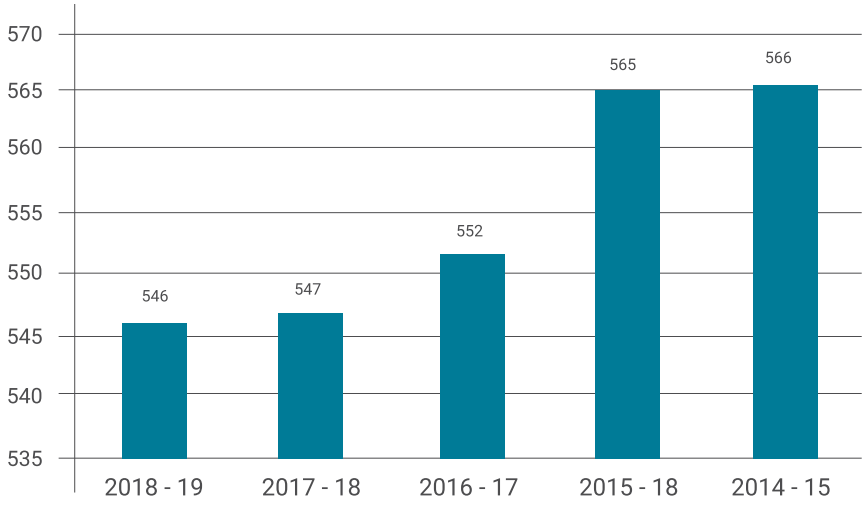
Total - 921

Faculty 2018-19

New Faculty Inducted during 2013-2018

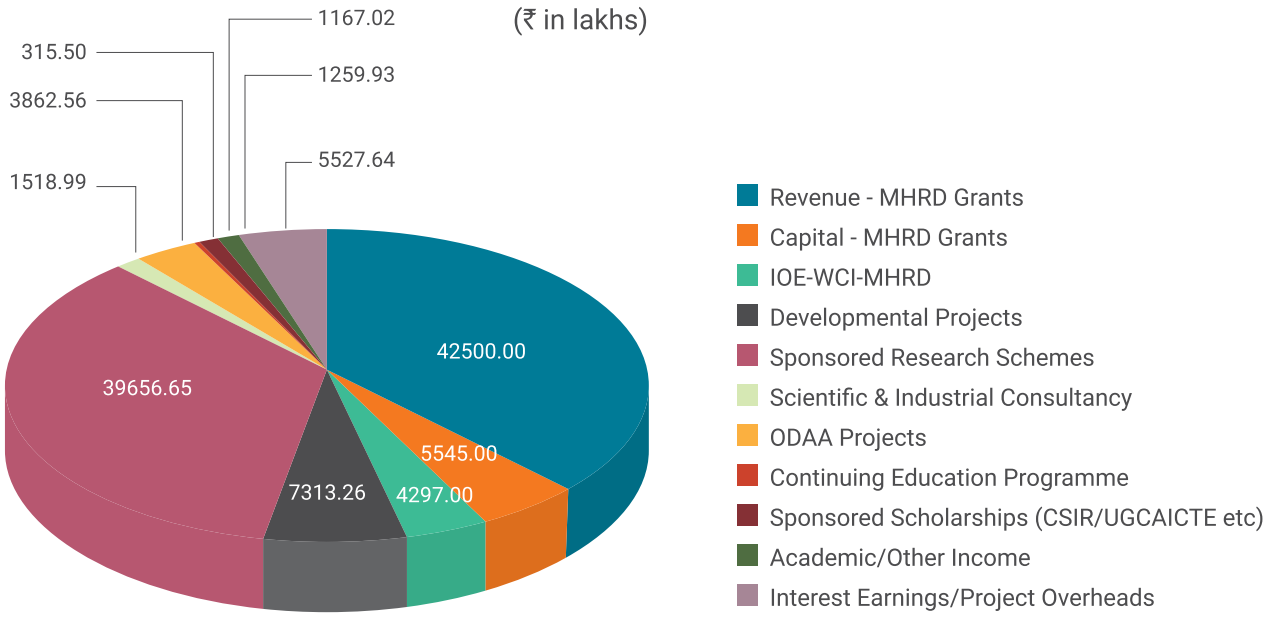


Academic, Scientific and Technical Staff On Roll from 2013-2018



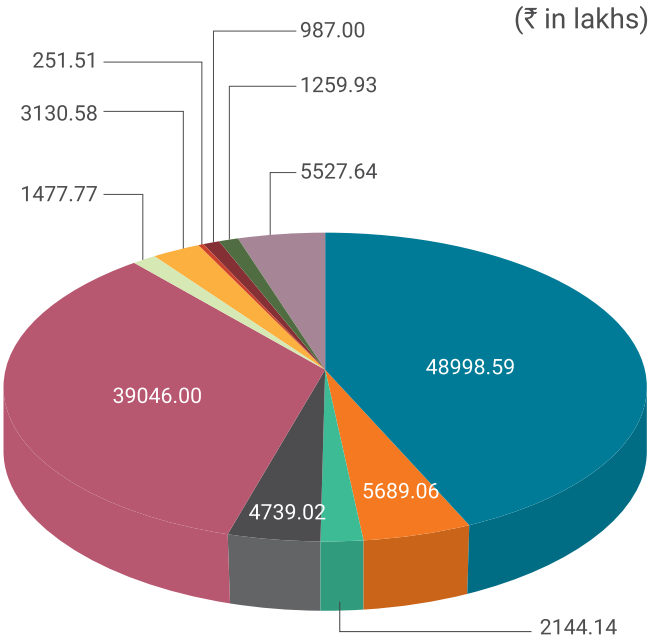
Finance 2018-19

Receipts



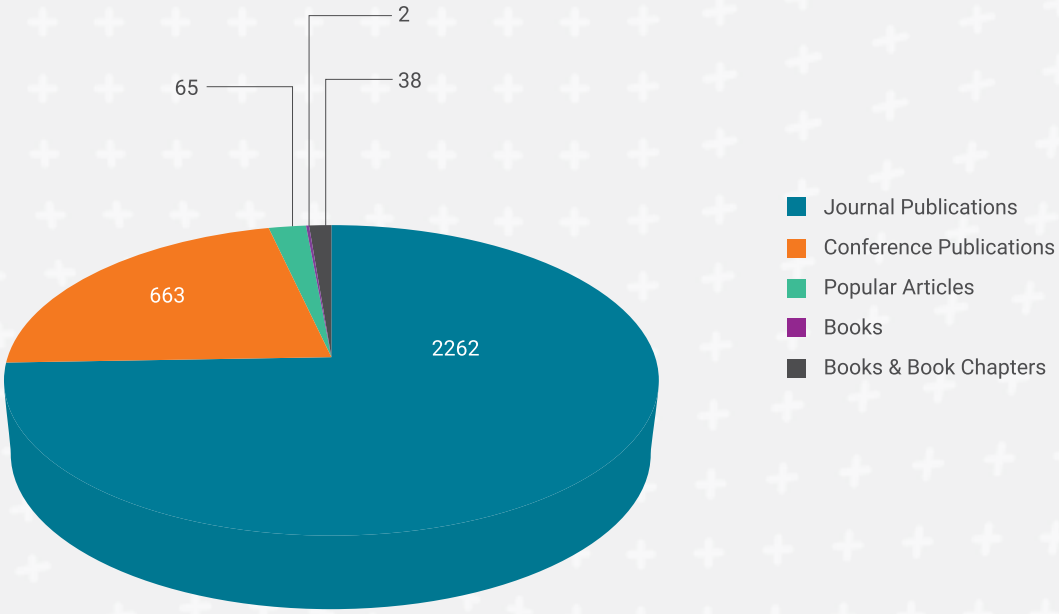
Total - 112963.55

Payments

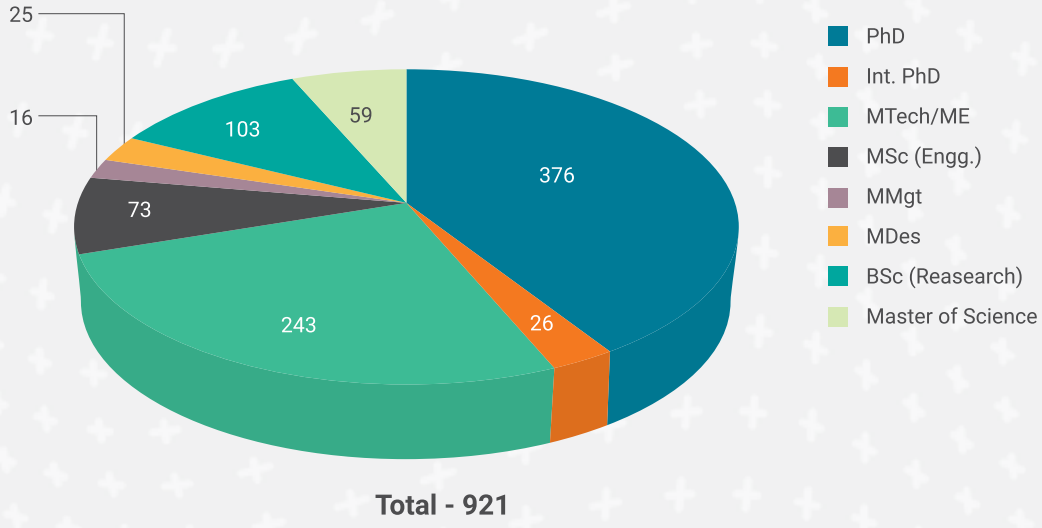


Total - 113251.24

Publications 2018



Degrees Awarded 2018-19



Total - 921

Programmes

Research

PhD Int.PhD BSc (Res)

SCIENCE

- Biochemistry
- Ecological Sciences
- Microbiology and Cell Biology
- Molecular Biophysics
- Molecular Reproduction Development and Genetics
- Neurosciences
- Inorganic and Physical Chemistry
- Materials Research
- Organic Chemistry
- Solid State and Structural Chemistry
- Mathematics
- Physics
- Astronomy and Astrophysics
- High Energy Physics
- Interdisciplinary Programme - IMI
- Undergraduate Programme

Course / Research

PhD MTech (Res) MTech M Des MMgt

ENGINEERING

- Civil Engineering
- Earth Sciences
- Computer Science and Automation
- Electrical Engineering
- Electrical Communication Engineering
- Electronic Systems Engineering
- Aerospace Engineering
- Chemical Engineering
- Mechanical Engineering
- Materials Engineering
- Product Design and Manufacturing
- Atmospheric and Oceanic Sciences
- Instrumentation
- Computational and Data Science
- Nanoscience and Engineering
- Energy Research
- Management Studies
- BioSystems Science and Engineering
- Water Research
- Sustainable Technologies
- Cyber Physical Systems
- Climate Change

Courses offered 2017-18

Division	100 level	200 level	300 level	400 level	0 level	Total
Biological Sciences	1	14	18	0	0	**33**
Chemical sciences	0	15	14	0	0	**29**
Physical & Mathematical Sciences	0	51	53	1	0	**105**
Electrical, Electronics, and Computer Sciences	0	119	22	0	0	**141**
Mechanical Sciences	1	104	41	1	0	**147**
Centres /IDP	0	8	3	0	0	**11**
Undergraduate (BS)	12	17	37	13	0	**79**
General Academic & Research Provisisons	2	12	18	2	0	**34**
Total	**16**	**340**	**206**	**17**	**0**	**579**

1 The Institute

The Indian Institute of Science is an institution of higher learning and research established in 1909 under the Charitable Endowments Act 1890. With the establishment of the University Grants Commission in 1956, the Institute came under its purview as a Deemed University. The principal authority governing the Institute is the Council, which is advised by the Court in the formulation of policies. The Director is the Chief Executive of the Institute and is assisted in its management by the Senate and the Faculties of Science and Engineering.

1.1 The Court

The membership of the Court is drawn from different cross sections of the country such as Industry, Universities, Scientific Institutions, etc. In addition to eminent persons of science, learning and industry, it also contains the nominees of the Government of India, the Government of Karnataka and the Tata Trusts. The Professors of the Institute and the members of the Council are also ex-officio members of the Court. The following are the members of the Court:

N CHANDRASEKARAN
President of the Court Chairman, Tata Sons Ltd Bombay House, 24, Homi Mody Street Mumbai 400 001

PRAHLADA RAMARAO
Formerly Distinguished Scientist and Chief Controller, DRDO, NEW DELHI Adjunct Faculty, Dept of Management IISc and NIAS Bengaluru

ANIL D SAHASRABUDHE
Chairman, The All India Council for Technical Education Nelson Mandela Marg, Vasant Kunj
New Delhi – 110 067

MANJULA N
Commissioner, Office of the Commissioner Dept. of Collegiate Education 2nd Floor, DTE Building Palace Road Bangalore 560 001

R K KRISHNA KUMAR
Director, Tata Sons Ltd Bombay House, 2nd Floor 24, Homi Mody Street Fort, Mumbai 400 001

PANKAJ R PATEL
President: FICCI & Chairman & Managing Director, Cadila Healthcare Ltd., Zydus Tower Satellite Cross Roads Ahmedabad 380 015

S N AGARWAL
Chairman, Bhoruka Power Corporation Ltd., 5th Floor Hitananda-II, 48, Lavelle Road Bangalore 560 001

VIJAY PADATE
Director General, The Employers Federation of India, 1703, World Trade Centre-I, Cuffe Parade Mumbai 400 005

SHEKHAR C MANDE
Director General Council of Scientific & Industrial Res. Anusandhan Bhawan 2, Rafi Marg, NEW DELHI

P RAMA RAO
Former Vice-Chancellor, Univ. Of Hyderabad Chairman, Governing Council, IISc "NAIMISAM"
Flat No. 301, Plot No. 22 , Srinagar Colony, Hyderabad 500 073

M K BHAN
Former Secretary Dept. Of Biotechnology Govt. of India, Min. Of Science and Technology New Delhi

R S BAWA
Vice Chancellor Chandigarh University Gharuan, District Mohali Punjab 140 413

SANDEEP SANCHETI
Vice Chancellor SRM Institute of Science & Technology SRM Nagar, Kattankulathur Kancheepuram District Chennai 603 203

RAKESH BHATNAGAR
Vice Chancellor Banaras Hindu University Varanasi 221005

M P RAVINDRA
President, IISc. Alumni Association IISc Campus, Bengaluru 560 012

ANURAG KUMAR
Director (Ex-officio)

ALL PROFESSORS OF THE INSTITUTE
(Ex-officio)

ALL MEMBERS OF THE COUNCIL
(Ex-officio)

V RAJARAJAN
Registrar (Ex-officio Secretary)

During the year, the Court met once on Mar 15, 2019.

1.2 The Council

The Council is the principal governing authority of the Institute and its membership includes the Nominees of the Court, Parliament, Government of India, Government of Karnataka, Tata Trusts, Representatives of Indian Universities, University Grants Commission and Scientific bodies. The following are the members of the Council.

P RAMA RAO
Chairman of the Council Former Vice Chancellor University of Hyderabad Hyderabad (Nom. GOI)

R SUBRAHMANYAM
Secretary, Min. of Human Resource Development Dept. of Higher Education, Govt. of India Shastri Bhavan, New Delhi 110001

V L V S S SUBBA RAO
Senior Economic Advisor Ministry of Human Resource Development Higher Education Department, Govt. of India 107-C, Shastri Bhawan
New Delhi 110 001

A S KIRAN KUMAR
Former Secretary Department of Space Antariksh Bhavan New BEL Road
Bangalore 560 231

B H ANIL KUMAR
Additional Chief Secretary, Higher Education Dept Govt. of Karnataka, Bangalore 560 001

I S N PRASAD
Additional Chief Secretary Finance Dept., Govt. of Karnataka
Bangalore 560 001

J J IRANI
Director, Tata Sons Ltd. # 7, Beldih Lake Northern Town Jamshedpur 831 001

RAJENDRA PRASAD
Director, Amity Institute of Biotechnology
Amity Univ Gurgaon
(Haryana) 122413

NARENDRA JADHAV
Hon'ble Member of Parliament (RS)
304, Shalaka, 4th Floor, Maharshi Karve Road Near Cooper age Telephone Exchange
MUMBAI 400021

SURESH C ANGADI
Hon'ble Member of Parliament (LS) "Spoorthi" Sampige Road Vishweshwarayya Nagar
Belgaum 590 009

M K BHAN
Former Secretary, Dept. of Biotechnology Govt. of India, Min. of Science & Technology, New Delhi

R S BAWA
Vice Chancellor, Chandigarh University Gharuan, District Mohali
Punjab 140 413

SANDEEP SANCHETI
Vice Chancellor, SRM Institute of Science & Technology SRM Nagar, Kattankulathur Kancheepuram District
Chennai 603 203

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NEW DELHI 110 067

SHEKHAR C MANDE
Director General, Council of Scientific & Industrial Res. Anusandhan Bhawan, 2, Rafi Marg
NEW DELHI 110 001

ANURAG KUMAR
Director (Ex-officio)

BIMAN BAGCHI
(Ex-officio)
Dean, Science Faculty

K KESAVA RAO
(Ex-officio)
Dean, Engineering Faculty

V RAJARAJAN
Registrar (Ex-officio Secretary)

The Council met quarterly on Jun 23, 2018; Oct 6, 2018; Dec 22, 2018 and Mar 16, 2019.

1.3 Finance Committee

The following are the members of the Finance Committee.

P RAMA RAO
Former Vice Chancellor University of Hyderabad, Chairman of the Council (Ex-officio)

PAVAN KUMAR MALAPATI
Deputy Secretary (Budget & Resources)
Finance Department
Bangalore (Nom. GOK)

ASHISH W DESHPANDE
Secretary & Chief Financial Officer Sir Ratan Tata Trust, Bombay House, Homi Mody Street, MUMBAI – 400 001

R F SAVAKSHA
Secretary & Chief Accountant Sir Dorabji Tata Trust
Mumbai (Nom. Tata Trusts)

DARSHANA M DABRAL
Joint Secretary & Financial Adviser
Dept. of Higher Education
MHRD GOI (Nom. GOI)

M K BHAN
Former Secretary, Dept. of Biotechnology, Govt. of India Min. of Science and Technology
New Delhi

V L V S S SUBBA RAO
Senior Economic Advisor, Ministry of Human Resource Development, Higher Education Department, Govt. of India, 107-C, Shastri Bhawan
New Delhi 110001

R NARESH
Pr. Accountant General (G&SSA)
Karnataka, Bangalore (Ex-officio)

ANURAG KUMAR
Director (Ex-officio)

V RAJARAJAN
Registrar (Ex-officio Secretary)

The Finance Committee met quarterly on Jun 22, 2018; Sep 28, 2018; Dec 21, 2018 and Mar 14, 2019.

1.4 The Senate

The Senate is one of the authorities of the Institute that consists of the Director as the Chairman, all Professors and Associate Professors, one elected representative (Assistant Professor) from each of the Faculties, the Librarian, and the Registrar (Secretary). The Senate meets at least once in a term.

This principal academic body functions to (a) plan and coordinate the research activities of the Institute, (b) regulate and organise courses of instruction and study, admission of students, examinations, etc., (c) formulate conditions for the award of degrees of the Institute, and (d) recommend names to the Council for the award of degrees.

During the year, the Senate met on May 30, 2018; Sep 6, 2018; Nov 16, 2018 and Feb 11, 2019.

The Senate recommended the award of various degrees as follows:

• PhD	376
• Int. PhD	26
• MSc (Engg)	73
• ME/MTech	243
• MDes	25
• MMg	16
• BSc (Research)	103
• Master of Science	59
Total	**921**

1.5 Faculties

The Science Faculty and Engineering Faculty act as advisory bodies to the Senate and assist in the discharge of its duties. Each Faculty consists of the respective Dean as Chairman, all Professors, Associate Professors, Chief Research Scientists, Principal Research Scientists, Assistant Professors and Senior Scientific Officers as members and the Assistant Registrar as the Secretary.

The Science Faculty met on Apr 13, 2018 and Oct 10, 2018. The Engineering Faculty met on Apr 11, 2018 and Oct 11, 2018 during the year.

The joint meetings of Faculty of Science and Faculty of Engineering were held on Aug 21, 2018 and Jan 4, 2019. The Director chaired the joint meetings.

2 Staff

Director: Anurag Kumar

Dean (Science)
Biman Bagchi

Deputy Director (Infrastructure and Planning)
Rudra Pratap

Chair, Division of Biological Sciences
Umesh Varshney

Chair, Division of Electrical, Electronics, and Computer Sciences
Y Narahari

Chair, Division of Mechanical Sciences
Vikram Jayaram

Dean (Engineering)
K Kesava Rao

Deputy Director (Administration and Finance)
Jayant M Modak

Chair, Division of Chemical Sciences
P K Das

Chair, Division of Interdisciplinary Research
G Rangarajan

Chair, Division of Physical & Mathematical Sciences
Rahul Pandit

UG Programme: P S Anil Kumar

Registrar
V Rajarajan, MSc
(TNAU, Coimbatore)

Financial Controller
Indumati Srinivasan, MA (JNU)
MPhil (JNU), PGDPPM (IIMB)

Deputy Registrar
V Nagaraja, MA (Mysore)
M C Jayaprakash, MCom, MBA, BL

Deputy Financial Controller
M Krishna Murthy, MCom,
MBA (Bangalore), PGDPM & IR
(Bangalore), PhD (Bangalore)
P Manivannan, MA (Madras)

Administrative Officer
Umashankar Apali

Assistant Registrars
Aparna Kandi, BE (Gulbarga)
Veeranna Kammar, MSc (Bangalore)
B N Sreedhar, MBA (KSOU)
P Selva Kumar, MA (KSOU)
Krishna Kant Kumar, MA(IGNOU)
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(Nagarjuna University)

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BSc (Mysore), LLB (Bangalore)

Sr. Hindi Officer
V Thilagam, PhD (Bangalore)

Sr. Sports Officer
C P Poonacha
BA (Mysore), MPEd (Karnataka)

Internal Auditor
Gurumurthy, M. Com

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C Sathish Rao, MBBS (Mysore)
L Sharada, MBBS, DGO (CMC, Vellore)
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G Lohithesh Kumar, BE (Kuvempu),
MTech (Visvesvaraya)
Manjunath S, BE (BMS)

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B Sridhar MSc (Hort) (UAS, Bangalore)

GYMKHANA
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Ambedkar Dukkipati, PhD (IISc)

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Rajeev Tanjan, PhD (BHU)
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Prabal K Maiti, PhD (IIT/K)
Partha Pratim Mondal, PhD (IISc)
Ravishankar Narayan, PhD (IISc)
Annapoorni Rangarajan, PhD (NCBS)
Abha Misra, PhD (IIT Bombay)

3 Divisions

3.1 Division of Biological Sciences

IN NUMBERS

- 74 FACULTY MEMBERS
- 360 PhD STUDENTS
- 51 INTEGRATED PhD STUDENTS

The Division of Biological Sciences forges important links between basic science and innovative research. It is committed to enhancing frontline studies in almost all aspects of modern biology: Neuroscience in health and disease, Infectious Disease, Structural Biology, Oncology, DNA Repair and Genomic Stability, Systems Biology and Bioinformatics, Immunology, Enzymology, Reproductive and Developmental Biology, Diverse Ecological Studies and more.

THEMES

Investigators in the Division focus on numerous processes central to the understanding of life, emphasising on areas with considerable translational potential, namely, Cognition and Neuronal Reprogramming, Infectious Diseases, Drug and Molecular Design, Diagnostics and Therapeutics in Cancer, Gene Targeting, Genetic Disorders and Genetic Diversity.

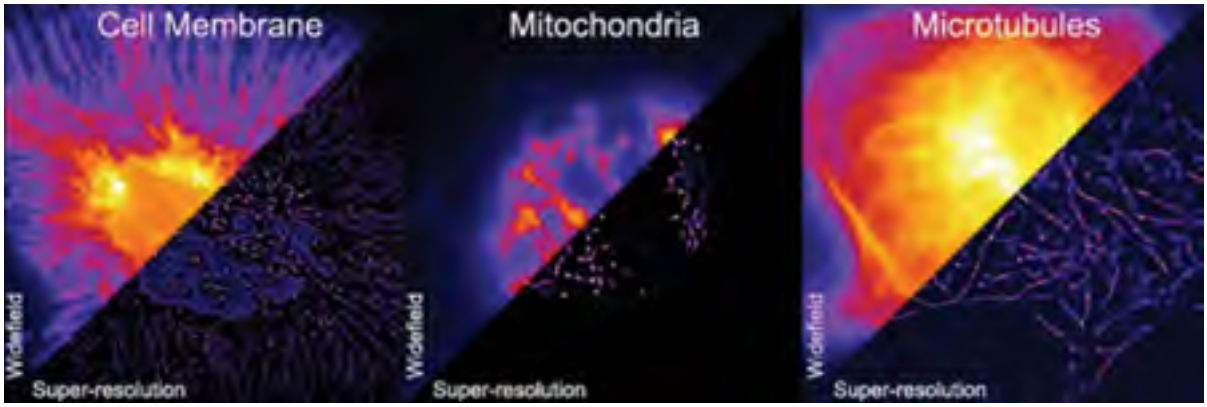
RESEARCH HIGHLIGHTS

The Division of Biological Sciences consists of the Departments of Biochemistry, Microbiology & Cell Biology, Molecular Reproduction, Development & Genetics, Molecular Biophysics Unit, Ecological Sciences, Centre for Neuroscience, Centre for Infectious Disease Research and Central Animal Facility including Primate Research Laboratory.

DEPARTMENTS | CENTRES | UNITS

- BIOCHEMISTRY
- CENTRAL ANIMAL FACILITY
- CENTRE FOR ECOLOGICAL SCIENCES
- CENTRE FOR INFECTIOUS DISEASE RESEARCH
- CENTRE FOR NEUROSCIENCE
- MICROBIOLOGY AND CELL BIOLOGY
- MOLECULAR BIOPHYSICS UNIT
- MOLECULAR REPRODUCTION, DEVELOPMENT AND GENETICS

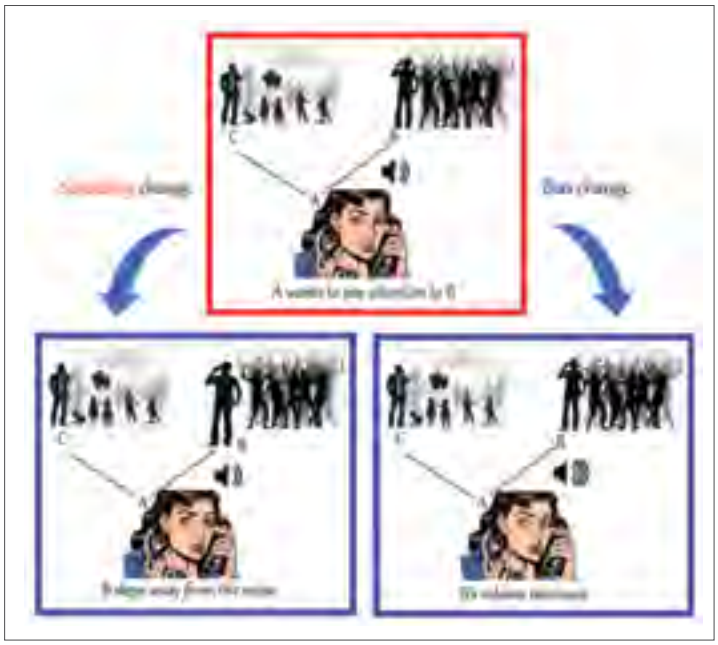
Research Snapshots 2018-19



Deepak Nair (CNS)

Fluorescence-Activating and absorption-Shifting Tag (FAST) is a novel genetically encoded optical highlighter probe. Since the fluorescence of FAST originates from the stochastic and reversible diffusive association of a fluorogenic ligand, we investigate the application of FAST using Super-Resolution Radial Fluctuations (SRRF) to achieve routine imaging below the diffraction limit in a widefield epifluorescence microscope. We show that intensity fluctuation analysis like SRRF allows the imaging of FAST-tagged proteins with sub – 100 nm resolution in live cells. FAST co-labeled with conventional fluorophores enables real time multicolour 2D and 3D super-resolution imaging, indicating that FAST can be used for observation of sub-diffraction limited structures in both living and fixed samples.The development of improved FAST variants with orthogonal fluorogen selectivity in the future could allow efficient, cost-effective, multicolour super-resolution imaging in any widefield epifluorescence microscope, improving our understanding of fundamental molecular organization in cell biology.

Live cell super resolution imaging by radial fluctuations using fluorogen binding tags
M Venkatachalapathy, V Belapurkar, M Jose, A Gautier, D Nair Nanoscale 11 (8), 3626-3632, 2019

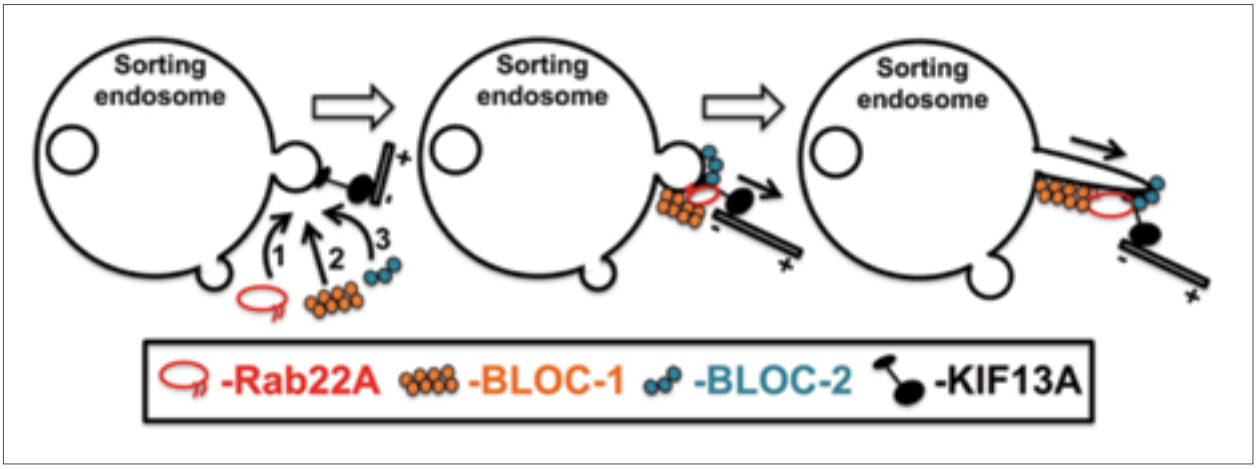


Sridharan Devarajan (CNS)

Attention is the remarkable ability that allows us to selectively process relevant information from the world around us, but is “attention” a single (unitary) phenomenon? In two behavioral studies conducted with human participants we show that attention is not a unitary phenomenon, but can be divided up into two components: “sensitivity” (improving information encoding) and “bias” (enhancing information weightage). The cartoon alongside illustrates these concepts: Say, individual A is having two conversations (over two phones) simultaneously with individuals B and C, who are themselves in noisy environments. And say, A is more interested in hearing what B has to say, and wants to pay attention selectively to B’s voice. She could ask B to step away from the noisy dance floor to increase the clarity of B’s voice over his background noise (increasing “sensitivity”). Alternatively, she could increase the volume on the receiver over which she hears B’s voice, to make B’s voice (and his background noise) louder, and more audible, compared to C’s (increasing “bias”). We show that both of these mechanisms are at play regardless of whether participants pay attention voluntarily, instructed by an attention cue (“endogenous” attention, Banerjee et al, 2019) or have their attention captured automatically, by a bright flashing stimulus (“exogenous” attention, Sagar et al, 2019). These findings form the basis for future research on brain mechanisms of these components of attention.

Banerjee S, Grover S, Ganesh S and Sridharan D. Sensory and decisional components of endogenous attention are dissociable. *Journal of Neurophysiology* (in press). https://doi.org/10.1152/jn.00257.2019

Sagar V, Sengupta R, and Sridharan D. Dissociable sensitivity and bias mechanisms mediate behavioral effects of exogenous attention. *Scientific Reports* (in press). https://doi.org/10.1038/s41598-019-42759-w



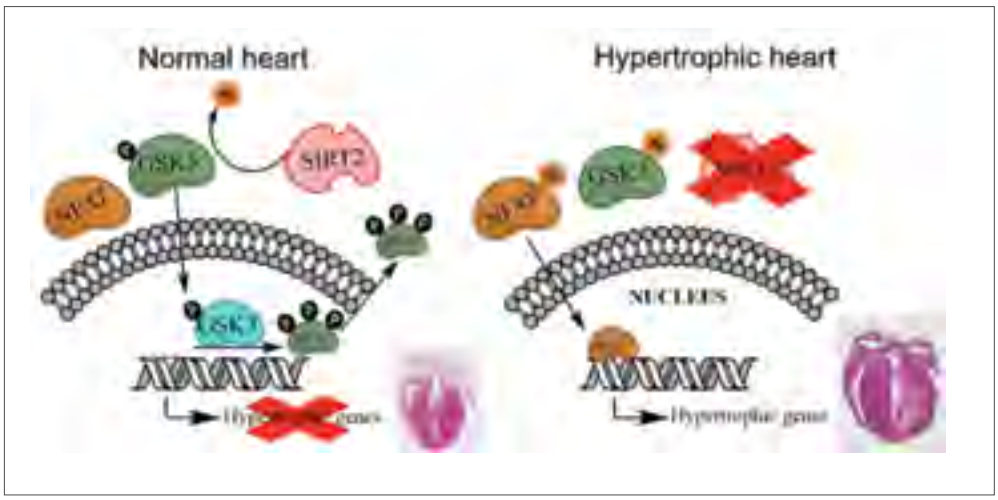
Subba Rao Gangi Setty (MCB)

Recycling endosomes (REs) are transient endosomal tubular intermediates of early/sorting endosomes (E/SEs) that function in cargo recycling to the cell surface and deliver cell type-specific cargo to lysosome-related organelles such as melanosomes in melanocytes. Members of Subba Rao's lab study the mechanism of RE biogenesis. By using an endosomal Rab-specific RNAi screen, they have identified Rab22A as a critical player during RE biogenesis. Rab22A-knockdown results in reduced RE dynamics and cargo accumulation in the E/SEs. Rab22A forms a complex with BLOC-1, BLOC-2 and the kinesin-3 family motor KIF13A on E/SEs. Consistently, the RE-dependent transport defects observed in Rab22A-depleted cells phenocopy those in BLOC-1-/BLOC-2-deficient cells. These findings suggest that Rab22A promotes the assembly of a BLOC-1-BLOC-2-KIF13A complex on E/SEs to generate REs that maintain cellular and organelle homeostasis.

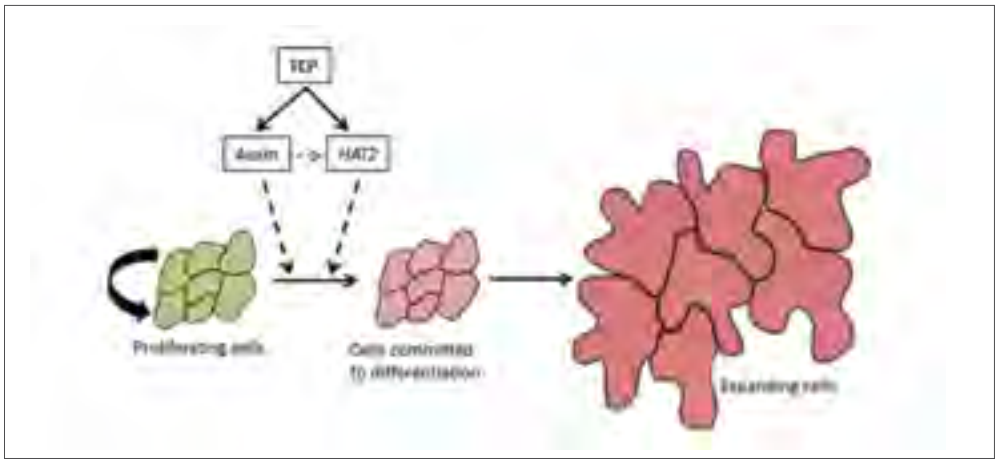
Shakya, S., Sharma, P., Bhatt, A. M., Jani, R. A., Delevoye, C. and Setty, S. R. (2018). Rab22A recruits BLOC-1 and BLOC-2 to promote the biogenesis of recycling endosomes. *EMBO Reports 19,* e45918.

N. Ravi Sundaresan (MCB)

In humans, development of pathological cardiac hypertrophy involves complex molecular events occurring at the level of cardiac myocytes. Studies suggest that Glycogen synthase kinase 3 (GSK3) play a critical role in antagonizing the development of cardiac hypertrophy. Interestingly, the enzymatic activity of GSK3 isoforms is inhibited by phosphorylation-independent mechanisms during cardiac failure, although the mechanism(s) are not understood. Studies in Ravi Sundaresan's lab have identified acetylation as a novel modification of GSK3, which plays a critical role in the development of cardiac hypertrophy. Molecular modeling and/or molecular dynamics simulations indicate that acetylation of GSK3 would hinder both the adenosine binding and prevent stable interactions of the negatively charged phosphates. They found that SIRT2, a class III histone deacetylase blocks cardiac hypertrophy by deacetylating the GSK3 isoforms.



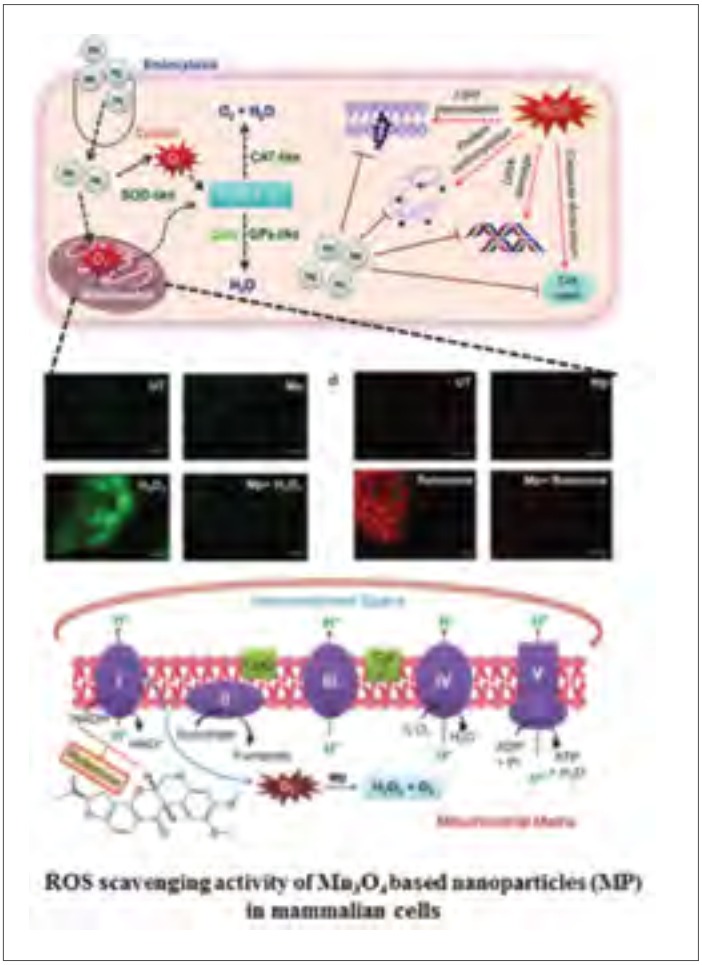
Sarikhani, M., Mishra, S., Maity, S., Kotyada, C., Wolfgeher, D., Gupta, M. P., Singh, M. and Sundaresan, N. R. (2018). SIRT2 deacetylase regulates the activity of GSK3 isoforms independent of inhibitory phosphorylation. *Elife. 7.* e32952.



Utpal Nath (MCB)

Cells in young organs undergo active proliferation at an early stage to generate sufficient number, before exiting proliferation and entering differentiation. How these proliferating cells acquire differentiation potential is unclear. Utpal Nath's lab studies this process in plants by analyzing the role of TCP transcription factors which promote cell maturation. By inducing the activity of TCP4 at various developmental stages of Arabidopsis leaf primordium, they have shown that TCP4 acts as a switch for the transition from proliferation to differentiation. A 24-hour pulse of TCP4 activity is sufficient to impart irreversible differentiation competence to dividing cells. Possibly to ensure the transition, these proteins promote cell differentiation by a two-prong strategy; indirectly by promoting the maturity-inducing hormone auxin, and directly by activating another maturity protein, HAT2.

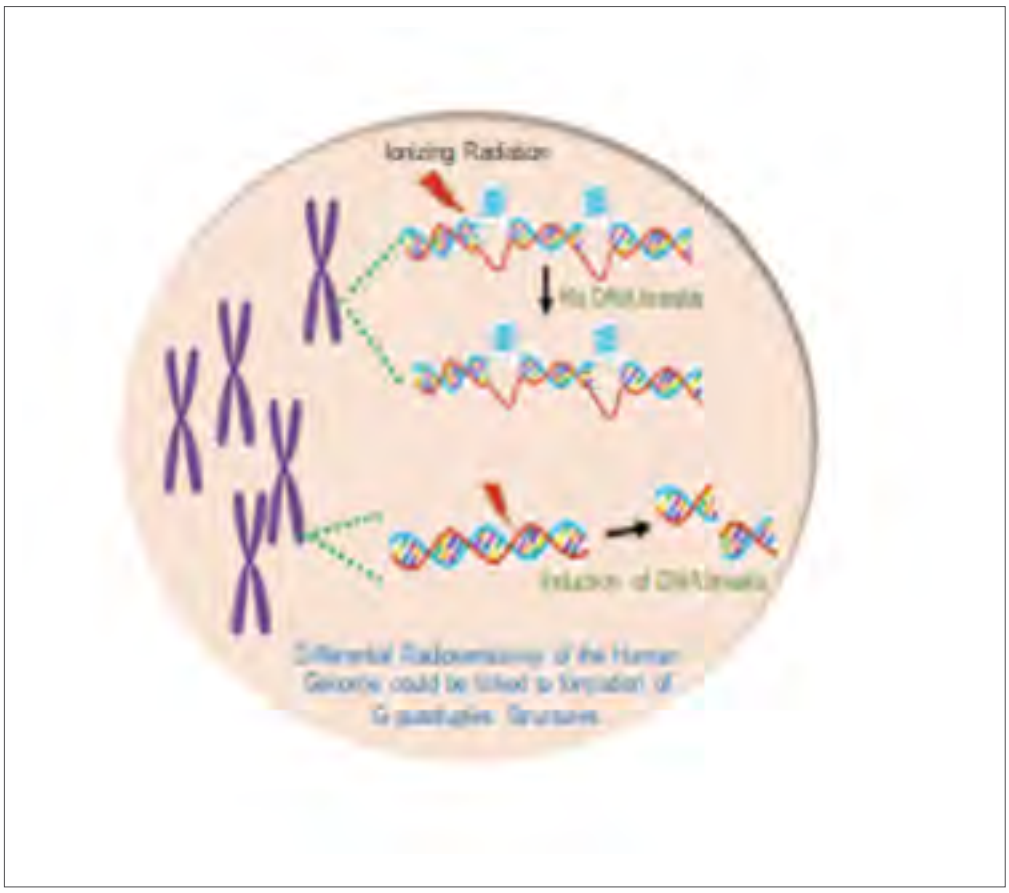
Challa, K. R., Rath, M. and Nath, U. (2019). The CIN-TCP transcription factors promote commitment to differentiation in Arabidopsis leaf pavement cells via both auxin-dependent and independent pathways. *PLoS Genet. 15,* e1007988.



Patrick D'Silva (BC)

The maintenance of an optimum level of reactive oxygen species (ROS) and their stringent regulation is the primary criteria for normal cellular health. The imbalance in the ROS levels due to either excessive production or inefficient in the antioxidant defense mechanism results in several pathological conditions, including cardiovascular, diabetes, cancer, and neurodegenerative diseases. This evokes the need for an efficient enzyme-mimic nanomaterial that can function under physiological conditions, circumventing the detrimental effects of excess ROS without perturbing the cellular machinery. We report here, the ability of Mn3O4 nanoparticles to mimic the functions of three major antioxidant enzymes (catalase, glutathione peroxidase, and superoxide dismutase). The nanoparticle prevented the oxidative damage of cellular components such as DNA, protein, and lipids. Our observations highlight that the ROS-scavenging activity of Mn3O4 nanoparticles functions synergistically with the endogenous antioxidant machinery. Based on our findings, we envisioned that the multienzyme mimic Mn3O4 nanoparticles possess great potential in suppressing the oxidative stress-mediated pathophysiological conditions under which the antioxidant system is overwhelmed.

Singh N, Savanur MA, Srivastava S, D'Silva P*, Mugesh G*. (2019) "A manganese oxide nanozyme prevents the oxidative damage of biomolecules without affecting the endogenous antioxidant system". *Nanoscale.* 2019 Feb 28;11(9):3855-3863. doi: 10.1039/c8nr09397k.PMID:30758009 (*Equal contribution).



Sathees C Raghavan (BC)

DNA, the fundamental unit of human cell, generally exists in Watson-Crick base paired B-DNA form. Often, DNA folds into non-B forms, such as four stranded G-quadruplexes. It is generally believed that ionizing radiation (IR) induces DNA strand-breaks in a random manner. In an interesting new study, we observed that regions of DNA enriched in G-quadruplex structures are less sensitive to ionization radiations such as γ- or X-rays compared to B-DNA. Importantly, cells in S-phase of the cell cycle are less radiosensitive due to higher propensity of G-quadruplex formation. Thus, our results reveal that formation of G4 structures contribute towards differential radiosensitivity of the human genome and can be modulated in a cell cycle dependent manner.

Reference: Nitu Kumari*, Supriya V. Vartak*, Vidya Gopalakrishnan*, Sumedha Dahal*, Sagar S. Desai**, Susmita Kumari**, Bibha Choudhary and Sathees C. Raghavan# (2019). Differential Radiosensitivity of the Human Genome is linked to G-quadruplex Structures and could be modulated in a Cell Cycle Dependent Manner (To be published).

Rohini Balakrishnan, Kavita Isvaran (CES)

Predation is considered a powerful force of natural selection, shaping the evolution of diverse traits, including signals and behaviours related to animal communication. In systems where males produce long-range acoustic signals to attract females from a distance, signal production increases conspicuousness and thereby the risk of predation. This has led to the assumption that the signaling male faces higher risk of predation than the silent female that moves to locate the signal. These assumptions have however rarely been tested empirically. Using a tree cricket species as a model system, Torsekar et al. (2019) provide one of the first empirical, quantitative estimates of the predation risk faced by signaling males and localising females in the wild. Given the difficulty of observing predation events in the wild, predation risk was estimated using a set of constituent probabilities, including co-occurrence with a predator on a bush, encounter and escape probabilities.

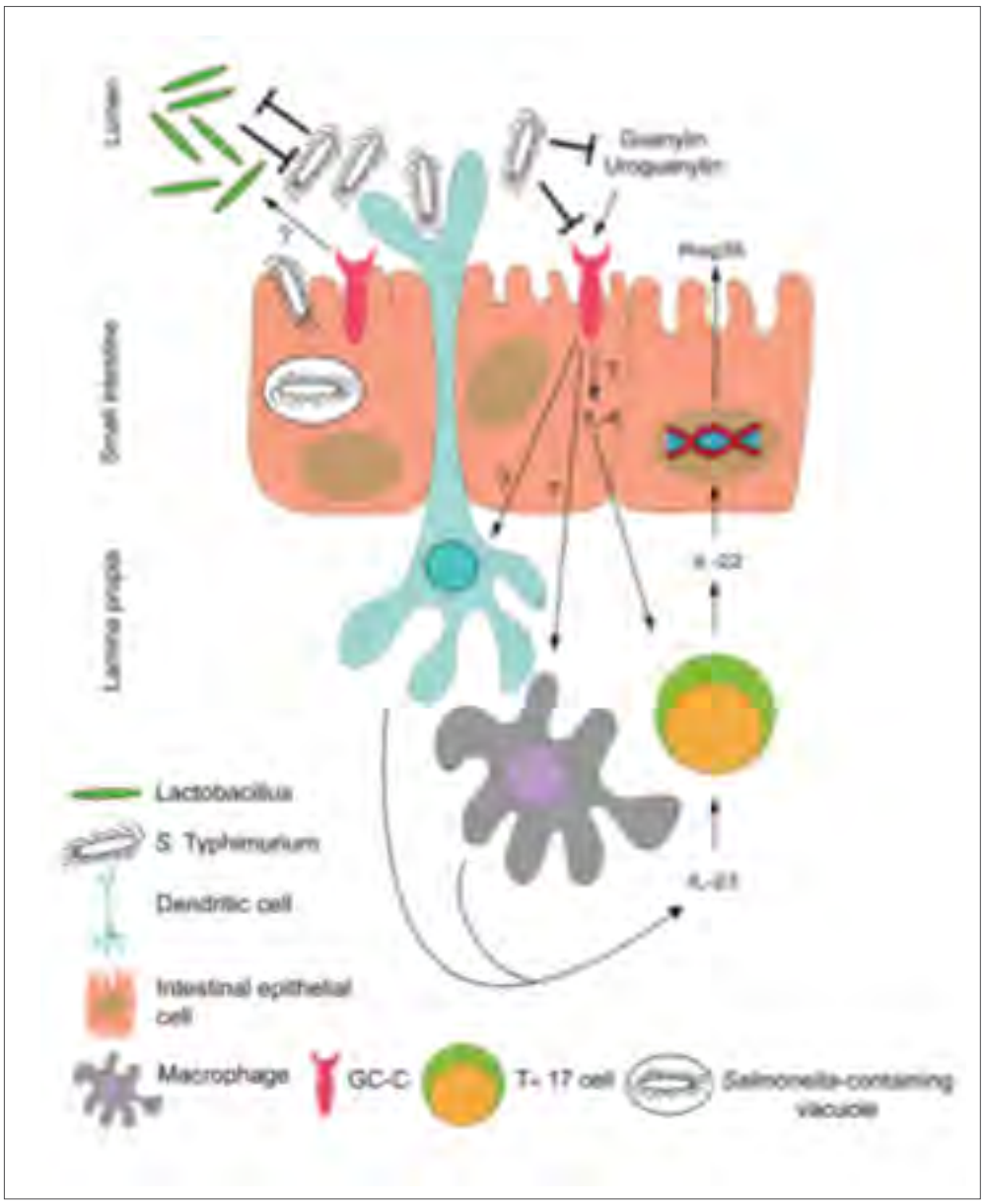
The results showed that predation risk was equivalent for signaling males and responding females, challenging the long-held idea that signaling is riskier than searching, and thereby that males are the sex taking the higher risk in the context of communication and mate-finding. This finding has implications for our understanding of sexual selection in the context of communication. In addition, the overall level of predation risk was low for both males and females, also questioning the role of predation as a major force shaping the evolution of signaling behaviour.

Torsekar, V. R., Isvaran, K. & Balakrishnan, R. (2019) *Evolutionary Ecology 33:* 329-343. https://doi.org/10.1007/s10682-019-09982-3

Maria Thaker (CES)

Bright and conspicuous colours are used by many animals to attract mates and to communicate with each other. However, these conspicuous colours can also attract the attention of unintended audience, such as predators. Therefore, expressing bright colours may be risky to animals. In the Indian rock agama lizard (Psammophilus dorsalis), males dramatically change their colours and display different colour combinations when they are fighting with other males, and when they are courting females. Though visual modelling, we discover that the courtship colours of males are highly conspicuous not only to lizards, but also their predators such as birds, dogs and snakes. On the other hand, colours displayed by males when fighting and the colours of females are comparatively less conspicuous. We then placed lizard-shaped models in the wild and found that the courtship-coloured male models were attacked more than models of any other colour combination. Together, these results indicate that the courtship colour combination of males is risky to them. Therefore, colour change in these animals may have evolved as an elegant solution for the males to gain the advantages of bright colours for communication but still reduce the risk of being noticed by predators at other times.

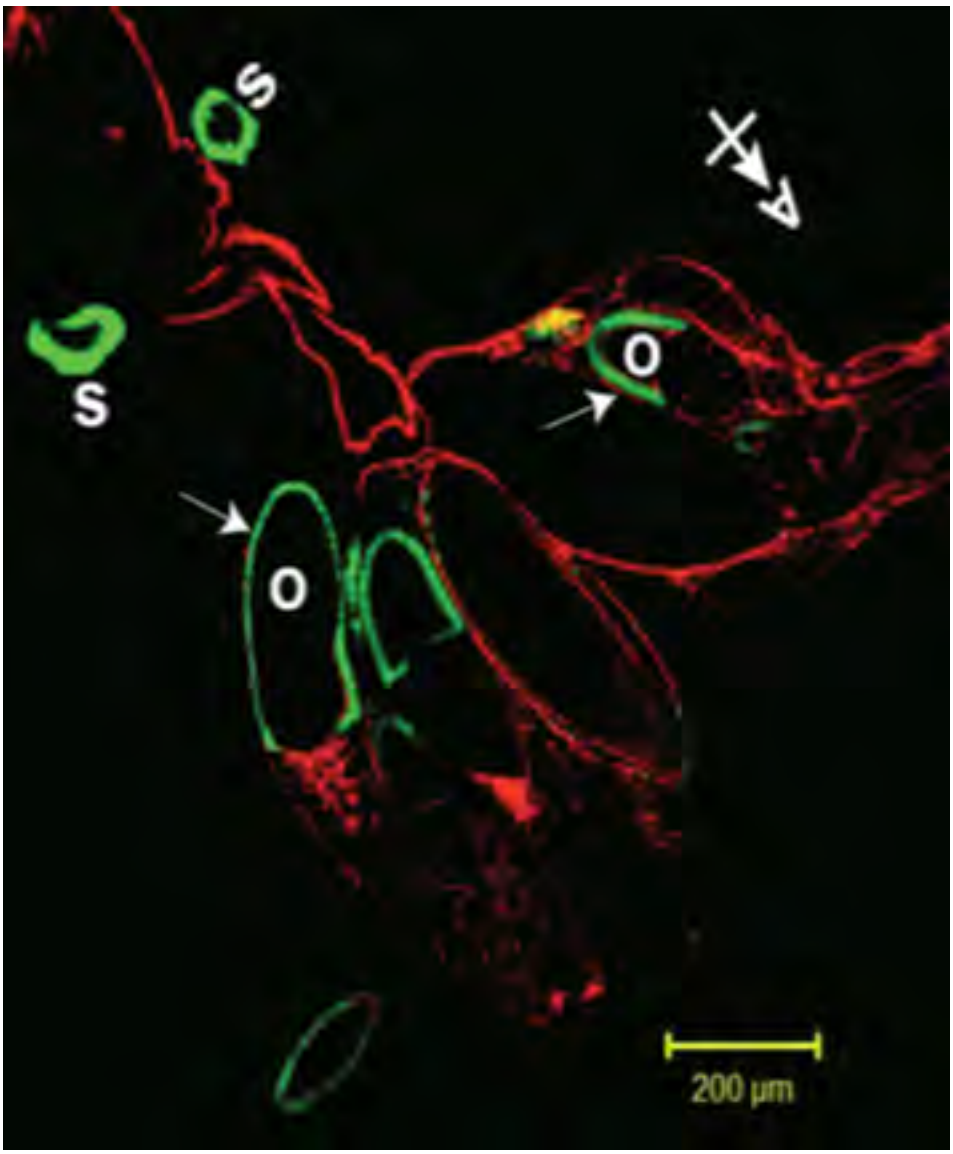
Amdekar, M. S., & Thaker, M. (2019). *Risk of social colours in an agamid lizard: implications for the evolution of dynamic signals. Biology Letters, 15(5), 20190207.*



Sandhya Visweswaraiah (MRDG)

The group of Prof. Sandhya S. Visweswariah is interested in understanding the role of receptor guanylyl cyclase C in the gut of mammals. Using knock out mice and working in collaboration with Prof. Dipankar Nandi and his group from the Department of Biochemistry, it appears that this receptor is involved in providing protection from infection by the gut pathogen, Salmonella Typhimurium. Mechanisms underlying this protection include a poorer immune response generated in the intestine as a result of lower cytokine production by immune cells in the gut.

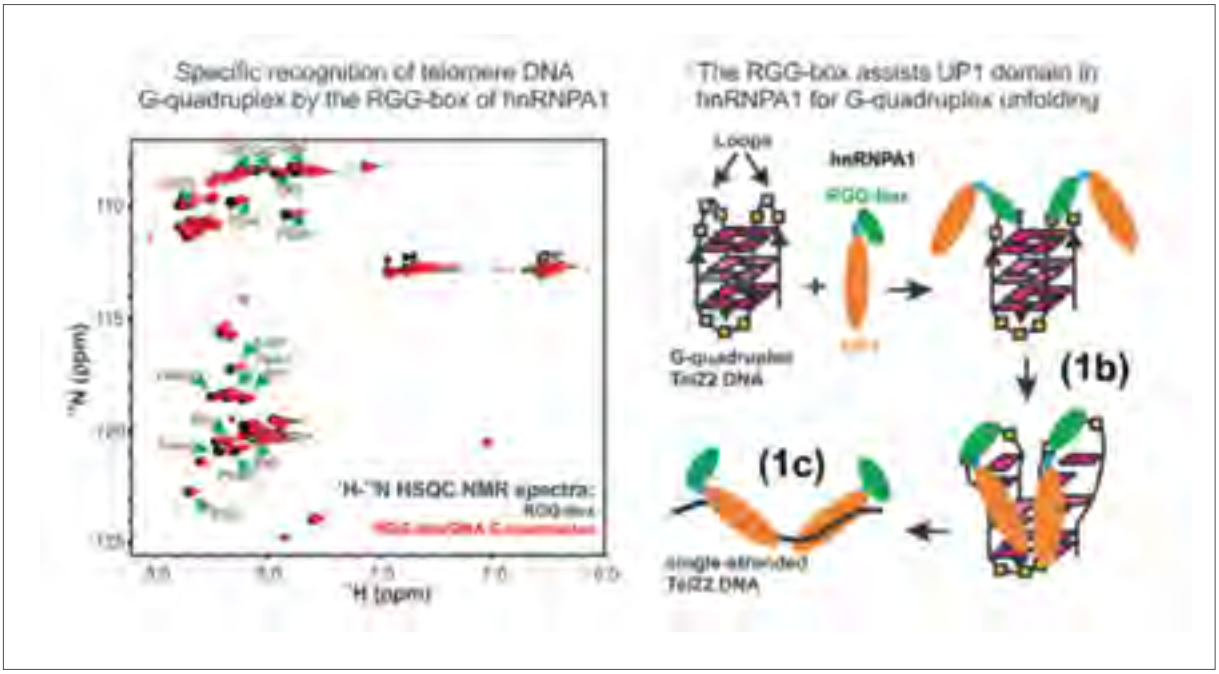
Majumdar, S., Mishra, V., Nandi, S., Abdullah, M., Barman, A., Raghavan, A., Nandi, D. and Visweswariah, S.S. (2018) Absence of receptor guanylyl cyclase C enhances ileal damage and reduces cytokine and antimicrobial peptide production during oral Salmonella Typhimurium infection. *Infect. Immun. 86: 799-817*



Upendra Nongthomba (MRDG)

Bx function in follicle cells is important for normal egg development and fecundity in Drosophila. Two enhancer trap Gal4 lines, c323a and c204, which were reported to be expressed in follicle cells were selected to knock down Bx in follicle cells. These drivers show GFP expression in follicle cells (white arrow in A) surrounding oocyte (O), and also in the cells of spermathecae (S). Beadex is essential for egg development and fertility.

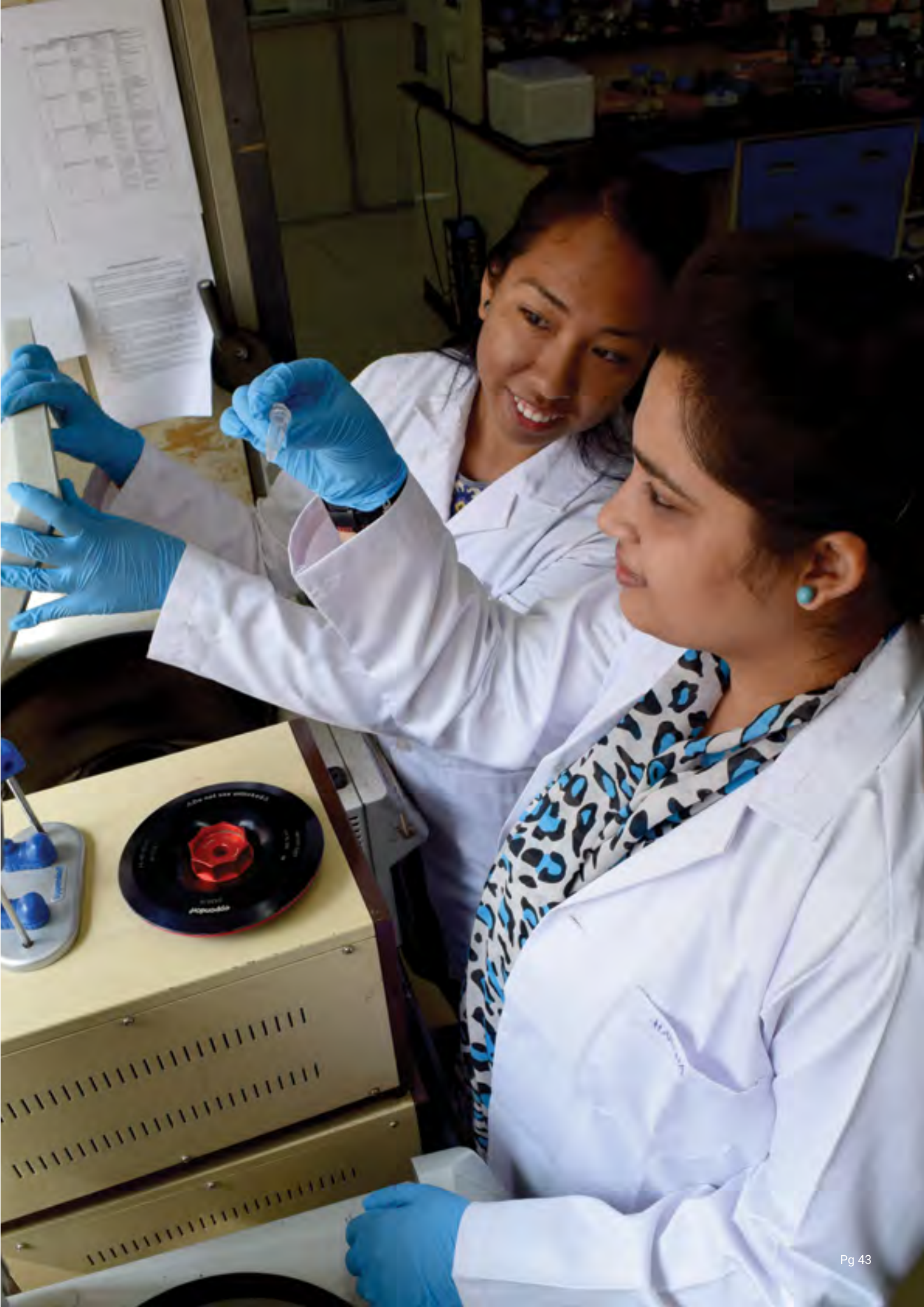
Subhash Kairamkonda, Upendra Nongthomba, Beadex, a Drosophila LIM domain only protein, function in follicle cells is essential for egg development and fertility, *Experimental Cell Research 367* (2018) 97–103



Mahavir Singh (MBU)

Maintenance of telomere DNA has implications in both cellular aging and cancer. Controlled remodeling of highly ordered and organized telomere nucleoprotein structure is critical during DNA replication. Several proteins (e.g. hnRNPA1, TRF2, RTEL1 etc.) and a non-coding RNA called TERRA (telomere repeat containing non-coding RNA) play important roles in telomere DNA remodeling, however the precise mechanism of the process is not well understood. Mahavir Singh's lab focuses on understanding the interplay of various proteins, telomere DNA and TERRA RNA that is critical for coordinated telomere DNA remodeling. Recently, Mahavir Singh's lab has shown that an intrinsically disordered, arginine and glycine rich domain (RGG-box) of hnRNPA1 specifically recognizes the higher order telomere DNA and TERRA RNA G-quadruplex structures but not the single-stranded DNA or RNA. This helps adjacent the UP1 domain in hnRNPA1 to unfold G-quadruplex structures more efficiently. The lab is currently pursuing the understanding of role of arginine methylation the structure of the RGG-box and G-quadruplex binding.

Ghosh, M. and Singh, M. "RGG-box in hnRNPA1 specifically recognizes the telomere G-quadruplex DNA and enhances the G-quadruplex unfolding ability of UP1 domain". *Nucleic Acids Research.* (2018). 46(19):10246-10261. doi: 10.1093/nar/gky854.



3.1.1 Biochemistry

CHAIRPERSON
C JAYABASKARAN

The Department of Biochemistry started in 1921. It was recognized as Centre of Advanced study by UGC in 1965. There are 12 members of the faculty, 1 Honorary Professor, 3 Emeritus Scientists, 82 PhD students, 30 PDF/ DST Young Scientists/UGC Kothari Fellows, administrative staff, 4 permanent helpers and 40 temporary staff in the department.

Current Research

PROTEIN, NATURAL PRODUCTS AND METABOLIC ENGINEERING

In the past year, there has been intensive research on anticancer compounds of fungal isolates from marine algae collected from Kerala, Tamil Nadu and Goa. A total of 101 fungal strains were isolated which were cultivated for 21 to 28 days in PDB medium. MTT assay against different human cancer cell lines showed that 11 fungal extracts showed significant cytotoxicity. The ethyl acetate extract of Chaetomium globosum isolated algae collected from Goa coastal region displayed high cytotoxicity against the MCF-7 cell line (IC50 = 7.2 µg/ml) and this was then subjected to GC-MS analysis. The anticancer compound was purified by preparative TLC on silica gel and the UV and FTIR spectra of the purified compound matched with standard chrysin. The results indicated that chrysin induced apoptosis in MCF-7 cells via ROS mediated mitochondrial dependent pathway. In vivo anticancer experiments are in progress.

FACT FILE

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IN NUMBERS

12 Academic Staff
67 PhD students
15 Int PhD Students
100 Publications
2 Int PhD Conferments
23 PhD Conferments

Core Research

Proteins, Natural products and metabolic engineering; DNA repair, RNA transactions and genomic stability; Biology of chaperones; Immunobiology.

One of the key global health care concerns is the emergence of antibiotic resistance in bacteria. To address the problem of drug resistance, a long short-term memory (LSTM) language model was used to understand the underlying grammar in known antimicrobial peptide sequences. Two most effective antimicrobial peptides displayed activity against multidrug-resistant clinical isolates of a variety of bacteria by selectively interacting with and disrupting bacterial cell membranes. Several chemicals present in the environment, e.g. herbicides, phenolics etc, are capable of inducing higher incidences of antibiotic resistance. The effects of sodium salicylate on E. coli strain MG1655 and its isogenic mutant strain lacking Lon protease were previously studied. MarA, a key transcription factor is a known substrate of Lon protease; not surprisingly, the strain lacking Lon is also more resistant to antibiotics due to higher amounts of endogenous MarA. Four commonly used non-steroidal anti-inflammatory drugs (NSAIDs), Sodium salicylate, Acetyl salicyclic acid, Acetaminophen and Ibuprofen, identified to induce high amounts of phenotypic antibiotic resistance. In addition, the roles of marA and acrB in the induction of antibiotic resistance by the four NSAIDs were dissected Mxr1p, a zinc finger protein was identified as a key regulator of ethanol metabolism of the methylotrophic yeast, Pichia pastoris. Rtg1p, a basic/helix-loop-helix- leucine zipper protein was shown to be a novel cytosolic, post-transcriptional regulator of multiple metabolic pathways of P. pastoris. Apolipoprotein L9, a phosphatidylethanolamine binding mouse protein was shown to interact preferentially with lipidated form of Lc3/Gabarap and localize to mitochondria and lysosomes in autophagy arrested cells.

In addition, a massive resource of three-dimensional definitions of small molecule ligand binding pockets called the augmented pocketome of PDB was employed. Putative ligand associations are made for more than a million sites through novel computational analysis. This analysis provides a basis to systematically probe allostery in proteins and explore them for drug discovery.

DNA REPAIR, RNA TRANSACTIONS AND GENOMIC STABILITY

The bacterium Helicobacter pylori is one of the most common infectious agents found in the human stomach. H. pylori has an unusually large number of DNA methyltransferases (MTases), prompting speculation that they may be involved in the cancerization of epithelial cells. To better understand the role of M.HpyAXVII in H. pylori biology, Prof. DN Rao's laboratory cloned and over-expressed the hp1369-70 fusion construct in Escherichia coli BL21 (DE3) cells. Results from size-exclusion chromatography and multi-angle light scattering analyses suggested that M.HpyAXVII exists as a dimer in solution.

Kinetic studies including product and substrate inhibition analyses, initial velocity dependence between substrates, and isotope partitioning suggested that M.HpyAXVII catalyzes DNA methylation in an ordered BiBi mechanism in which the S-adenosylmethionine (AdoMet) binding precedes DNA binding and AdoMet's methyl group is then transferred to an adenine within the DNA recognition sequence. Altering the highly conserved catalytic motif (DPPY/F) as well as AdoMet binding motif (FXGXG) by site directed mutagenesis abolished the catalytic activity of M.HpyAXVII. These results provide insights into the enzyme kinetic mechanism of M.HpyAXVII. It is possible that AdoMet binding conformationally "primes" the enzyme for DNA binding.

Cyclic di-GMP and cyclic di-AMP are second messengers produced by a wide variety of bacteria. Cyclic di-AMP has been shown to negatively regulate the expression of Mycobacterium smegmatis recA and attenuate DNA strand exchange through binding to the C-terminal motif of mycobacterial RecA proteins. Anionic phospholipids of the bacterial plasma membrane have been shown to act as a scaffold for RecA storage and regulate its recombinational DNA repair and the SOS functions. Phamacologically relevant small ligands were synthesized and shown to bind to the DNA secondary structural motifs embedded in the promoter sequences of the human acetyl-CoA carboxylase gene and oncogenes and regulate their expression.

Studies carried out in the department have shown that efficient DNA double strand break repair takes place in diffuse large B cell lymphoma. They have identified novel miRNA that could modulate RAG1 expression in B cell development stages. Their results reveal that formation of G-quadruplex structures can impart differential radiosensitivity to human genome and this can be modulated in a cell cycle dependent manner. Preliminary studies suggests that Caffeine could act as a radioprotector. In addition, they have also conducted investigation to establish DNA double strand break repair mechanism in mammalian mitochondria.

Investigation of the role of cohesin in gene expression is being investigated by researchers. Cohesin is an important determinant of chromosome architecture due to its DNA binding and tethering ability. They investigated the role of cohesin near telomeres of budding yeast chromosomes. In budding yeast, transcription within 20 kb of telomeres is repressed, in part by the histone-modifying silent information regulator (SIR) complex. However, extensive subtelomeric repressed domains lie outside the SIR-binding region, the mechanism of silencing within these regions remains unexplored. They reported a role for cohesin in subtelomeric silencing that extends even beyond the zone of SIR binding. Clusters of subtelomeric genes were preferentially derepressed in a cohesin mutant, whereas SIR binding was unaltered. Genetic interaction analysis indicated that cohesin operates independent of the SIR-mediated pathway for telomeric silencing. They found that compaction of subtelomeric domains and tethering to the nuclear envelope were impaired in cohesin mutant cells. Their findings provide evidence for a unique SIR-independent mechanism of subtelomeric repression mediated by cohesin. In this period they also continued studies on phenotypic defects arising from cohesin mutations in yeast cells, and extended ongoing work with other Smc protein complexes.

Another strand of research in teh department demonstrated that a subset of RAD51 paralogs, XRCC2/FANCU and its binding partner RAD51D, restrain active DNA synthesis during dNTP alterations. The absence of XRCC2 was found to be associated with increased levels of RRM2, the regulatory subunit of RNR. This in turn resulted in elevated nucleotide pools, unrestrained fork progression and accumulation of DNA

damage during dNTP alterations. Also, it was shown that clinically relevant mutations of XRCC2 identified in Fanconi anemia (FA) and breast cancer are defective in fork slowdown. They also demonstrated that two RAD51 paralog complexes (DX2 and CX3) are differentially regulated by ATR signaling, through phosphorylation of XRCC2 and XRCC3. XRCC2 was shown to be phosphorylated at Ser247 by ATR kinase. However, in contrast to the DSB-specific activation of XRCC3, phosphorylation of XRCC2 was specifically induced by replication stress. Functionally, this activation of XRCC2 was found to be crucial for restraining fork progression, thus preventing the generation of post-replicative gaps, fork degradation, and genome wide DSBs. Notably, cells defective in XRCC2 phosphorylation were found to undergo early activation of XRCC3 during replication stress, which allows HR-mediated repair of accumulated DNA damage and cell survival.

The roles of self-association of RGG-motif proteins in translation control were investigated and it was observed that self-association likely affects the activity of RGG-motif repressor proteins. In addition, they are also addressing the role of arginine methylation of Sbp1 in regulating its activity.

One of the primary interest of faculty in the department is to understand the regulation of mammalian translation. They have identified 4 mammalian genes (AGO1, MTCH2, NNAT and FEM1B) whose mRNAs undergo translational read through, a process where protein translation continues beyond the stop codon. This generates longer proteins with different functions. Studies on AGO1 translational read through have revealed a global microRNA sponge. It is generally believed that human mature erythrocytes don't perform protein translation. However, it is not clear how they manage to survive 120 days in circulation without fresh protein synthesis. Their laboratory has demonstrated that mature erythrocytes can indeed translate at low level. At present, the regulation of translation in different physiological stresses such as fever and hypoxia is being investigated.

BIOLOGY OF CHAPERONES

Over the last two decades, department has contributed to better understanding of the roles of heat shock protein 90 (Hsp90) in the pathogenesis of diseases caused by a number of organisms, e.g. Plasmodium, Giardia, Trichomonas, Entamoeba, Trypanosoma, Babesia, Theileria etc. Using a variety of protozoan parasites of human and veterinary importance as model systems, the potent role of Hsp90 inhibitors in specifically targeting their virulence and growth has been shown. The current focus is on understanding the mechanistic aspects of the post-transcriptional repair of Hsp90 pre-mRNAs to generate the mature message in G. lamblia with the aim to identify unique molecular components which may be facilitating this process. In addition, a new area of interdisciplinary research in understanding flagellar motility in G. lamblia has been initiated. Also, unique metabolites released from Plasmodium infected RBCs have been identified and their potential as clinical biomarkers is being evaluated. Finally, the pathophysiology and potential alternate modes of transmission of sexually transmitted parasite T. vaginalis is being understood.

Recent studies have focused on the elucidation of the organization of pre-sequence translocase and mechanisms of protein translocation across the mitochondria. Their laboratory has uncovered on the roles of maintenance of mitochondrial quality control during human health. In addition, their laboratory has uncovered Reactive Oxygen Signalling (ROS) networks in eukaryotes. The design, synthesis and characterization of ROS-scavenging Nano-enzymes and drug delivery vehicles for therapeutic applications has been evaluated.

IMMUNOBIOLOGY

Glycodelin is an immunomodulator and known to be important for the maintenance of pregnancy in humans. The immunosuppressive effects of Glycodelin were addressed in an allograft nude mouse model. Glycodelin treatment reduced the numbers of activated T cells and expression of pro-inflamamtory cytokines, therby promoting increased graft survival. Sepsis is a complex syndrome caused due to excessive host-mediated inflammatory responses during infections and is the leading cause of death in intensive care units. In our laboratory, we have standardized a Salmonella Typhimurium (S. Typhimurium) infection-induced peritonitis model of sepsis in mice. We have shown that NOS2-derived NO is a critical mediator of inflammatory responses, including cytokine burst and neutrophil recruitment to the peritoneal cavity, which most likely contributes to the protection from sepsis-induced organ damage and survival of mice. In addition, the effect of genetic heterogeneity on the immune response of an individual to the influenza virus through a new mathematical model connecting genomic information to the disease susceptibility phenotype was investigated. It was shown that larger the genetic diversity, higher is the protection against the spread of influenza in a population and protection against epidemic breakoutsand in some cases sequence motifs. Using this knowledge, a genome-wide scan was carried out in M. tuberculosis, from which more than a thousand ATP binding proteins were identified. Several of these were validated experimentally using a chemical proteomics approach in a collaborator's laboratory.

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3.1.2

Central Animal Facility

CHAIRPERSON
K SOMASUNDARAM

The Central Animal Facility (CAF) breeds, maintains and supplies pure and inbred strains of experimental animals for biomedical research activities at the Institute. The animal species includes New Zealand white rabbits, Wistar rats, Sprague Dawley rats and several strains of mice (Swiss albino, BALB/c, FVB/N, CD1, C57BL/6, C3HeJ) including knockout mice (IFNg, KO, INoS KO, etc.).

Faculty & Staff

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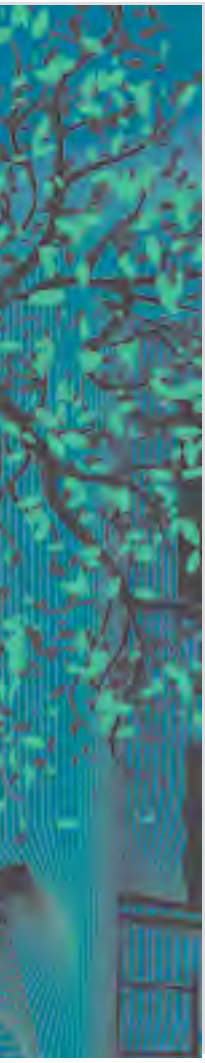
Core Research

The experimental animals are provided to several investigators who are using animals for research activities in the Division of Biological Sciences (Biochemistry, Microbiology and Cell Biology, Molecular Reproduction, Development and Genetics, Molecular Biophysics Unit, Centre for Neuro Sciences) and other Departments such as Department of Mechanical Engineering, Materials Research Centre, Materials Engineering, Inorganic and Physical Chemistry and Centre for Nanoscience and Engineering.

3.1.3

Centre for Ecological Sciences

CHAIRPERSON
ROHINI BALAKRISHNAN



Centre for Ecological Sciences (CES) has continued to do cutting-edge research in diverse areas of ecology, behaviour and evolutionary biology. We study a range of systems from insects, herpetofauna and birds to the largest land mammals, the Asian elephant, including climate change. We employ diverse tools from molecular ecology to mathematical modelling of ecosystems.

Current Research

CES has continued to conduct cutting-edge research in the field of ecology and evolution. Many ecosystems exhibit tipping points, wherein systems abruptly switch from one stable state to another. New methods have been developed to detect signs of such impending tipping points. Long-term monitoring of forests at Mudumalai reserve forest continue to provide deep insights into the role of climate, fire, invasive species and mammalian herbivory on forest dynamics, carbon stock changes, and diversity changes. Anthropogenic alterations have many unintended effects on ecosystems. A study of elephants that raid cultivated crops outside protected forested areas show that they are in better body condition than those in protected areas as they reap the benefit of higher diet quality and consequently suffer lower stress. Long-term space-use and population patterns of the endemic and threatened blackbuck antelope in a typical fragmented grassland landscape

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10 Academic Staff
2 Scientific Staff
55 PhD students
5 Int PhD Students
60 Publications
4 PhD student Conferments
1 Honorary Professor

Core Research

The Centre carries out research in Animal Behaviour, Behavioural Ecology, Bioacoustics, Biogeography, Chemical Ecology, Climate Change, Community Ecology, Ecosystem Ecology, Evolution, Forest and Grassland Dynamics, Marine and Coastal Ecology, Mathematical Ecology and Modelling, Molecular Ecology, Movement Ecology, Nutrient Cycling, Phylogenetics, Phylogeography, Plant–Animal Interactions, Predator–Prey Interactions, Sensory Ecology, Stress Physiology.

show that these animals appear to respond to anthropogenic risk factors but these social and space-use responses may not be sufficient since the population continues to decline. Lizards seem to cope effectively in urban areas by adjusting their immune responses, altering their social behaviour and modulating their hormone levels. A multi-year study of the ecological effects of green energy shows that wind-farms have the same effects on ecosystems as top predators. The study was carried out by altering prey density, as well as their morphology, behaviour and physiology. In the field of animal behaviour, a new conceptual modelling framework was developed to understand social partner choice. Positive interspecific interactions strongly structure biological communities, particularly mixed-species foraging groups in bird and marine reef fish. The foraging behaviour of the lesser false vampire bat in fragmented habitats was studied, and field experiments on bat foraging decisions were carried out. Multimodal courtship behaviours and the effects of nutrition on animal communication were better understood in katydids and crickets. In most primitively eusocial wasps, the emergence of division of labour among the nest foundresses was experimentally unravelled. Ongoing long-term study that tracks individuals over their lifetime show how space use and territoriality patterns of rock agamas shift over their lifespan. Through lab and field-based experiments on Aedes mosquitoes, evidence was found that adult females make complex decisions about where to lay their eggs depending on predators. Study of diverse systems ranging from figs

and fig wasps to ant-plants, ants, nematodes, crab and ant-mimicking spiders, and nocturnal bees have shown how vision and/or chemoreception interact with physiology to impact the ecology and evolution of multitrophic interactions. New collaborations with civil engineers enable an integrated understanding of termite mound construction. From work in the fields of molecular systematics, species delimitation and biogeography, increasing evidence now shows that the Indian dry zone harbours higher biodiversity than expected. Use of new community phylogenetic approaches allow for the better understanding of the biogeographical history of India, and these include determining drivers of distribution, and patterns of diversity across a range of taxa including amphibians, reptiles, birds and plants in terrestrial habitats, and inter-tidal fauna along the coast. These studies also reveal both the adaptive and non-adaptive factors that have led to the diversification of lineages and the consequences for endemism and diversity. Among non-human primates, primate-specific pathogens were found to have far wider distribution in their host than previously reported. The evolutionary origin and diversification of cnidocytes (the first venom delivery apparatus in the animal kingdom) was studied, as was the transcriptomic, proteomic, and clinical investigation of the lesser banded hornet, and the spatiotemporal shifts in venom profiles of the starlet sea anemone.

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3.1.4 Centre for Infectious Disease Research

CONVENER
DIPANKAR NANDI

The main goal of Centre for Infectious Disease Research (CIDR) is to integrate research activities in the area of infectious diseases with interactions and collaborations and provide avenues for multidisciplinary activities with translational outcomes. CIDR hosts fellows with a fully equipped and functional laboratory and a state of the art BSL-3 facility to perform their research. Research activities in CIDR are spearheaded by faculty or scientists with senior level fellowships, e.g., DBT-Wellcome, Ramalingaswami, Ramanujan, etc., through which competitive grants have been procured for studies related to infectious disease research.

Current Research

An important area of study is the understanding of the mechanisms by which *Mycobacterium tuberculosis* evades immunity. A comparative analysis of some 5000 whole genome sequences of *Mycobacterium tuberculosis* isolates curated from India identified precise amino acids that are recognized by CD4+ T cells, resulting in the bacterium escaping immune recognition. These studies have significant potential impact on TB vaccine design. In addition, key markers have been identified in chronically activated CD4+ T cells during *Mycobacterium tuberculosis* infection. The second area of investigation is in protecting *Mycobacterium tuberculosis* from oxidative stress by

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5 Publications

condensing the DNA. Modulating the levels of WHiB4, an intracellular redox sensor, attenuated the ability of Mycobacterium tuberculosis to survive inside macrophages and in an animal models of experimental tuberculosis. This study points to the critical role of redox in the biology of Mycobacterium tuberculosis. This study points to the critical roles of redox in lowering drug resistance in Mycobacterium tuberculosis.

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Shashank Tripathi | PhD (Delhi), Assistant Professor

Core Research

On-going work is directed towards understanding and targeting drug tolerance in Mycobacterium tuberculosis and application of network biology to identify new drug combinations. Another area of research is focused on the principal immune mechanisms that contribute to reactivation of tuberculosis in the context of HIV infection. A new area of research in virus-host interactions has been added.

3.1.5 Centre For Neuroscience

CHAIRPERSON
ADITYA MURTHY

Understanding the structure, function and development of the brain in health and disease requires studying the brain across different levels of organization using molecular, cellular, systems, cognitive, and computational approaches. These are the main focus areas of the Centre for Neuroscience (CNS). It recruits faculty across wide-ranging disciplines to establish a strong program in basic neuroscience and builds links to existing expertise in IISc as well as with clinical centres to develop translational research.

Current Research

CNS is a multidisciplinary department with the common goal of understanding brain functions in health and diseases. The department currently has nine faculty members, one Wellcome-DBT India Alliance Intermediate Fellow, two Ramalingaswami Fellows and one INSPIRE faculty fellow.

In the context of motor control, it is commonly thought that visuomotor adaptation is mediated by the cerebellum while reinforcement learning is mediated by the basal ganglia. In contrast to this strict dichotomy, we demonstrate a role for the basal ganglia in visuomotor adaptation in patients with Parkinson's disease (PD) by comparing the degree of motor learning in the presence and absence of dopamine medication, in the

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9 Academic Staff
44 PhD students
22 Publications
3 Int PhD Students
1 MS (Science)
8 PhD Conferments

presence and absence of subthalamic deep brain stimulation. We also report that reinforcement is an essential component of visuomotor adaptation by demonstrating the lack of motor learning in patients with PD during the ON-dopamine state relative to the OFF-dopamine state in the absence of a reinforcement signal. Our results suggest that the basal ganglia modulate the gain of visuomotor adaptation based on the reinforcement received at the end of the trial.

In the context of sensory information processing, we have obtained several insights into how the brain performs object recognition: (1) Symmetric objects are special in perception despite being governed by generic computations in single neurons; (2) There is a temporal hierarchy of object invariances in single IT neurons whereby size and position invariance develop earliest, followed by viewpoint invariance; (3) Humans use targets, non-targets and scene context to guide object detection in natural scenes; (4) Human scene priors can be used to improve computer vision algorithms and (5) Fine-grained face classification reveals systematic differences between humans and machines.

In the context of attentional processing, we have developed a model for the analysis of behavior that decouples perceptual from decisional mechanisms of attention. We are currently using this model in conjunction with neuroimaging (functional MRI, diffusion MRI, EEG) and neurostimulation (TMS, tACS) techniques to understand the neural correlates of these attention components. We are also developing machine learning models to understand the neural bases of attention deficits in neurodegenerative disorders like Alzheimer's dementia. In the context of neural oscillations, it was found that large visual stimuli generated two gamma oscillations in the visual cortex of monkeys and humans, and these gamma oscillations were highly tuned to reddish colours.

In the context of emotion and motivation, the laboratory focuses on understanding how emotional and motivational factors influence perception and cognition at multiple levels: brain, behaviour and physiology. To probe these interactions, we plan to use behavioural paradigms in combination with high-resolution functional MRI and physiological skin conductance recording.

In the area of Molecular, Cellular and Developmental Neuroscience, the laboratory studied the molecular mechanisms regulating reactive astrogliosis in the mouse brain. It was found that the transcription factor, SRF, may regulate generation of protective reactive astrogliosis. Lipid metabolism has been shown to hold the key to major fundamental processes including neuronal differentiation. Work on delineating the role played by astrocytes in modulating mood-related behaviour is also being carried out. Molecular, behavioural and histological techniques and transgenic mouse models are used to understand the signalling pathways responsible for astrocyte-neuron communication and subsequent modulation of behaviour. Another aspect of work focuses on unravelling the molecular mechanisms underlying neuronal polarity and how it contributes to neuronal differentiation and development. Towards deeper understanding of the molecular architecture of the synapse, the functional units of neuronal communication, the Nano Organization laboratory utilizes ultra-high resolution imaging approaches to investigate assembly and regulation of synaptic transmission machinery. Novel imaging paradigms like nanoscale imaging combined with optical and chemical stimulations is used to observe real-time organization of a chemical synapse.

In the area of disorders of the nervous system, the research is focused on elucidating the early pathogenic mechanisms leading to Alzheimer's disease (AD), a progressive neurodegenerative disorder often seen in the elderly and manifests clinically as memory loss and cognitive impairment.

Core Research

Motor Control, Neurobiology of Disease, Neural mechanisms of Selective Attention, Neuronal differentiation and development, Astrocyte biology, Neurobiology of Learning and Memory, Molecular organization of synapse, Neuronal receptor biology, Visual perception and recognition, Neurobiology of Stress and Depression, Interactions between Emotion Motivation and Cognition

It has been shown that synaptic dysfunction including loss of activity-dependent protein translation and cytoskeletal F-actin occurs in AD long before the manifestation of disease pathology. Loss of synaptosomal F-actin is associated with impaired recall upon fear conditioning and can be reversed by actin polymerizing agents. Studies are being carried out on how ubiquitination and deubiquitination of metabolic G-protein coupled receptors and their adaptor protein, β-arrestin2 contribute to the agonist induced synaptic functions in cellular models and mouse models of Alzheimer's disease. These findings may provide new avenues for therapeutic intervention and prevention of AD progression.

In the context of learning and memory, declarative memories represent our life events enables us to retrieve, recollect and relive these very moments. Research in our laboratory has focused on asking how memories of related memories (related in content/character) are organized and if such an organization of storage can modulate new learning. In doing so, we found that such organized storage of memories can bias how the new information in encoded in the brain as well as play a critical role in determining the animal's behavior in a novel scenario. In order to perform these studies, we had to develop both behavioral and optical methodologies to probe these processes at the scale of neurons and synapses. In a related but distinct area of research, the Centre is studying how hippocampal network creates a coherent representation of events within their spatial context. Specifically, the studies focus on the interplay between sensory derived spatial and non-spatial information brought in by the lateral entorhinal cortex (LEC) and the internally generated, path-integration-based spatial representation in the medial entorhinal cortex (MEC).

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3.1.6 Molecular Biophysics Unit

CHAIRPERSON
N SRINIVASAN

The Molecular Biophysics Unit (MBU) is currently engaged in frontline research in contemporary areas of Biophysics, Structural Biology and Physiology. Research activities in the Unit focus on the structure, conformation and interactions of biomolecules and their functions, with the main objective of explaining biological activity in molecular terms.

Current Research

The projects handled in the unit include biophysical, structural, and computational studies of biomolecules with the aim to understand the biological phenomenon at the molecular level.

Tools to characterize the complex phase organization in membrane using ideas from non-affine deformation and topological rearrangements in lipids were developed. Membrane heterogeneity was correlated in terms of packing defects and showed the implications in peripheral protein membrane association. Recently, molecular-level insight, into how the bulging of membrane at the EHD1 scaffold leads to fission, was revealed.

Neurotransmitter transporters are vital for the control of neural communication and serve as targets for anti-depressants, addictive drugs and drugs to treat chronic pain. In this context, recently the X-ray structure, of a neurotransmitter transporter in complex with

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IN NUMBERS

13 Academic Staff
72 PhD Students
09 Int PhD Students
80 Publications
11 PhD Conferments
2 Int. PhD Conferments

medication popularly used to treat neuropathic pain and fibromyalgia, was elucidated. Antimicrobial efflux is a mechanism leading to multi-drug resistant pathogens. Recent work on a proton-driven antibacterial efflux transporter QacA, has provided insights into the promiscuous substrate recognition observed in efflux transporters.

Two new research areas on understanding the molecular mechanism behind the mammalian circadian rhythms and metamorphic proteins have commenced.

Research is underway towards characterization of large multi-protein complexes that mediate intra-cellular RNA levels in Staphylococci. Also, the molecular mechanism(s) that link environmental conditions with the transcription mechanism in Mycobacteria will be understood. A recent prominent finding was that RNA degradation mechanisms are directly regulated by other information pathways in bacteria.

Incorporation of thioamide into the peptide backbone of a cyclic peptide results in enhanced local rigidity. The increased local rigidity translates into global rigidity of the peptide backbone. This increased rigidity results into extremely well-defined conformation of the peptide that could be used to pre-design the orientation of pharmacophores for target recognition. This was utilized to develop cyclic peptides that have very high affinity to integrins in-cellulo. The structural rigidity also results into increased metabolic stability of the peptides in human serum ex vivo.

Maintenance of telomere DNA has implications in cellular aging and cancer. Several proteins and telomere repeat containing non-coding RNA, TERRA play roles in this process. Recently, it was shown that the RGG-box in hnRNPA1 specifically recognizes the telomere DNA and RNA G-quadruplex structures and helps adjacent UP1 domain to unfold DNA G-quadruple efficiently. The structural and bioinformatics analysis revealed that the SWI/SNF protein, BAF250a contains a C-terminal ARM-repeat domain along with the N-terminal ARID domain, implicating these domains in function and assembly of the BAF remodeling complex.

The derivatives of the HIV-1 envelope surface protein were designed and it was demonstrated that these elicited broadly neutralizing sera in guinea pigs and broadly protective antibodies in rabbits and macaques. In other studies, a gp120 derived fragment was expressed on the surface of proteinaceous nanoparticles and was explored different immunogen combinations to elicit neutralizing antibodies and used diverse protein engineering strategies to design and test derivatives of the outer domain of HIV-1 gp120 as potential immunogens. immunogens derived from the conserved stem of the influenza virus surface protein, hemagglutinin were designed. Using the methodology of yeast surface display, the immunogen libraries were screened to isolate a derivative that was thermally stabilized over previous design by about 24°C. This will be tested in future vaccine studies.

Models of medial entorhinal cortical stellate neurons exhibited degeneracy, whereby models with disparate channel combinations were endowed with similar physiological characteristics. The generation of dendritic spikes and the consequent sharp tuning of neuronal responses are together attainable even when iso-feature synapses are randomly dispersed across the dendritic arbor. Targeted synaptic plasticity converts silent cells to place cells for specific place fields in models with disparate channel combinations that receive dispersed synaptic inputs from multiple locations. The research demonstrated a unique convergence of cellular- and network-scale degeneracy in the emergence of channel decorrelation in the dentate gyrus, whereby disparate forms of local and afferent heterogeneities could synergistically drive input discriminability. It unveiled a pivotal role for dendritic voltage-gated ion channels in actively amplifying

Core Research

Protein folding and dynamics, protein-protein interactions, protein-DNA/RNA interactions, lectin-carbohydrate interactions, peptide synthesis and design, X-ray crystallography of proteins and viruses, solution NMR studies of proteins and nucleic acids, CryoEM studies of biomolecular complexes, computational modelling and dynamics of biological molecules, theoretical studies on the conformation of peptides, proteins, and nucleic acids, unusual nucleic acid structures and control of transcription, ionophores and drugs and their interaction with membranes, genome organization, synthetic protein and vaccine design, ion channels and electrophysiology, neurophysiology and computational neuroscience.

or suppressing biochemical signals and their spatiotemporal spread.

The structural basis for the allosteric inhibition via feedback mechanisms have been investigated for the enzyme Acetohydroxy acid synthase. High resolution structures of the regulatory subunit in complex with effector molecules have provided an insight into the above mechanism.

Structural studies of polyketide synthase, pore forming toxin bacterial secretion system, bacterial ion channels and GPCRs are underway using cryo-electron microscopy. Cryo-EM techniques are used to characterize the protein structure, conformational changes and dynamics of very small (100 kDa) protein complexes to extremely large biological macromolecules (2.6 MDa).

Extensive analysis of 3-D structures of protein-protein complexes highlighted the importance of interactions of protein-protein interface residues with the protein in which the interface residues are housed. Extensive analysis of toxin-antitoxin systems in Mycobacterium tuberculosis enabled recognition of novel systems, cross talks and cross regulation. A protocol has been designed for repurposing FDA approved drugs against infectious diseases as well as cancer.

The crystal structures of the coiled-coil region of nonstructural protein 4 (NSP4), from two strains of the rotavirus as two novel antiparallel tetrameric forms, were determined. The study demonstrates the structural diversity of the protein under different conditions. DNA damage-inducible 1 (Ddi1) is a multidomain protein with one of the domains being retropepsin-like. HIV-1 protease inhibitors were found to reduce opportunistic infections caused by pathogens like Leishmania and Plasmodium, and some of them were shown to inhibit the growth of these parasites. The crystal structure of the retropepsin-like domain of Ddi1 from Leishmania major was determined and its binding with one of the HIV-1 protease inhibitors was characterized in solution.

Studies on the sensitivity of the longer isoform of human brain TREK1 leak potassium ion channel to hypoxia, that has neuroprotective role using single-ion channel molecule patch clamp recordings on excised inside-out patches of hTREK-1 channels expressed in HEK293 cells indicates an increase in the activity of hTREK-1 channel during hypoxic conditions. Polymodal regulation by ischemic factors like pH and lactate are being investigated. The role of lactate whose concentration in the brain rises during epileptic activity is being investigated for its neuroprotective role in hippocampal subicular neurons and identifying the ion channel mechanisms. In vitro brain slice experiments are being conducted on the medial entorhinal cortex stellate cells (that show grid cell firing in vivo), subjected to in-vivo like stochastic synaptic activity through the dynamic clamp, to understand mapping between the speed-direction modulated excitatory inputs, and firing rate modulation.

A novel therapeutic approach targeting both a metabolic pathway in Mtb essential for its survival and the host machinery crucial for its survival in the host was developed. The compound targets an allosteric site in the essential enzyme, ArgJ, of Mtb not found in human or its commensals sparing the humans of harmful effects of currently used therapy. While the genetic basis for a number of neuropsychiatric disorders afflicting millions is increasingly being appreciated, for the first time a link between immunity and obsessive-compulsive disorder (OCD) was establised by demonstrating incursion of TH17 cells in the thalamic and brain – stem circuit of the brain.

UV cross-linking experiments and ITC revealed that the association of 32 P azido-labeled ppGpp with RNAP was weaker without ω subunit. Altered distribution of RNA polymerase lacking the omega subunit was found within the prophages along the E. coli genome. ChIP-chip analysis of wild-type and rpoZ-defective mutant strains elucidated the functional role of omega subunit. Substrate-induced domain movement in a bifunctional protein DcpA regulates cyclic-do-GMP turnover C-di-GMP homeostasis in M. smegmatis is supported by DcpA, a bifunctional protein. FRET experiments were used to gain insight into how interactions and

movement among these three domains affect the DcpA activity.

High-throughput in vitro and in silico analyses have been carried out to understand the influence of flanking sequences outside the cognate sites in binding of three transcription factors (TF) families in vertebrates. It is found that local structural features of flanking sequences are instrumental in determining the binding affinity of TFs for their core consensus motifs.

Structural studies on mycobacterial proteins involved in maintaining genomic integrity and mycobacterial and archeal lectins were carried out. The mode of cation of second single stranded DNA binding proteins RecGwed and MutT2 has been elucidated. A major long-range collaborative program on the design of inhibitors against selected TB proteins, has been kicked off.

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Manju Bansal | PhD (IISc), FASc, FNASc, FNA, INSA Senior Scientist
MRN Murty | PhD (IISc), FASc, FNASc, FNA, FTWAS, INSA Senior Scientist
M Vijayan | PhD (IISc), FASc, FNASc, FNA, FTWAS, NASI Senior Scientist
Saraswathi Vishveshwara | PhD (New York), CSIR Emeritus Scientist

3.1.7

Microbiology Cell Biology

CHAIRPERSON
USHA VIJAYRAGHAVAN

The origin of the department of Microbiology & Cell Biology (MCB) traces to the Pharmacology Laboratory and the Fermentation Technology Laboratory, both established in the early 1940's, which were amalgamated in 1968. MCB has 17 faculty members: 8 Professors, 4 Associate Professors and 5 Assistant Professors. The major research activities include investigations on microbial pathogenesis and eukaryotic cellular processes.

Current Research

PATHOGENESIS AND GENOME BIOLOGY OF HUMAN PATHOGENS

One of the mechanisms by which the human Pathogen Salmonella enterica causes infection is by surviving inside dendritic cells (DCs) and suppressing antigen presentation. Mechanistic studies revealed that Salmonella infection induces a host epigenetic modulator SIRT2, which produces nitric oxide (NO) in amounts required to inhibit the T cell response. This inhibition of T cell via SIRT2-mediated NO production impaired antigen presentation, facilitating the establishment of Salmonella infection. Similarly, examination of host-pathogen interaction in the context of Tuberculosis (TB)-causing bacteria (Mycobacterium tuberculosis [Mtb]) identified an epigenetic mechanism coordinated by c-ABI-TWIST1 to deregulate inflammatory response during Mtb infection. This study proposed to use c-ABI inhibitors in potentiating innate immune response against TB infection. Further

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IN NUMBERS

16 Academic Staff
1 Scientific Staff
72 PhD Students
10 Int PhD Students
63 Publications
1 Int PhD Conferments
17 PhD Conferments

Some areas where MCB department has a long tradition of excellence are (i) Host-Pathogen Interaction, (ii) Gene Regulation, (iii) Cancer and Cell biology, (iv) Vaccine and Drug development, and (v) plant biology. Some newer areas where we are expanding include (i) Systems Biology, (ii) Molecular Virology, (iii) Microbial Ecology, and (iv) Cardiovascular and Muscle Research.

investigation on Mtb revealed a crucial role for a protein WhiB4 in protecting the TB bacteria from oxidative stress by condensing the DNA (nucleoid). Compacted DNA has reduced surface area and hence lower vulnerability to oxidative stress. Modulating the levels of WhiB4 attenuated the ability of Mtb to survive inside macrophages and in animal models of experimental TB. Asymmetric cell division and heterogeneity in cell length also modulate mycobacterial stress response. It was shown that mycobacteria secrete Diadenosine polyphosphates, Ap to induce variations in the length of mycobacterial cells during cell division. In the context of protein translation, studies have identified the evolutionary lineages of initiator and elongator methionine tRNAs. This study led to identification of a single mutant tRNA capable of initiating and elongating protein synthesis in bacteria, thus indicating that initiator and elongator methionine tRNAs might have originated from a single 'dual function' tRNA. Using Mycobacterium smegmatis as a model system, it has been demonstrated that modulation of DNA gyrase expression has a wide-spread influence on cell division, nucleoid structure, chromosome condensation, and gene expression. Knocking down DNA gyrase also led to increased susceptibility of bacteria towards clinically relevant anti-TB drugs.

VIRAL PATHOGENESIS AND VACCINE DESIGN

Hepatitis C Virus (HCV) is a liver-specific pathogen, which manipulates the host machinery to establish a chronic infection. Studies have identified the role for a host factor, Human antigen-R (HuR) and a micro-RNA (miR-125b) in mediating HCV replication. Furthermore, a long non-coding RNA, Highly Upregulated in Liver Carcinoma (HULC), was found to increase the number and the size of lipid droplets (LDs), which enhanced the association of the viral core protein with LDs and facilitated the release of the virus particles. In the field of flavi-virology, comparison of immune response elicited by the highly efficacious live attenuated

vaccine SA14-14-2 against JEV to those generated by circulating wild type strains of JEV resulted in new insights on the correlates of protection. The live attenuated SA14-14-2 vaccine stimulated far more robust CD8+ T cells than seen in natural infections, and to a wider repertoire of viral proteins. Cell biological investigations of virus-infected cells have revealed that the SA14-14-2 vaccine induces ER stress and the unfolded protein response, leading to enhanced autophagy in infected cells, which is well known to generate vesicles that can be cross presented by dendritic cells.

CELLULAR PROCESSES, CELL DIVISION, AND CANCER BIOLOGY

Correct orientation of the mitotic spindle during metaphase is fundamental for dictating the future plane of the cell division axis. It is well known that the evolutionarily conserved dynein adaptor NuMA regulates the correct spindle orientation. Further studies discovered that Polo-like kinase 1 (Plk1) directly phosphorylates NuMA and regulates proper spindle orientation by orchestrating the cortical localization of NuMA/dynein. Inhibition of Plk1 in metaphase robustly enriches NuMA and dynein at the cell cortex, which affected spindle orientation on cell grown on the L-shape micro-patterns. In humans, several lysosomal disorders are mediated by alterations in the mechanisms of cargo segregation, vesicle biogenesis and transport, and vesicle fusion. Work in this direction, identified a major role for Rab22A in recycling endosome biogenesis and Rab4A in organizing cargo-specific domains on sorting endosomes. Efforts are also ongoing to understand microRNA (miRNA) metabolism in Caenorhabditis elegans (C. elegans), especially how these regulatory RNAs themselves get regulated by the turnover pathway. In the field of cancer biology, genetic and epigenetic landscapes were identified during glioma (adult brain tumor) development. It was discovered that RNA methylase METTL3 and m6A modification are essential for glioma stem cell growth. Furthermore, it was found that GBMs with Calcitonin receptor (CALCR) mutations defines a subtype with poor prognosis.

GENE REGULATION, DEVELOPMENT AND LIFESTYLE DISEASES

FFundamental mechanisms underlying cardiovascular diseases and pathologies are not completely understood. In parts, we lack basic tools to study heart failure in vitro and in vivo. A simple and cost-effective method was developed for culturing cardiomyocytes using keratin derived from human hair to study the cardiac hypertrophy. This resulted in elucidating the role for SIRT2 deacetylase in the development of heart failure. The SIRT2 deficiency hyperactivated NFAT signaling pathway in the heart thus induced spontaneous pathological cardiac hypertrophy. Another SIRT family member, SIRT6 played an important role in inducing metabolic shift associated with the remodeling of failing heart. In the area of plant development biology, genome-wide datasets of OsMADS1 transcription factor-chromatin interactions and comparative gene expression generated snap shots of two temporal gene regulatory networks. One of its indirectly downstream target, a transcription factor OsbZIP47, was shown to partner with OsMADS1 thus establishing a regulatory loop between these factors that likely controls floral development. Intron splicing is an essential step in post-transcriptional fine-tuning of eukaryotic gene expression to give functional mRNA. Using yeast as a model system, the role of an essential fission yeast splicing RNA helicase in intron context specific splicing and its role in centromere heterochromatin formation was uncovered.

The timing of transition to flowering in plants is crucial for their reproductive success. Two transcription factors, VASCULAR PLANT ONE–ZINC FINGER1 (VOZ1) and VOZ2, were found to promote flowering in Arabidopsis by modulating the activity of another flower-promoting transcription factor, CONTANS. The molecular control of epidermal cell shape in Arabidopsis, especially trichomes, is

still not clear. Studies show that the CIN-TCP transcription factors suppress trichome branching in Arabidopsis leaves and inflorescence stem by direct transcriptional activation of GLABROUS INFLORESCENCE STEMS (GIS), a known negative regulator of trichome branching.

Faculty & Staff

P Ajitkumar | PhD (IISc), Associate Professor
KN Balaji | PhD (IISc), FNA, FASc, FNASc, Professor
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Saibal Chatterjee | PhD (IICB), Assistant Professor
Saumitra Das | PhD (IICB), FNA, FASc, FNASc, Professor (On-Lien)
Sachin Kotak | PhD (Goethe University), Assistant Professor
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Amit Singh | PhD (ICGEB), Associate Professor
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S Vijaya | PhD (IISc), Professor
Usha Vijayraghavan | PhD (Caltech.), FNA, FASc, FNASc, Professor
William R Surin | PhD (Lucknow), SSO

3.1.8

Molecular Reproduction, Development and Genetics

CHAIRPERSON
SANDHYA S VISWESWARIAH

Research in the Department of Molecular Reproduction, Development and Genetics (MRDG) is diverse and ranges from molecular to organismal scales. Groups within the department conduct research in bacterial and human genetics, signal transduction, mammalian reproduction, endocrinology, developmental biology, aging, cancer, stem cells and cryo-electron microscopic analysis of large macromolecular complexes.

Current Research

Following are the important on-going research projects in the Department.

GPCRS AND INFLAMMATION

The main highlight of this work has been on the elucidation of the role of a GPCR, CXCR4 in regulation of inflammation during aging and anti-cancer therapy. We have identified the pathway by which this receptor drives enhancement in inflammation when cellular DNA is damaged. Using a targeted drug screening approach, we have also identified lead molecules which can be repurposed to suppress inflammation and showed their efficacy in animal model of aging.

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IN NUMBERS

14 Academic Staff
50 PhD students
9 Int PhD Students
32 Publications
1 Int PhD Conferment

Core Research

The core research areas of the department are as follows: Gene regulation in prokaryotes & eukaryotes, Host- Pathogen Interactions, Human Genetics, X-inactivation, Signal Transduction, Developmental Biology and Ageing, Morphogenesis, Mouse Embryo Development, Stem Cells and Differentiation, Reproductive Biology, Endocrinology, Cancer Biology and Cancer Stem Cells, and protein translation and its regulation

UTILIZATION OF BETA-GLUCOSIDES BY BACTERIA

Sustained work in the laboratory over the past two decades has explored the evolutionary significance of bacteria maintaining genetic systems in their genomes that are silent and uninducible. Results from the laboratory over the past year using the bgl operon of E. coli as a paradigm have highlighted the fact that rather than being silent, enhanced expression of the bglG gene has a significant role in the physiology of the organism, particularly in stationary phase. Using genomic and genetic approaches, it could be shown that regulation of the ridA gene that encodes a deaminase by BglG has a significant impact in reducing the toxicity associated with the catabolism of amino acids such as serine in stationary phase. These studies have also helped to identify regulators involved in diverse physiological functions that are influenced by BglG.

STRUCTURAL BIOLOGY OF TRANSLATION

During translational initiation in eukaryotes, the 40S ribosomal subunit forms a 43S pre-initiation complex (PIC) with eukaryotic initiation factors eIF1, eIF1A, eIF3, ternary complex (eIF2-GTP-Met-tRNAMeti) and eIF5. The mRNA bound to eIF4 complex is recruited to the ribosomal 43S pre-initiation complex (PIC) to form 48S PIC. The 48S PIC, in an open conformation, scans the 5' untranslated region (UTR) of mRNA to locate the start codon. The recognition of the start codon in the scanning-

arrested closed state of 48S PIC leads to the release of eIF1. We observed in the cryo-EM structure of 48S PIC, captured after start codon recognition and eIF1 release, that the N-terminal domain (NTD) of eIF5 occupies the position on 40S left vacant by eIF1.

SIGNAL TRANSDUCTION, INFECTION AND TRANSGENIC MOUSE MODELS TO STUDY GASTROINTESTINAL FUNCTION

We have shown that receptor guanylyl cyclase C is important to provide protection against Salmonella Typhimurium infection. Transgenic mice harbouring activating mutations in guanylyl cyclase C have been obtained and characterized at the molecular and phenotypic level. In the area of Pore Forming Toxins, we have shown that ClyA needs cholesterol to induce a conformational change required for pore formation, using single molecular and supported lipid bilayer approaches.

METABOLIC DISORDERS ASSOCIATED WITH PREGNANCY AND LACTATION

Research on understanding development of glucose insensitivity and sensitivity during pregnancy and lactation effect of steroids on glucose utilization in muscle and adipose tissue is being conducted.

MUSCLE DEVELOPMENT

LIM domain, constituted by two tandem C2H2 zinc finger motif, proteins regulate several biological processes. They are usually found associated with various functional domains like Homeodomain, kinase domain and other protein binding domains. LIM proteins that are devoid of other domains are called LIM only proteins (LMO). LMO proteins were first identified in humans and are implicated in development and oncogenesis. The Drosophila LMO protein (dLMO), Beadex (Bx), regulates various developmental processes like wing margin development and bristle development. We have shown that Beadex is essential follicle cells of the Drosophila oocyte for development.

EPIGENETICS OF DEVELOPMENT

A novel putative methyltransferase protein enriched on the inactive X-chromosome is being studied. We are trying to link the reprogramming of primed to native pluripotent state and X-chromosome reactivation. Molecular and functional characterization of an Xist-antisense long non-coding RNA is also being investigated.

ADIPOCYTE DIFFERENTIATION

In general, white adipose tissue (WAT) expands massively during obesity and aging with lipid overload. Conversely, brown fat, a distinct tissue dissipates energy in the form of heat through uncoupled respiration and increasing activity of brown adipose tissue (BAT) is considered an attractive therapeutic strategy to help reduce obesity and associated metabolic disease. Screening small molecules to increase BAT function and reprograming of WAT to BAT conversion is being carried out. We have identified a small molecule that positively regulates brown adipocyte function and energy homeostasis in mice.

GENETICS OF HUMAN DISEASE

Mutations in the glucocerebrosidase (GBA) gene have been associated with Parkinson's disease (PD). Several variants in the gene have been identified as risk factors for the development of PD, but there is difference in the prevalence of the mutations in various ethnic groups and countries. There is no published study related to this field on the Indian population. The aim of the study was to investigate the frequency of mutations in the GBA gene in Indian patients with PD. To perform the mutation analysis of the GBA gene, we amplified its entire coding region. We screened a total of 100 PD patients for mutations in the GBA gene. The sequence analysis identified five variants in this gene. All the variants were detected in homozygous as well as in heterozygous states. Our results suggested that GBA mutations may not be so common in Indian patients with PD as compared to the other ethnic populations.

HOST-MICROBE INTERACTION

We utilize a genetically tractable nematode, Caenorhabditis elegans, to study its interactions with pathogenic and non-pathogenic microbes in the soil, many of which are medically relevant human pathogens. C. elegans uses its olfactory neurons to smell a pathogenic bacterium Pseudomonas aeruginosa and run away from it. Specific bacterial metabolites that stimulate host sensory neurons have been identified. Additional projects in the laboratory have shown that infection causes the nematode host to quickly utilize stored fats to facilitate better survival during infection.

EARLY MAMMALIAN EMBRYONIC DEVELOPMENT

Studies on the cellular and molecular regulation of blastocyst hatching and, pluripotent stem cell (PSC) differentiation are in progress. We use experimental systems such as (i) in vitro development of blastocysts through zona-hatching; (ii) in vitro cell-lineage commitment and differentiation of PSCs to neural or cardiac cell types i.e., neural stem cells (NSCs) and cardiovascular progenitors (CVPs); (iii) human embryo biomarkers analysis in embryo-spent medium employing ELISA and metabolomics approaches. Overall, we examine (i) blastocyst-derived hatching enabling regulators in terms of their gene expression, (sub)-cellular localization and function and (ii) the enrichment and expansion of NSCs and CVPs, for potential use in stem cell transplantation (translational) research. These study outcomes have implications in the clinical management of human infertility and stem cell-based cell transplantation.

CANCER STEM CELLS

Major focus in the laboratory is to understand the biology of cancer stem cells and their role in drug resistance and metastasis. The work has identified a central role for the cellular energy sensor AMPK in the regulation of stemness and cancer drug resistance. More recently we have identified feedback loops between AMPK and other kinases like Akt and Erk in matrix-detached cancer cells that contributes to their anchorage-independent survival properties which is fundamental for cancer metastasis

CANCER GLYCOBIOLOGY

The relationship between cancer (breast and ovarian) cells and their tissue microenvironments in the context of invasion and metastasis is being investigated using approaches including experimentation and computation to understand how changes in glycans that contribute to cell and tissue structure, and are aberrantly regulated and in turn impact affect cancer cell phenotypes. In this context, we have focused in the past year on the functions of galectins (galactose-binding lectins) and sialic acids, terminal sugars of glycoproteins and how their altered levels affect the behavior of cancer invasion.

CANCER AND CELLULAR SIGNALING

Our group is studying the pathways that regulate breast and brain cancers. We have been able to establish that cancer associated fibroblasts are essential for breast cancer promotion in vivo which is comparable to the role of TGF-β over expressing fibroblasts. In glioblastoma, we were able to identify differential DNA methylation pattern in the tissues of recurrent glioma patients compared to the primary tumors. Also, we established the pathway of IGFBP2 actions that involve regulation of HIF1α and β-catenin. With respect to Activin mediated signaling, we identified several regulators notably ERK in the activation of SMAD2 and this involves activation of EGFR and AKT pathways.

Faculty & Staff

Ramray Bhat | MBBS (Calcutta), PhD (NYMC), Assistant Professor
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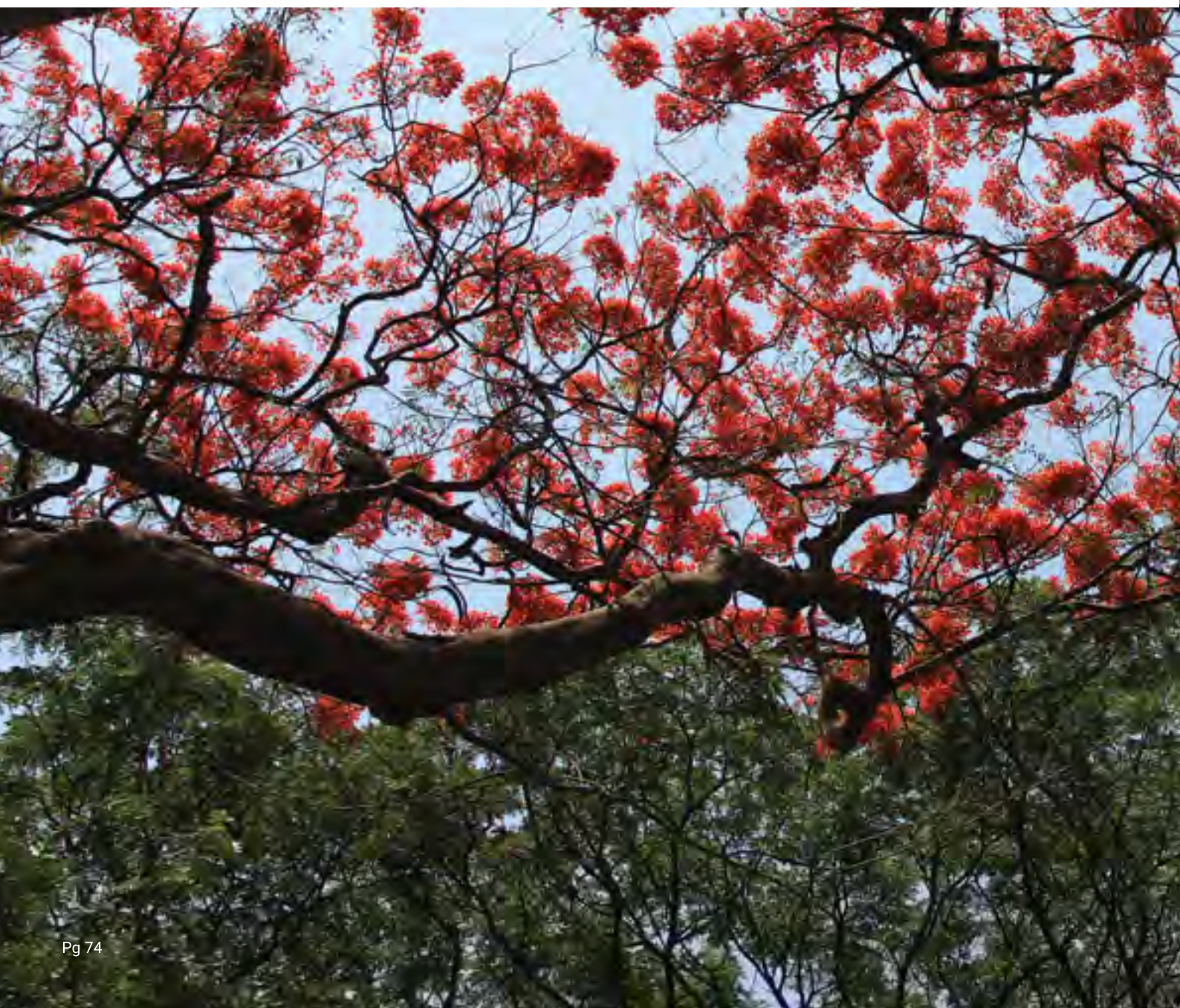
Sandhya S Visweswariah | PhD (IISc), FASc, FNA, FTWAS, Professor



3.2 Division of Chemical Sciences

IN NUMBERS

- 57 FACULTY MEMBERS
- 268 PhD STUDENTS
- 72 INT PhD STUDENTS

The faculty members of the Division work on all contemporary topics in chemistry, ranging from Chemical Synthesis, Drug Design, Chemical Biology, Materials Chemistry, Surface and interface Science, Nanochemistry, Molecular Spectroscopy, Ultrafast Chemical Dynamics, Computational and Theoretical Chemistry, Solid State Chemistry and Nuclear Magnetic Resonance spectroscopy.

THEMES

The Division of Chemical Sciences has consistently maintained its position among the top 50 chemistry departments in world rankings over the past decade. It is a globally competitive Division with clear focus on top quality research in specific current areas such as bio-inorganic chemistry and chemical biology of drugs with a particular aim on disease control and cure, ultrafast spectroscopy and dynamics of molecules towards

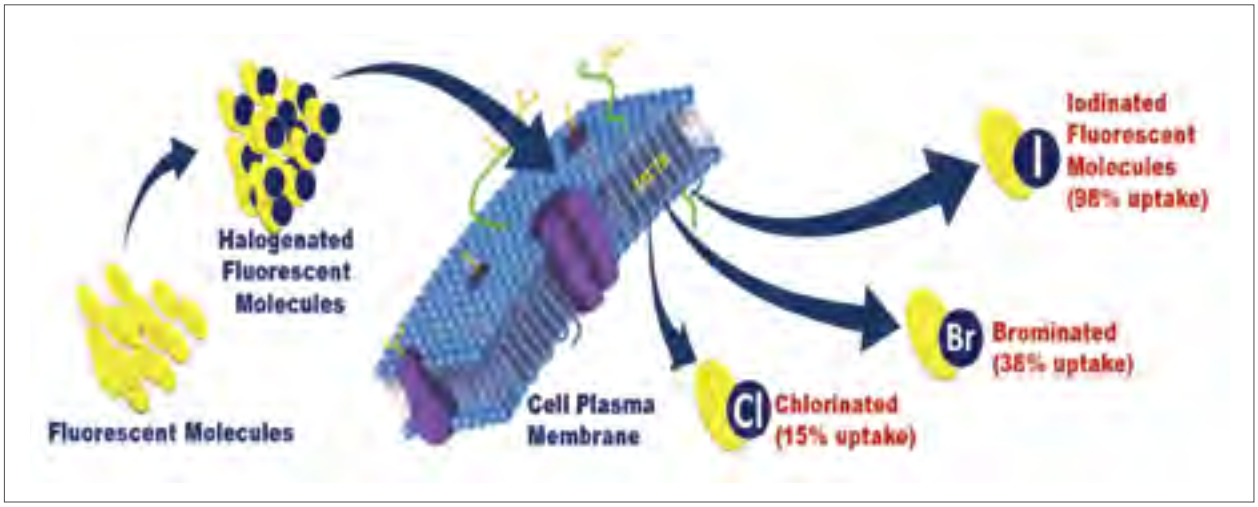
RESEARCH HIGHLIGHTS

The Division of Chemical Sciences comprises the Department of Inorganic and Physical Chemistry, Department of Organic Chemistry, Solid State & Structural Chemistry Unit, Materials Research Centre and NMR Research Centre

DEPARTMENTS | CENTRES | UNITS

- INORGANIC AND PHYSICAL CHEMISTRY
- MATERIALS RESEARCH CENTRE
- NMR RESEARCH CENTRE
- ORGANIC CHEMISTRY
- SOLID STATE AND STRUCTURAL CHEMISTRY UNIT

Research Snapshots 2018-19



G. Mugesh (IPC)

For decades, scientists have used fluorescent probes to detect molecules, monitor cellular activity and deliver drugs inside cells. Probes based on a compound called naphthalimide are especially popular because they can easily be made in large quantities and their fluorescence can be tweaked by changing their constituent atoms. But they are usually absorbed by cells only in small quantities, which hampers their effectiveness. In addition, little is known about how they cross the cell membrane to reach inside.

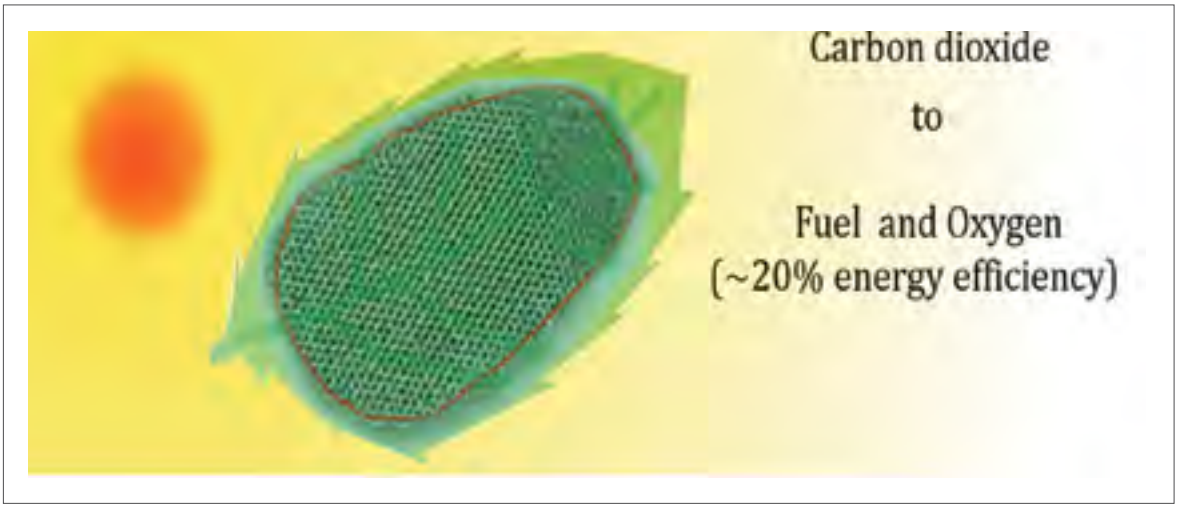
In a new study, researchers from the Indian Institute of Science (IISc) have figured out a way to boost the cellular uptake of such fluorescent probes. They found that simply replacing two hydrogen atoms with iodine in their structure dramatically increases the amount transported into mammalian cells — up to 98%.

The Remarkable Effect of Halogen Substitution on the Membrane Transport of Fluorescent Molecules in Living Cells, *AngewandteChemie International Edition,* May 2018. https://onlinelibrary.wiley.com/doi/abs/10.1002/anie.201804128

Abhishek Singh (MRC)

The application of machine learning (ML) to develop structural and functional materials is relatively new, however, has great potential to accelerate the discovery of materials for a desired application. A foremost requirement in designing predictive models is the availability of high quality scientific data in the form of shared materials databases. Continuous update and establishment of new databases are crucial for targeted applications. In this regard, Materials Theory and Simulations Group at Materials Research Centre has developed an open-access online repository of functional materials. The database is called aNANt and hosts the structures and electronic properties of more than 10000 functionalized MXene. It is expected to grow to host 25000 functionalized MXene within few months. Using information from this database, we have recently developed a ML model to predict the accurate band gap of functionalized MXene.

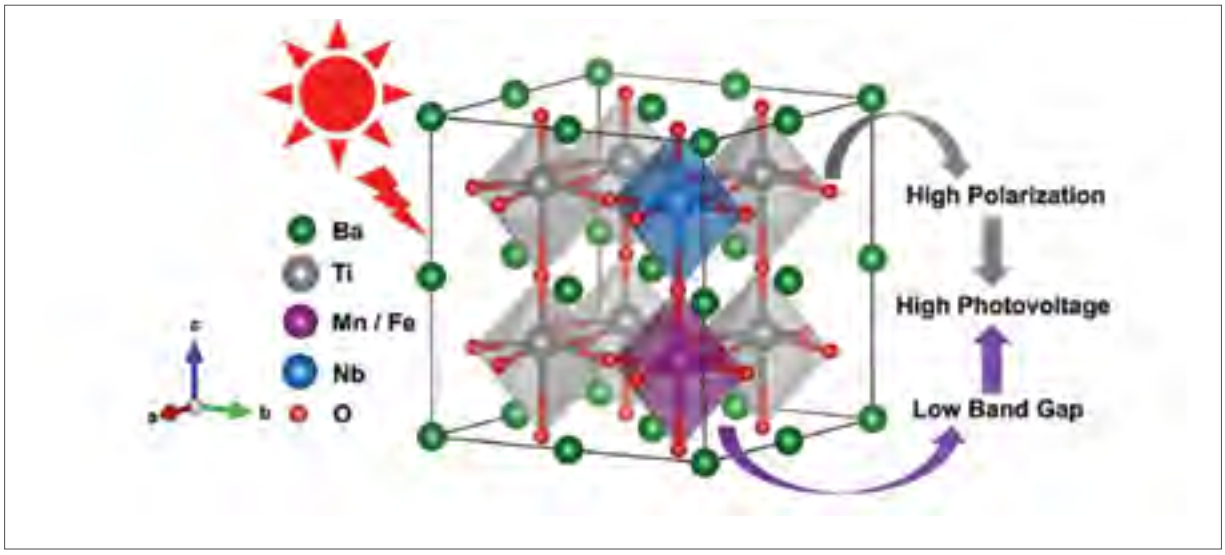
A. C. Rajan, A. Mishra, S. Satsangi, R. Vaish, H. Mizuseki, K. R. Lee and A. K. Singh. Machine Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene. Chem. Mater. 30, 4031 (2018)



Anshu Pandey (SSCU)

Artificial photosynthesis is a very promising idea, since it can directly help capture atmospheric carbon dioxide and convert to a fuel or an industrial feedstock.
While extensive efforts have been made towards electrically assisted CO2 reduction, exclusively photocatalytic reduction remains in a relatively nascent state. In this work we have designed and prepared CuAlS2/ZnS quantum dots that can reduce aqueous bicarbonate ions to formate under visible light. We are able to get high turnover numbers (>7×10^4 molecules of sodium formate produced per quantum dot) and also solar to chemical energy conversion efficiencies as high as 20%. This efficiency is roughly 100 times greater than what is typically achieved in natural photosynthesis.

Bhattacharyya, B.; Simlandy, A. K.; Chakraborty, A.; Rajasekar, G. P.; Aetukuri, N. B.; Mukherjee, S.; Pandey, A. Efficient Photosynthesis of Organics from Aqueous Bicarbonate Ions by Quantum Dots Using Visible Light. *ACS Energy Lett.* 2018, 3, 1508-1514



D D Sarma (SSCU)

Any ferroelectric material is potentially an efficient solar energy converter. Unfortunately, all known ferroelectric materials have large band gaps with little overlap with the solar spectrum and therefore, poor ability to absorb and convert sunlight to electricity. We recently discovered an efficient way to reduce the band gap of a classical ferroelectric material, BaTiO3, without compromising its ferroelectric polarization significantly with the help of a charge-neutral dipole doping of Mn3+-Nb5+ pair replacing two Ti4+ ions.

Shyamashis Das, Somnath Ghara, Priya Mahadevan, A. Sundaresan, J. Gopalakrishnan, and D. D. Sarma; Designing a Lower Band Gap Bulk Ferroelectric Material with a Sizable Polarization at Room Temperature *ACS Energy Lett.* 2018, 3, pp 1176–1182; (DOI: 10.1021/acsenergylett.8b00492)

3.2.1

Inorganic and Physical Chemistry

CHAIRPERSON
ARUNAN ELANGANNAN

Established more than a century ago in 1909, when the Institute was founded, the Inorganic and Physical Chemistry Department (IPC) has excelled in both fundamental and applied research.

Current Research

BIO AND MEDICINAL INORGANIC CHEMISTRY

On this topic the following research areas are being undertaken by the department faculty.

Curcumin-based metal complexes as photochemotherapeutic agents have been developed and the compounds show significant photo-induced cytotoxicity in visible light while being minimally toxic in dark. BODIPY – Copper conjugates are reported to show mitochondrial localization with singlet oxygen mediated visible light-induced apoptotic cell death.

Metal oxide nanomaterials that are capable of mimicking all the three major cellular metalloenzymes have been shown for, controlling the level of reactive oxygen species (ROS) inside cells. The nanomaterials appear promising candidates for therapeutic applications against oxidative stress-induced neurological disorders, particularly Parkinson's.

Direct delivery of proteins into cells has been an emerging area of research at IPC. By exploiting the power of halogen bonding mediated interactions, protein as large as 28 kDa was successfully incorporated into cells with great efficiency.

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IN NUMBERS

20 Academic Staff
3 Scientific Staff
100 PhD Students
35 Int PhD Students
119 Publications
3 Int PhD Conferments
15 PhD Conferments

Core Research

Currently, the department has 20 faculty members working in rich and diverse areas of chemistry including molecular spectroscopy, magnetic resonance spectroscopy, chemical dynamics, bio photonics, analytical and computational theory, electrochemistry, polymer chemistry, transition metal and non-metal chemistry, bioinorganic and biophysical chemistry, chemical biology, and functional materials

Challenging membrane bound metallo-enzymes that play crucial roles in hydrocarbon biosynthesis in Nature are being investigated.

CHEMICAL DYNAMICS AND SPECTROSCOPY

Several faculty members of the department work in this area.

The department has been at the forefront in the emerging area of inter-molecular bonding: Some highlights: 1. Using the home-built pulsed nozzle Fourier transform microwave spectrometers, hydrogen bonding in the hydrogen sulphide dimer has been revealed, very much like water dimer. This is against conventional wisdom given in text books on chemistry and biology. The work was featured in Chemical and Engineering News and Chemistry World and news papers and Science based websites in India. 2. First paper to discuss interstellar hydrogen bonding. 3. Protonated methane is an important cation that has attracted enormous interest. Work at IPC showed that it has five covalent bonds and no H-H bond, contrary to popular characterization. On the other hand, protonated silane and germane exhibit a tetrel bond between TH3+ and H2. It appeared in the cover of the

Blue-shifted H-bonded species have been investigated using Fourier Transform Infrared Spectroscopy (FTIR) in gas phase complexes at room temperature and the origin of such bonding which is “not normal” has been explored. Protein nanoparticle interaction has been investigated using second harmonic light scattering in solution and various thermodynamic quantities such as binding constant, free energy change, enthalpy and entropy change of the protein adsorption on the nanoparticle surface have been explored at concentrations much lower than what is accessible by other standard techniques.

Ultrafast surface reactions are being studied, including catalytic oxidation of CO monoxide, desorption of CO and CO2 on transition metal and metal oxide nanoparticle surfaces. Ultrafast initial steps in the laser ignition of energetic molecules like propellants and plasticizes are also being investigated. Steps are being taken towards development of X-Ray spectroscopy. Theoretical studies in attochemistry are also done.

Research in condensed matter theory, including the statistical mechanics of complex fluids, polymer physics and stochastic processes is actively pursued in the department. Recent efforts have been to explore the statistical mechanics of the coil-stretch transition, and to throw light on a hitherto unresolved aspect of dynamically disordered Brownian motion.

The effect of system reservoir coupling on currents flowing through quantum junctions is under investigation. Two simple double-quantum dot configurations coupled to two external fermionic reservoirs have been considered and the net current flowing between the two reservoirs is being investigated. The net current is partitioned into currents carried by the eigenstates of the system and by the coherences between the eigenstates induced due to coupling with the reservoirs. It has been found that the current carried by populations is always positive whereas current carried by coherences are negative for large couplings. This results in a non-monotonic dependence of the net current on the coupling strength. It has also been found that in certain cases, the net current can vanish at large couplings due to cancellation between currents carried by the eigenstates and by the coherences.

An understanding of vibronic dynamics in the gas and solution phases via theory is being developed. Most recent studies were on molecular dynamics simulations of H-atom abstraction reaction by CN radical from ethanol, and also the topology and mode involvement in the low-lying conical intersections of aniline involving the first pi-sigma* state.

POLYMER CHEMISTRY

Periodically grafted amphiphilic copolymers are polymeric chains where pendant segments are located at long equally-spaced intervals; immiscibility between the backbone and pendant segments was shown to lead to the folding of the chain, which in turn helps collocate the backbone segments in the middle while the pendant segments are located above and below. By suitable design alteration, a polymer has been prepared that carries two different segments, namely PEG and fluorocarbon, at alternating locations but in a periodic manner; such a system folds to generate a system that carries PEG chains on one side and fluorocarbon on the other, thereby desymmetrizing the folded chain. Such desymmetrized folded chains could be used to explore several interesting properties, such as polar ordering of chromophores in solution, surface modification, etc.

ORGANOMETALLIC AND COORDINATION CHEMISTRY

In this sub-discipline, the departmental faculty members have contributed to the following.

Catalytically active ruthenium metal nanoparticles of very small dimensions (2-10 nm) were generated in solution and used for catalysis. This in situ generated nanoparticle is stabilized by the solvent, capping organic ligand and other Lewis bases making them more or less stable depending on the Lewis bases present under fairly mild conditions. It has been shown that half-sandwich organometallic complexes with NHC ligands have extra stability and can have have been shown to be very efficient for reduction and C-C coupling reactions. The particles lose some of their catalytic activity

if the solution is allowed to cool to room temperature. They aggregate and precipitate.

The development of a relatively new strategy to obtain transition metal sigma complexes of H2, R3SiH, H3NaBH3, and CH4 was carried out in the hope of realizing methane conversion catalysts. A series of novel iridium and rhodium complexes bearing PNP pincer complexes has been developed. Creation of vacant coordination site in these complexes followed by binding of these small molecules resulted in sigma-complexes in the cases of H2, R3SiH, H3Nâ€¢BH3. Further, catalytic hydrogenation reactions of several different substrates including hydrogenation of CO2 to formic acid using these iridium complexes has been carried out. A thorough understanding of the underlying mechanisms of the formation of a core-shell nanostructured material and its transformation into an alloy has been achieved. For this, the Au-Ag system was used. Certain metal nanosponges was developed and exploited for their potential in catalytic hydrogenation reactions. The metal nanosponges have wide substrate scope and exhibited high catalytic efficiencies.

SUPRAMOLECULAR CHEMISTRY/ CATALYSIS

Pd(II) and Pt(II) cages and molecular barrels were synthesized and their confined space was used for studying chemistry of photochromic molecules. Newly designed organic cages were used as templates for nucleation of Au nanoparticles and uses as photocatalysts.

MAIN GROUP CHEMISTRY

In this area, the following contributions have been made.

• Development of cost effective, earth abundant, less toxic base metal catalysts or main group catalysts for the synthesis of organoboranes, which are important synthetic intermediates in pharmaceuticals and organic light-emitting diodes as exemplified by the Suzukiâ€“Miyaura cross-coupling reaction has been carried out. Considerable effort has been committed to the preparation of organoboranes using precious metals (such as Pd, Rh, Ir, etc.) and more recently, using non-precious metals (Cu, Ni, Fe). High cost, human toxicity, and limited natural abundance are few drawbacks associated with precious metals. These drawbacks have sparked interest for the development of cost effective earth abundant, less toxic metals or even metal free catalytic systems to promote selective synthesis of organoboranes efficiently. Recently, she developed an efficient catalyst system based on Co(II)-NHC complex for the the borylation of aryl halides.

• The design and synthesis of new molecules/ materials containing BORON for the potential application in the field of Catalysis, Molecular Electronics (OLEDs, TFTs and solar cells), and Chemosensory materials s going on. Also the Lewis acidity of tri-coordinated boron for the development of boron based proteasome inhibitors (BPI) and understanding the differences in the catalytic activity of multiple proteolytic sites in both eukaryotic and bacteria proteasomes is going on.

THEORETICAL CHEMISTRY

Work is being carried out on the development of a multicoordinate three-electronic potential surface for NH2 group's photodynamics in aniline as well as coding for the dynamics itself. The former involves a series of computationally intensive ab initio calculations and subsequent fits, which are ongoing. A coordinate system for the dynamics was carefully chosen, where only a few coordinates are non-orthogonal. Calculations are ongoing for the CN radical's reactions with solvents like chloroform. The construction of a full dimensional potential surface for the H-atom tunneling in catecholate is being carried out. This is with a wider view to investigate multidimensional tunneling. The Distributed Gaussian Empirical Valence Bond approach to build the potential surface is being used; even with a single Gaussian coupling, the results are already promising.

ELECTROCHEMISTRY, LAYERED MATERIALS AND DEVICES

Layered semiconductors based on metal phosphochalcogenides (MPX3 (M=Ni,Fe,Mn etc; X=S,Se)) have been synthesized and exfoliated in to few and single layers. Electrocatalysis of small molecule redox chemistry has been demonstrated. Electrical transport studies have been conducted and devices fabricated using NiPS3, FePS3 and MnPS3. Rechargeable metal-air batteries, particularly zinc-air and lithium-oxygen systems have been fabricated using the layered materials and studied. 1T phase of MoSSe has been stabilized and strain associated stability studied. Humidity sensing using flexible sensors for real time monitoring has been demonstrated with short response and recovery times.

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Binny J Cherayil | PhD (U Chicago), Professor
Debasis Das | PhD (U Michigan), Assistant Professor
P K Das | PhD (Columbia U), FASc, Professor
K Geetharani | PhD (IIT Madras), Assistant Professor
Upendra Harbola | PhD (JNU), Associate Professor
Balaji R Jagirdar | PhD (Kansas State U), FASc, Professor
G Mugesh | PhD (IIT Bombay), FASc, FNASc, FNA, Professor
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Sanjay Prasad | MTech (Anna), Scientific Officer
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Honorary Professor

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3.2.2 Materials Research Centre

CHAIRPERSON
K K NANDA

The Materials Research Centre (MRC) was established in 1978, to foster interdisciplinary research in different areas of materials science and technology with an emphasis on electronic and functional materials. Recently the centre has diversified into biomaterials, multiscale simulation and properties of nanomaterials. The slogan of the centre, "From basic science to device prototypes," would aptly sum up its research efforts.

Current Research

ENERGY HARVESTING MATERIALS

Faculty of the centre are involved in addressing the challenges associated with development of efficient energy harvesting materials using state-of-the-art density functional theory-based methods. An extensive study is in progress to develop guidelines for designing high ZT thermoelectric materials and ambient condition efficient hydrogen and Li storage materials. Nanostructurization of transition metal silicides is carried out for high temperature thermoelectric application.

2D MATERIALS AND METAMATERIALS

Faculty of the centre are working on 2D materials as they are considered as materials for next generation devices. In order to use 2D materials as building blocks in electronic, optical, and sensing applications, their electronic properties need to be modified. A

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IN NUMBERS

8 Faculty
1 INSA Faculty
80 graduate students
47 PhD Students
6 Int PhD Students
100 publications

focussed effort aiming towards gaining the ability to modify the band gaps of these materials in a controlled and non-invasive way in currently underway. Meta-structure based on Vanadium oxide phase change materials for perfect absorbers at IR and microwave frequencies is demonstrated.

WHITE LIGHT-EMITTING-DIODES FOR GREEN ENERGY

The LED project evolved for this initiative dealt with “White” LEDs, typically blue LEDs working in conjunction with yttrium aluminium garnet (YAG) phosphor, used for lighting applications. A commercial white LED produces 110 lm/W at an injection current of 700 mA, exemplifies the state-of-the-art in solid-state lighting. The work at MRC developed highly efficient white LEDs higher than commercially available LEDs in three phases over the last 6 years in collaboration with an industry.

BIOMATERIALS FOR ORTHOPAEDIC AND DENTAL APPLICATIONS

One of the on-going projects as per of the centre of excellence on biomaterials for orthopaedic and dental applications is related to the acetabular socket materials based on hybrid polymer-ceramic composite for Total Hip Joint Replacement and the deliverables of this specific project hold promise for immediate commercialization for use as acetabular sockets in THR. The Zirconia-toughened Alumina (ZTA) based femoral ball head prototype will be developed using integrated manufacturing steps to obtain smoothly polished femoral ball heads with better strength, fracture toughness and wear resistance. Development of dental implants with Ti6Al4V-based dual ceramic coated abutment and screw implants are being developed.

NANOSTRUCTURED MATERIALS FOR ENERGY AND ENVIRONMENT APPLICATIONS

Faculty of our centre are involved in designing nanostructured based catalysts for water splitting, water purification, batteries and fuel cells. Few faculties are associated with the development of materials for gas sensing applications at room temperature, infra-red and UV detection.

Faculty & Staff

Bikramjit Basu | PhD (Kuleuven, Belgium), Professor
Prabeer Barpanda | PhD (Rutgers), Assistant Professor
Karuna Kar Nanda | PhD (IOP), Professor

Core Research

The efforts of the faculty of the centre covers the following broad areas of research: Semiconducting materials for blue LEDs, phosphors for white light applications, absorber for photovoltaic applications, infra-red and UV detection, gas sensing, etc. Biomaterials for musculoskeletal applications, catalytic materials for water splitting, water purification, energy harvesting and storage materials for thermoelectric, Li-ion/ Na-ion battery, and hydrogen storage, fuel cells, etc and thermoelectrics and meta-materials are pursued in the centre.

3.2.3

NMR Research Centre

CHAIRPERSON
S VASUDEVAN

The primary focus of the NMR Research Centre is the development of new NMR spectroscopic methods and their application to important and challenging problems in Chemistry and Biology.

Current Research

NMR based identification and quantification of metabolites allows direct mapping of related biological pathways and helps in understanding their flux in the cell. However, this requires recording data on a large number of samples to arrive at a statistically relevant information, which increases the time required for data collection. We develop new techniques, which allows one to significantly reduce the time required for acquiring multidimensional NMR data. We have also developed methods for automated data analysis, which address the important problem of rapidly identifying metabolites from NMR spectrum and mapping them to metabolic pathways. We have applied these methods for finding biomarkers in human in-vitro fertilization (IVF) and for studying cancer cell metabolism.

A simple ternary ion-pair complexation protocol has been developed for rapid testing of enantiopurity and the assignment of absolute configurations of various acids and ester derivatives employing 1,1'-[binaphthalene]-2,2'-diamine (BINAM) as a novel chiral solvating agent (CSA) in the presence of trifluoromethanesulfonic acid (TFMS) as a third ingredient. The protocol also permits the unambiguous assignment of stereospecific configurations

FACT FILE

080-2293-2536 (Office);
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IN NUMBERS

Students 13
Academic Staff 3
Publication 30

Core Research

NMR Spectroscopy, Elucidation of molecular structures, Chiral Analysis, Weak Molecular Interactions, Metabolomics, Structural Biology, Bionanomaterials

of different acids and ester derivatives. Bifurcated intramolecular hydrogen bond in the dibenzoyl oxalamide derivatives.Orchestrated approaches have been developed using pure shift NMR for the extraction of spectral parameters, ultra-high resolution, and sensitivity enhancement

Faculty & Staff

Hanudatta S Atreya | PhD (Bombay), Associate Professor
N Suryaprakash | PhD (Bangalore), FNASc, Professor
Soumya S Roy | PhD (Univ. Of Massachusetts), Assistant Professor

3.2.4 Organic Chemistry

CHAIRPERSON
N JAYARAMAN

The Department of Organic Chemistry (OC) is one of the oldest departments in IISc, which started in the year 1911. Core strength of the Department relies on the broad areas of organic chemistry, covering all aspects of organic synthesis and application of organic chemistry principles at the interface of biological and materials chemistry.

Current Research

Organic Synthesis Synthesis of N-Heterocyclic compounds: A novel route for the diastereoselective construction of diversely substituted N-heterocyclic ring systems as valuable scaffolds for natural products and pharmaceuticals, starting from an easily accessible prochiral Î±-phenyl-Î²-enamino ester has been developed. The reaction sequence relied on the unexplored reactivity of Î±-phenyl-Î²-enamino ester as a nucleophilic partner in the Mitsunobu reaction to forge the N-tethered alkeneâˆ’alcohol/thiol/amine intermediate, which was subjected to an intramolecular hetero-Michael addition reaction under mild conditions to furnish the respective N-heterocyclic compounds embedded with an exocyclic chiral center in high yields and excellent diastereoselectivities.

Development of the first catalytic enantioselective iodoetherification of Î³,Î´-unsaturated oximes - Development of the first iridium-catalyzed enantioselective vinylogous allylic alkylation of coumarins - Visible light-mediated aerobic oxidation of boronic acids is

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53 PhD students
13 Int PhD Students
Publications 65
2 Int PhD Conferments
6 PhD Conferments

Core Research

Organic Synthesis; Peptides; Enantioselective Catalysis; Synthetic Methodologies; Asymmetric Synthesis; Transition Metal Catalysis; Total Synthesis of Natural Products; Medicinal Chemistry; Chemical Biology; C-H Activation and Functionalization; Hydrogen Economy; Cross Dehydrogenative Coupling Reactions; Green Chemistry; Carbohydrate Chemistry; Macromolecular Chemistry; Biophysical Chemistry; Organocatalysis; N-Heterocyclic Carbenes; Aryne Chemistry; Asymmetric Catalysis; Material Chemistry; a-Helical Turn Mimics; Helix Folding; Amyloidogenesis; Supramolecular Chemistry; Lanthanide Photoluminescence; Enzyme Sensing; Hydrogels; Applied Supramolecular Chemistry; Analytical Chemistry

unveiled using CdSe nanocrystal quantum dots (QDs) as the photoredox catalyst.

Total synthesis of bio-active pyrone cryptopyranmascatone B is accomplished and the structure assigned for the natural product was confirmed and the NMR data was revised by synthesis. Also, the total synthesis of the macrolactone natural product Sch 725674 was accomplished from commercially available deoxyribonolactone. A very concise stereospecific synthesis of vonduramine was accomplished from chiral pool tartaric acid. Short route for chiral diphenylpyrrolidine

methanol privileged Ligands in asymmetric catalysis was accomplished from non-racemic sulfinimines.

Water has been used as a hydride source via Pd(II)/Pd(0) catalysis. As proof of concept, an effective hydroarylation method has been developed. A stereodivergent synthesis of Z/E- olefins using H2O as the H2 source and diboron compound as the mediator under homogeneous Pd-catalytic conditions. A Co(III)-catalyzed desilylation direct ortho-vinylation of N-methyl benzamide derivatives and ortho-alkenylation of N-methyl benzamide derivatives and the alkenylation of indole at the C2-position were uncovered. An Rh(III)-catalyzed ortho-C-(sp2)-H amidation of ketones and aldehydes and novel switchable reaction to obtain either oxidative Heck-type product or 1,4-addition coupled product at the C4 position of indole with maleimide using COCF3 as a weak directing group have been achieved. A selective amination reaction has been disclosed under metal-free reaction conditions.

Modification of monosaccharides through stereocontrolled routes is conducted on unsaturated sugar synthons. A number of C1 - C2 modified sugars are secured through application of judiciously chosen rearrangement reactions. A novel latent-active concept of glycosylation is developed in O-allyl protected glycosides, through radical halogenation-mediated glycosyl activation, followed by reaction with glycosyl acceptors. Synthesis and thermodynamic studies of a conceptually new cyclic pentasaccharide, constituted with glycosidic bond expansion by a methylene moiety are accomplished. Supramolecular control on band gap opening in single-walled carbon nanotubes is demonstrated through wrapping of mannose functionalized poly (propyl ether imine) dendrimer molecules.

A conceptually new NHC-catalyzed imine umpolung for the synthesis of 4-difluoromethylquinolines has been developed. N-Heterocyclic Carbene-Catalyzed Michaelâ€“Michaelâ€“Lactonization Cascade for the Enantioselective Synthesis of Tricyclic Î´-Lactones has been demonstrated. N-Heterocyclic Carbene-Catalyzed Enantioselective Synthesis of Spiro-glutarimides via Î±,Î²-Unsaturated Acylazoliums has been uncovered. Oxidative NHC-Catalysis for the Generation of Imidoyl Azoliums for the Synthesis of Benzoxazoles has been developed. Enantioselective N-Heterocyclic Carbene-Catalyzed Cascade Reaction for the Synthesis of Pyrroloquinolines via Nâ€“H Functionalization of Indoles was developed.

Synthesis of laterally size controlled 2D single/thin-layer molecular assemblies by chemical synthesis/possessing (top-down/bottom-up method) from their corresponding precursors such as single molecular unit, single crystals, etc. have been developed. The supramolecular application of these assemblies especially in molecular recognition such as protein, DNA and macromolecular interaction has been explored. Following the synthesis, stabilization and surface fictionalization of layered assemblies, various supramolecular applications including, but not limited to, molecular recognition, sensing and catalytic applications were studied.

First access to 3(10)-helical structures in coded tripeptide sequences - by replacing an imaginary i+3-->i H-bond with a covalent H-bond surrogate (HBS) and by planarizing of the i+1st nitrogen through N-carbamation has been studied. . The resulting peptide shows 1D, 2D NMR, FT-IR and CD data consistent with the 3(10)-helical turn. The first alpha-helical turn peptides by replacing the transient i+4-->i H-bond formed in short tripeptides with a covalent H-bond surrogate (HBS) and rigidify the conformation by introducing minimal number of sp2 atoms in the cyclic ring (7 out of 13) were studied. The tertiary amide is an unavoidable feature at the i+3-i+4 junction of any HBS model; the

cis isomers at this bond are unproductive for a-helical structures.

A mild acid treatment converted green emitting Au nanoclusters to blue emitting ones. The hybrid in a bile acid-based hydrogel stabilized the luminescence. Toxic Pb2+ was detected by a turn-off luminescence. Capped CdSe quantum dots were uniformly incorporated into an organogel without affecting their photophysical properties, even when taken through a gelâ€“solâ€“gel cycle. Single nanofibers of a hybrid of CdSe/S nanorods with an organogel exhibited sharp polarized red luminescence or dual perpendicularly polarized blue/red luminescence. QROM revealed the nanorod/nanofibre alignment with high order parameters. A paper based assay using a Eu/Tb based hydrogel matrix was developed for the detection of alkaline phosphatase, and Î²-galactosidase. Rapid detection of enzyme inhibitors was also achieved.

Various supramolecular biomaterials and utilized them in rather challenging biomedical applications were studied. ±-Tocopherylated cationic gemini lipids with hydroxylated heads and studied their gene transfection properties in high serum were studied. In addition, Î±-Tocopherylâ€“Lipoic Acid conjugates were also used in drug delivery to â€˜drug-resistantâ€™ cancer cells. Fluorescent Benzimidazole-carbazole ligands were developed for targeting G4 DNA structures as well as for ratiometric probing of human serum albumin. Pyrene-based probes (having terpyridine and bispicolyl moieties) were also designed and their stimuli-responsive self-assembly properties in phospholipid vesicles were exploited.

Faculty & Staff

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Santanu Mukherjee | PhD (Cologne), Assistant Professor
A T Biju | Associate Professor
Garima Jindal | Assistant Professors
E N Prabhakaran | PhD (IIT Kanpur), Associate Professor
K R Prabhu | PhD (IISc), Associate Professor
Kavirayani R Prasad | PhD (Pune), Professor

INSA Honorary Professor

S Chandrasekaran

3.2.5

Solid State and Structural Chemistry Unit

CHAIRPERSON
ANINDA J BHATTACHARYYA

The Solid State and Structural Chemistry Unit (SSCU) was founded in November 1976. The unit has provided major thrust to frontier areas of Chemistry. Besides developing its own research and teaching programs, unit members interact closely with other departments of the institute. The unit is a premier research centre of global repute in the areas of solid state and physical chemistry. Our faculty and students work in inter-disciplinary areas at the intersection of chemistry, physics and materials science.

Current Research

Experimental and theoretical research pursued in the unit aims at understanding diverse phenomena associated with solids and condensed phases as well as liquids at the fundamental level. There is also significant emphasis on research activities aimed at development of prototypes for commercialization. Some on-going cutting-edge research areas pursued in the Unit are as follows:

SYNTHESIS, STRUCTURE, ELECTRONIC AND MAGNETIC PROPERTIES OF OXIDES

Inorganic-organic hybrid framework compounds have been studied over the years with primary focus on understanding the structure and properties. In the course of this study, it has been found that new anions such as sulfates, thiosulfates, borates can be

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IN NUMBERS

11 Academic Staff
6 Scientific Staff
68 PhD Students
18 Int PhD Students
77 Publications
1 Int PhD Conferments
11 PhD Conferments

Core Research

The work of the faculty of the Unit broadly focuses on Materials, Physical, Solid State and Theoretical Chemistry with specific emphasis on: Inorganic and Organic Materials Synthesis for Energy Generation and Storage, Statistical Mechanics, Quantum Chemistry and Electronic Structure, Multidimensional Femtosecond Microscopy, Crystallography and Structural Chemistry, Molecular Magnetic Materials and Switches, Chemistry and Physics of Organic and Inorganic Materials, Multifunctional Materials.

incorporated as part of the framework leading to interesting new families of compounds. The use of organic acids along with nitrogen containing ligands led to new compounds that exhibit proton conductivity, (photo)catalysis, heterogeneous catalysis. Some of the framework solids have shown great potential in alkali metal-ion battery chemistries and hydrogen storage.

CRYSTAL ENGINEERING, CHARGE DENSITY AND RELATED ASPECTS

Application of crystal engineering in the development of pharmaceutical solids is the main topic of research here. The main objective of crystal engineering is to design functional molecular solids with tunable properties based on intermolecular interactions. The concept of supramolecular synthon or the recognition of molecules through intermolecular interactions plays a crucial role to correlate the structure and property of crystalline solids. A wide variety of weak interactions including hydrogen bonding, π-π, halogen-halogen interactions present in single component as well as multi-component molecular crystals or cocrystals have been studied. The understanding of molecular interactions aids in the design of pharmaceutical cocrystal with improved physicochemical properties.

ORGANIC PHOTOVOLTAIC MATERIALS

Synthesis of a new class of π-conjugated polymers, and correlating their structure and properties, has been pursued in great detail. New class of conjugated polymers by various chemical routes, which control the polymer chain conformations, intermolecular interactions and disorder by rational design were initiated and utilized to fabricate optoelectronic devices. The synthetic design principles helped in developing new class of n-type conjugated polymers, which exhibit enhancement of electron charge carrier mobility. Examples of this type are rare in the literature. The conjugated polymers exhibit band-like transport, which demonstrates the effectiveness of the rational molecular design and generate potential for new class of optoelectronic devices. Understanding the photophysical properties of such systems would lead to new and efficient photovoltaic materials.

SYNTHESIS, STRUCTURE AND ELECTRONICS PROPERTIES OF MOLECULAR SEMICONDUCTORS

The main activity centers on exploring novel properties of a range of materials with an emphasis on their electronic, magnetic, dielectric and optical properties. Besides seeking new materials and properties, a major thrust is in trying to understand the origin of such novel and interesting properties, based on advanced experimental techniques and state-of-the-art theoretical approaches. Some specific highlights of the research in such directions are (a) crystal structure engineering by fine tuning the surface energy in II-VI nanocrystals e.g. /CdSe, (b) tuning of dielectric properties and magnetism of oxide materials (c) discovery of multiglass properties in partially-disordered La2NiMnO6 (d) Magnetism in Fe/Cu co-doped ZnO nanocrystals (e) Discovery of effective Mass Driven Structural Transition in Mn-doped ZnS Nanoplatelet (f) The very first demonstration of Ultra-narrow and widely tunable Mn2+ Emission from Single Nanocrystals of ZnS-CdS alloy (g) Resolving the age-old controversy regarding NiS and proving it to be an unusual self-doped, nearly compensated antiferromagnetic metal (h) The pioneering work to demonstrate the feasibility of obtaining emission across the entire visible range from an atomic transition in doped quantum dots by strain engineering and (i) A microscopic description of how the local structure, distinct from the global average structure determined by XRD, evolves in to the global structure with an increasing length-scale of the description and its consequence on the widely used concept of a chemical pressure in solid solutions.

Other studies on this front have demonstrated the occurrence of ground state charge transfer between quantum dots. This leads to the emergence of strong electrostatic forces between quantum dots, leading to the formation of a quantum dot solid. These solids exhibit chemical properties such as stoichiometry, and bear a strong resemblance to ionic compounds except that the building blocks are hundreds of times larger. In another study, possible routes to low threshold quantum dot lasers have been proposed, and novel, low threshold continuous wave quantum dot based lasers have been developed. Other studies include the development of novel synthetic methods that enable copying the morphology of a nanostructure as well as the synthesis and spectroscopy of solar energy relevant quantum dots composed entirely of earth abundant, non-toxic elements.

MATERIALS ELECTROCHEMISTRY FOR RENEWABLE ENERGY

In this area, research of the unit faculty members focuses on the synthesis of electrode and electrolyte materials for various battery chemistries and supercapacitors. Critical understanding of materials properties, their correlation with structure and function is the primary focus. Many of these studies have also involved utilization of synchrotron facilities. Synthesis involved development of multifunctional high performance soft materials, inorganic nanomaterials along with networked gel polymer

electrolytes based on organic materials have been investigated as potential candidates for various rechargeable battery chemistries.

THEORETICAL STUDIES OF ELECTRONIC AND MAGNETIC PROPERTIES OF ORGANIC MATERIALS

Studies on the electronic and magnetic properties of strongly correlated low-dimensional systems and conjugated Entanglement entropy as a handle to study quantum phase transitions in frustrated spin chains was established. The scope of valence Bond (VB) method by using new symmetries of symmetrically substituted donor acceptor systems in polyenes and polyacenes to carry out ED studies on systems spanning nearly a billion dimensional Hilbert space was extended. This method was employed to study excited state tuning in substitute polyenes and Tetracene. In addition, systems such as fused azulenes can be in magnetic ground states due to intrinsic bond frustration in electron delocalization were also established.

STATISTICAL MECHANICS CONDENSED MATTER AND BIOLOGICAL SYSTEMS

The problems of protein folding and aggregation have important implications in several neurodegenerative diseases such as Alzheimer and Parkinson's. Our faculty have recently addressed a fundamental problem in the area of protein collapse. Single domain proteins are finite-sized heteropolymers and behave like random coils at high denaturant concentrations, and fold into specific three-dimensional structures at low denaturant concentrations to perform their functions. An interesting fundamental question is whether proteins akin to polymers undergo a coil-toglobule collapse transition during the initial stages of folding (burst-phase) organic molecules have been carried out. During the course of this study, new time dependent density matrix renormalization group (DMRG) algorithm was developed to study the effect of long-range correlations on spin charge separation in polyene chains. The studies, shown through entanglement entropy studies, reveal why the DMRG method is accurate for models with longrange interactions. The DMRG method was extended to study Bethe lattices and dendrimers. On the exact diagonalization (ED) front, for the first time how to exploit both spatial and spin symmetries of systems belonging to non-Abelian point groups was shown. as the conditions are made conducive for folding. The collapse transition in proteins is generally studied using single molecule fluorescence resonance energy transfer (FRET), and small angle X-ray scattering (SAXS) experiments. The FRET and SAXS experiments disagreed on whether Protein L, a model protein used to study protein folding, collapses during the burst-phase of folding. We studied the burst-phase of folding for Protein L using a coarse-grained protein model and molecular dynamics simulations to understand the impact of various approximations used in these methods to resolve the controversy between the FRET and SAXS experiments. We found that FRET experiments overestimated Rg of the protein due to the application of Gaussian polymer chain end-to-end distribution to extract Rg from the FRET efficiency and thereby suggesting pronounced compaction in the protein dimensions in the burst-phase. We further found that the decrease in Rg is close to the statistical uncertainties of the Rg data measured from SAXS experiments, which suggested no compaction, leading to a disagreement with the FRET experiments.

MOLECULAR SIMULATION AND THEORETICAL MODEL STUDIES

A detailed theory of the effects of intermediate metastable phases on the nucleation and growth of the thermodynamically stable phase has been developed. This theory explains such novel phenomena like the role of LDL phase in the nucleation of ice from supercooled water. A theory of surface tension under the same free energy conditions was developed. Studies on protein unfolding dynamics in aqueous binary mixtures demonstrated that while DMSO preferentially melts helices, urea does the same to beta sheets. The former

was not known before this work. A theory of pair hydrophobicity in mixed solvents was developed. Studies on the origin of hydrophobic force law between two hydrophobic surfaces were initiated. In another front, the first theory of the role of vitamin D in human immune response is being developed.

MAGNETIC MATERIALS AND SWITCHES

The world of digital information storage has been run mainly by bulk magnets, which have brought significant reduction in size together with enhanced storage capacity. Yet much betterment could be brought, both in terms of size and storage space, by opting for molecular magnets which have potential applications in the field of data storage, sensors, spintronics, quantum computing etc. Molecular systems are at par owing to their several advantages such as the chemical and structural versatility, low density, solubility towards conventional solvents making them fit for various device level applications.

Research activities of the group are directed towards the rational design, synthesis and details physical characterization of new molecular magnetic materials (organic, inorganic and nanoscale). The research being conducted is interdisciplinary in nature covering wide aspects of academically driven fundamentals of magnetism and challenges of applicative world. Highlights of group activities are Electron-transfer systems, Spin-Crossover compounds, Single Molecule Magnets, Single Chain Magnets, Magnetic Nanoparticles and Quantum Dots, Switchable Metal-Organic Frameworks, Magnetic Liquid Crystals etc. We are developing multi-functional materials where our interest in studying details (Photo)magnetism, Photoluminescence, Photo- and Thermo-induced electron transfer, Magnetocaloric effect, Magneto-Optical properties etc. The switchable materials being synthesised are also studied for their applications in various MEMS devices. Theoretical calculations are also being carried to enhance the present systems and design new materials.

MULTIDIMENSIONAL FEMTOSECOND MICROSCOPY

Multidimensional Femtosecond Spectroscopy coherently excites a manifold of vibronic states and resolves the ensuing coherent dynamics with conventionally high temporal and spectral resolution. Such information has provided valuable insight into the nature of System and Bath Hamiltonians for a number of systems spanning from proteins, organic photovoltaic polymers, singlet fission materials and perovskites.

The broad impetus of the group is to develop state-of-the-art multidimensional spectroscopic tools to probe matter through controlled interactions with femtosecond pulses and apply such tools to gain a better understanding of the fundamental physics of energy and charge transfer on femtosecond timescales. Such tools will integrate sub-micron spatial resolution with the conventional femtosecond temporal resolution and high spectral resolution of multidimensional spectroscopies. This will allow to probe fundamental processes ranging from electronic and nuclear interactions among a network of chromophores packed tightly inside a photosynthetic cell, to bridging the gap between the morphology of photovoltaic thin films and device performance by correlating morphology with sub-100 fs exciton delocalization physics.

Faculty & Staff

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KR Kannan | MSc (Engg) (IISc), Senior Scientific Officer
Abhishake Mondal | PhD (Paris), Assistant Professor
S Natarajan | PhD (IIT Madras), FASc, FNASc, Professor
Anshu Pandey | PhD (Chicago), Associate Professor
Satish A Patil | PhD (Wuppertal), Professor
Govardhan Reddy | PhD (Wisconsin), Assistant Professor
DD Sarma | PhD (IISc), FASc, FNASc, FNA, FTWAS, Professor
R Sathishkumar | MTech (Madras), Senior Scientific Officer
C Shivakumara | PhD (IISc), Principal Research Scientist
Vivek Tiwari | PhD (Boulder), Assistant Professor
NY Vasanthacharya | PhD (IISc), Senior Scientific Officer

Associate Faculty

Hanudatta S Atreya | PhD (Bombay), Associate Professor
Giridhar Madras | PhD (Texas A&M), Professor
N Suryaprakash | PhD (Bangalore), FNASc, Professor
S Vasudevan | PhD (IIT Kanpur), Professor

Honorary and Emeritus Professors

Gautam R Desiraju | PhD (Illinois), FASc, FNASc, FNA, FTWAS, Honorary Professor
J Gopalakrishnan | PhD (IISc), FASc, FNA, FNASc, FWIF, Emeritus and NASI Senior Scientist

3.3 Division of Electrical, Electronics, And Computer Science

IN NUMBERS

- 98 ACADEMIC STAFF
- 361 PhD STUDENTS
- 380 MASTER'S STUDENTS

The Division is assiduously seeking fundamental advances in the following core areas: Signal Processing, Communications, Networks, Microelectronics and Devices, Photonics, Theoretical Computer Science, Computer Systems and Software, Artificial Intelligence and Machine Learning, Control and Optimization, Power Systems, Power Electronics and High Voltage Engineering.

THEMES

A feature of the Division's R&D activities is its focus on rigorous innovation in contemporary, interdisciplinary themes: Cyber Physical Systems, Big Data Analytics, 5G Technologies, Devices for Healthcare, Electronics for Strategic Sector, Network Science, Cybersecurity, Neuromorphic computing, Image and Video Processing, and Smart Grids.

RESEARCH HIGHLIGHTS

The Division of Electrical, Electronics, and Computer Sciences comprises four Departments: Computer Science and Automation; Electrical Communication Engineering; Electrical Engineering; and Electronic Systems Engineering. A feature of the Division's R&D activities is its forays into contemporary, inter-disciplinary, and nationally relevant themes including Cyberphysical Systems, Cybersecurity, Data Science, and Neurocomputing. The Division is also actively participating in Institute level programs on Smart Energy, Smart Water, Smart Cities, and Devices for Healthcare, and Electronics for the Strategic Sector

DEPARTMENTS | CENTRES | UNITS

- COMPUTER SCIENCE AND AUTOMATION
- ELECTRICAL COMMUNICATION ENGINEERING
- ELECTRICAL ENGINEERING
- ELECTRONIC SYSTEMS ENGINEERING