Poornaprajna Institute of Scientific Research

(Promoted and managed by Admar Mutt Education Foundation)
{Recognized by DSIR, Govt. of India and Manipal Academy of Higher Education}

Annual Report 2018-19

Winter School in Chemistry, Physics and Biology was organized for undergraduate students of Poornaprajna College, Udupi at PPISR in November 2018.

Invited talk by Prof. C V Rode, Sr. Scientist, NCL Pune on August 21, 2018

The Founder's Day conference was organized at PPISR in July 4-5, 2019. Prof. Ramaswamy, Professor, JNCASR, Bengaluru was the Chief Guest for inaugural function.

Founder's Day Technical Session Talk by Prof. Ravishankar, Professor, Materials Research Centre, IISc, Bengaluru on July 5, 2018

The valedictory function of Founder's Day on July 05, 2019 was presided over by Prof. M. R. S. Rao, Professor, JNCASR, Bengaluru.


ದೇಶದ ಪ್ರಗತಿಗೆ ವಿಜ್ಞಾನ, ತಂತ್ರಜ್ಞಾನದ ಪಾತ್ರ ಮಹತ್ತರ

PPISR joins hand with Nagarjuna College of Engineering and Technology, Chikkaballapur to Conduct state level NECT Science Festival in January 2019.

3. MEMBERS OF BOARD OF TRUSTEES/ MANAGEMENT

H. H. Sri Vishwapriya Theertha Swamiji Peetadhipathi, Sri Admar Mutt, Udupi	Chairman
H. H. Sri Eeshapriya Theertha Swamiji	Junior Swamiji, Shri Admar Mutt, Udupi
Dr. K. Srihari, Professor (Rtd), UAS, Bengaluru	Hon. Secretary
Sri. M. Ashok Kumar, Chartered Accountant	Hon. Treasurer
Sri B.R. Prabhakara, IAS, Former Chief Secretary Govt. of Karnataka	Member
Sri V. V. Bhat, IAS, (Retd), Former Secretary to the Govt. of India	Member
Sri Rajendra J. Hinduja, Industrialist, Bengaluru	Member
Sri Laxmisha G. Acharya, Industrialist, Mumbai	Member
Dr. U. Shankar Rao, Medical Director, National Hospital, Chennai.	Member
Padma Shri Dr. V.R. Prahalada, Former Vice Chancellor, Defence Institute of Advanced Technology, Pune	Member
Sri. H. L. Suresh, Chairman, Axens India Pvt. Ltd., New Delhi	Member
Prof. V. Nagaraja, President, JNCASR, Bengaluru	Member
Dr. Anand B. Halgeri, PPISR	Director
Sri P. Sreenivasa Rao, PPISR	Financial Advisor
Padma Vibhushan Prof. P. Rama RaoFASc, FNA, FNASc, Ex. Secretary, Ministry of S &T, GOI	Special Advisor
Sri K. R. Prasad, Advocate, Bengaluru	Special Advisor

4. RESEARCH ADVISORY COMMITTEE

1. Padma Shri Dr. V. R. Prahalada, Former Vice Chancellor, Defence Institute of Advanced Technology, Pune
2. Prof. C. Sivaram, Professor, Indian Institute of Astrophysics, Bengaluru
3. Prof. K.R. Krishnamurthy, Chair Professor, National Centre for Catalysis Research, IIT Madras, Chennai
4. Prof. G. U. Kulkarni, Director CeNS and Professor, JNCASR, Bengaluru
5. Prof. A Jagannadha Rao, Professor, Raja Ramanna Fellow; DST, Department of Biochemistry, IISc, Bengaluru
6. Prof. T.N. Guru Row, Professor,SSCU, IISc, Bengaluru
7. Prof. Chandrabhas Narayana, Professor, CPMU, JNCASR, Bengaluru
8. Prof. S. Ramakumar, Professor, Bioinformatics Centre, IISc, Bengaluru
9. Prof. T. M. Aminabhavi, CSIR Emeritus Scientist, Former Professor, KUD
10. Prof. A. B. Halgeri (Member Secretary), Director, PPISR

5. DOCTORAL ADVISORY COMMITTEE

1.	Prof. C. Sivaram	Indian Institute of Astrophysics, Bengaluru
2.	Prof. T. N. Guru Row	SSCU, IISc, Bengaluru
3.	Prof. S. Ramakumar	Physics Dept., IISc, Bengaluru
4.	Prof. A. J. Rao	Biochemistry Dept., IISc, Bengaluru
5.	Prof. S Natarajan	SSCU, IISc, Bengaluru
6.	Prof. A. M. Umarji	SSCU, IISc, Bengaluru
7.	Prof. Shivashankar	Materials Research Center (MRC), IISc, Bengaluru
8.	Prof. B. R. Jagirdar	IPC Dept, IISc, Bengaluru
9.	Prof. Anjali A Karande	Dept of Biochemistry, IISc, Bengaluru
10.	Prof. Dipankar Nandi	Dept of Biochemistry, IISc, Bengaluru
11.	Prof. Rajeev Ranjan	Materials Engineering, IISc, Bengaluru
12.	Prof. Prabeer Barpanda	Materials Research Centre, IISc, Bengaluru
13.	Prof. B. S. Jai Prakash	Director, IEHMM, BIT campus, Bengaluru
14.	Prof. Chandrabas N.	JNCASR. Bengaluru
15.	Dr. Tapas Kumar Maji	CPMU, JNCASR, Bengaluru
16.	Dr. Sebastian C. Peter	JNCASR, Bengaluru
17.	Dr. Govindaraju T.	New Chemistry Unit, JNCASR, Bengaluru
18.	Dr. Meher K. Prakash	Biophysics group, JNCASR, Bengaluru
19.	Prof. Ramachandra	Chairman and Director, Centre for Fundamental Research and Creative Education, Bengaluru
20.	Prof. H. G. Nagendra	MVIT Engg. College, Bengaluru.
21.	Dr. R.Ravishankar	Deputy General Manager, HPCL, Bengaluru.
22.	Dr. P. Manikandan	Senior Manager, SABIC Research Centre, Bengaluru
23.	Dr. G S. Rao	Sr. Scientist, SABIC Technology Centre, Bengaluru
24.	Dr. N. S. Raviraja	Stempeutics Pvt. Ltd., Manipal.
25.	Prof. Rajeev Joshi	Central University Karnataka, Kalaburagi.
26.	Prof. N. Nagaraju	St. Joseph College, Bengaluru
27.	Prof. V Gayatri	Dept of Chemistry,Central College,Bangalore University
28.	Dr. Ramakrishna Matte	Centre for Nano and Soft Matter Sciences, Blru
29.	Dr. D. A. Nagegowda	Mol. Plant Biology & Biotech. group, GKVK, Blru
30.	Prof Rajeev Joshi	Central University of Karnataka, Kalburgi
31.	Prof. Y. S. Bhat	Emeritus Professor, PPISR and Former HOD, Chemistry Dept, BIT, Bengaluru.
32.	Dr. Chandrasekhar	Ex. HoD, Chem. Dept. Central University Gulbarga
33.	Dr. Shanti K.N.	PES University, Bengaluru
34.	Prof. S. K. Srivatsa	Atria Institute of Technology, Bengaluru

6. ORGANIZATION

Director: Dr. Anand B. Halgeri
Financial Advisor: Sri P. Sreenivasa Rao

Core Faculty:
Dr. Udupi A. Ramagopal
Dr. Sujit Sarkar
Dr. Srikanth R.
Dr. Ananda Kulal
Dr. Ganapati V. Shanbhag
Dr. Nalini G. Sundaram
Dr. Sanjeev P. Maradur
Dr. Suresh Babu Kalidindi
Honorary Professor:
Dr. Rajappan Vetrivel

Adjunct/ Honorary Faculty:

Prof. S. Asokan	IISc, Bengaluru (Glasses & Sensors)
Prof. T. N. Guru Row	IISc, Bengaluru (Crystallography)
Prof. K. G. Satyanarayana	Ex.Director, RRL (Polymers)
Prof. B. S. Jaiprakash	BIT/IEHMM, Bengaluru (Catalysis)
Prof. Y. S. Bhat	Former Professor, BIT, Bengaluru (Catalysis)
Prof. B. S. Ramchandra	CFRCE, Bengaluru (General relativity)
Prof. S. K. Srivatsa	Atria Institute of Technology, Bengaluru (Liquid Crystals)

Administration:

Senior Administrative Officer:	Mr. Kishore L. Gaikwad
Accounts Officer:	Mr. Nagarajan R.
PA to Director:	Mrs. Latha Srinivasan
PA to Financial Advisor:	Mrs. Nandini S.

Support staff:
Mr. Vishwaprakash A.
Mr. Praveen Kadam
Mr. Sriramappa S.
Mr. Shashidhara
Mr. Basavaraj

7. ABOUT THE INSTITUTE

Poornaprajna Institute of Scientic Research (PPISR) is situated near Bengaluru International Airport on a sprawling campus spread over 32 acres. It was conceptualized and founded by the pontiff of Admar Mutt H. H. late Sri Vibudhesha Theertha Swamiji. It was his vision to create a serene and congenial environment, where scientists would be inspired to carry out innovative and original research in fundamental and applied sciences. The foundation stone for the research campus was laid in 1998 by the then Prime Minister of India Sri Atal Behari Vajpayee. The institute is recognized by Department of Scientific and Industrial Research (DSIR), Govt. of India, New Delhi and Manipal Academy of Higher Education, Manipal, Karnataka, as an R&D centre. Currently, there are three departments; Theoretical Sciences, Materials Science and Biological Sciences, where advanced research activities are being conducted.

It is presently enthusiastically carried forward by the present Chairman HH Sri Vishwapriya Theertha Swamiji to make Poornaprajna Institute of Scientic Research a Centre of Excellence in order the realize the dreams of his Guruji H H Sri Vibudhesha Theertha Swamiji. H H Vishwapriya Theertha Swamiji has keen interest on the research activities of PPISR. The infrastructure is being constantly upgraded to meet the academic requirement and for scientists and student activities. In a short span of three years, H H Sri Vishwapriya Theertha Swamiji had inaugurated the new Biological Sciences laboratory, a new hostel building. Bharat Ratna Prof. C. N. R. Rao has donated a Materials Science Laboratory to carry out world class research at Bidalur campus.

The Institute has nine core faculty members, several distinguished professors as adjunct and honorary professors and 35 distinguished scientists from various renowned organizations. So far, eleven students from PPISR have obtained their PhD degree from MAHE, Manipal. Presently, 19 doctoral students, one postdoctoral fellow and several project assistants are actively involved in research activities on many sponsored projects both from Government agencies and as well as from industries. Till date, the Institute has published more than 230 papers in International peer reviewed journals. Three international patents have been filed in HPCL collaborative project, out of which, one US patent is granted in March 2018. The combined average impact factor of our publications is 2.8, higher than that of several leading institutions in the country.

PPISR is promoted and managed by Admar Mutt Education Foundation (AMEF). It is a part of a large family of sister institutions, which also includes around twenty nine Poornaprajna Schools, Poornaprajna Institute of Management and the Poornaprajna Institute of Faculty improvement, governed by the Udupi Sri Admar Mutt Education Council (AMEC). All these developments would not have been possible without the guidance, support and blessings from H H Sri Vishwapriya Theertha Swamiji and Sri Eeshapriya Theertha Swamiji. The excellent support from the management of Admar Mutt Education Foundation with the cooperation of all faculty members, students, and staff of PPISR has contributed immensely towards realising our founder chairman's vision.

8. DIVISION STRUCTURE

Faculty	Research Scholars/ Project Students
MATERIALS SCIENCE AND CATALYSIS	
Dr. A. B. Halgeri (Catalysis) Professor and Director	-
Dr. G. V. Shanbhag (Heterogeneous Catalysis) Associate Professor	Dr. Manjunathan P., Mr. Nagendra Kulal, Ms. Vaishnavi B. J., Mr. Manjunath D., Mr. Sujith S., Mr. Neehar P., Mr. Rahul R., Mr. Pandurang D., Mr. Subramanya K. S., Ms. Nimisha S., Mr. Madhav N.
Dr. Nalini Sundaram (Nanomaterials) Associate professor	Mr. Pradeep Shanbhog, Ms. Archana R., Ms. Chethana A.
Dr. Sanjeev P. Maradur (Heterogeneous Catalysis) Asst. Professor	Mr. Satyapal Churipard, Mr. Kempanna Kanakikodi, Ms. Arpana
Dr. Suresh Babu Kalidindi (Metal-organic frameworks) Asst. Professor(DST-INSPIRE)	Mr. Vasudeva Rao B., Ms. Marilyn E Dmello
BIOLOGICAL SCIENCES	
Dr. U. A. Ramagopal (Structural Biology) Associate Professor	Dr. Raghurama P.Hegde(Research Associate), Ms. Pavithra G. C., Ms. Swetha L, Mr. Shankar Kundapura
Dr. K. Ananda(Microbiology) Associate Professor	Ms. Kavitha K. N., Mr. Kirana M. P. Ms. Shrilakshmi S.
THEORETICAL SCIENCES	
Dr. Sujit Sarkat (Condensed Matter) Associate Professor	Mr. Rahul Sharma, Mr. Ranjith Kumar R., Mr. Kartik Y. R.
Dr. R. Srikanth (Quantum Information) Associate Professor	Mr. Shrikant Utagi, Mr. Vinod Rao

9. MISSION

* To carry out research in the selected frontier areas of basic and applied sciences

* To encourage and support sponsored research programmes by giving necessary infrastructure to them

* To encourage collaborations with industries for focused and application oriented research

* To promote collaborative research with scientists in academia in the country

* To produce PhDs of highest caliber and to make them highly competitive for their future career

* To provide a forum for scientific discussions on frontier scientific topics which are vital for the scientists of PPISR in particular and the institutes of the country in general

* To organize periodic summer and winter schools for the young undergraduate and graduate students

* To provide opportunities for talented young students to carry out short-term research projects

* To provide facilities to visiting scholars and faculty from all over India and abroad to work with the faculty of the institute.

* To publish research articles in reputed national/ international journals of high impact

* To file patents on research findings of potential commercial applications

10. CURRENT SPONSORED PROJECTS

10.1 Government sponsored projects

1. α-amylase and α-glucosidase inhibitors from endophytic fungi for treating Type 2 diabetes
   Principal Investigator: Dr. K. Ananda
   Funding agency: VGST-Karnataka (2017-2020)

2. Effect of electron beam radiation on endophytic fungi producing ligninase enzyme"
   Principal Investigator: Dr. K. Ananda
   Funding agency: DAE-BRNS, Govt. of India (2014-2018)

3. Chemical fixation of CO_2 by converting into value-added chemicals using metal modified nanoporous silicate catalysts
   Principal Investigator: Dr. Ganapati Shanbhag
   Funding agency: CESEM Grant, VGST, Govt. of Karnataka (2015-2019)

4. Feasibility study of a practical Realization of a protocol for semi-counterfactual quantum key distribution (QKD)
   Principal Investigator: Dr. R. Srikanth
   Funding Agency: DRDO, India (2018-2020)

5. Computational speedup in quantum mechanics and generalized probabilistic theories
   Principal Investigator: Dr. R. Srikanth
   Funding agency: DST-SERB, India (2017-2020)

6. Center for Excellence in quantum cryptography
   Principal Investigator: Prof. Anirban Pathak
   Co-Investigator: Dr. R. Srikanth, II
   Funding Agency: QuST (DST) (2019-2021)

7. Topological States of Superconducting Nanowires and interacting light-mattersystems at nano scales
   Principal Investigator: Dr. Sujit Sarkar
   Funding agency: DST-SERB, India (2016-2019)

8. Design of modified B7-1 (CD-80) and B7-2 (CD86) molecules to create potential reagents for cancer and auto-immune disorders", Vision Group on Science and Technology (VGST), Karnataka.
   Principal Investigator: Dr. Udupi A. Ramagopal

Funding agency: VGST-Karnataka (2014-2018)

9. Structural and evolutionary investigations on antibiotic resistance conferring rRNA methyltransferases for designing novel strategies of drug development, Department of Science and Technology, India.
   Principal Investigator: Dr. Udupi A. Ramagopal
   Funding agency: DST-SERB, India (2016-2019)

10. Design and Development Stable Metal Organic Frameworks with Multiple Functional Sites for Catalysis
    Principal Investigator: Dr. Suresh B. Kalidindi,
    Funding agency: DST under INSPIRE (2015-2020)

11. Transformative Crystalline Hybrid Porous Materials: Chemical Synthesis and Applications
    Principal Investigator: Dr. Suresh B. Kalidindi
    Funding agency: DST (2016-2019)

12. Phase Transitions in $BiMWO_6$ (M=Ce,fe,Cr) Smart Functional Nanomaterials
    Principal Investigator: Dr. Nalini G. Sundaram
    Funding agency: UGC-DAE CSR Mumbai Centre, India (2016-2019)

10.2 Industry sponsoredprojects

1. Catalyst and process development for aromatics alkylation to make higher aromatics(Sponsored by Deepak Novochem Technologies Ltd., Pune)
   PI: Dr. Ganapati V Shanbhag;
   Co-PI: Dr. Sanjeev P Maradur
   Year: 2018-2019

2. Design and development of a catalyst and process for regioselective nitration of O-Xylene to , 4-nitro-o-xylene (4-NOX) *(Sponsored by* Deepak Nitrite Ltd, Vadodara, India)
PI: Dr. Sanjeev P Maradur;
Co-PI: Dr. Ganapati V Shanbhag
   Year: 2019-2020

3. Design and development of a catalyst and process for C_1-C_3 hydrocarbon conversion to olefins and aromatics *(Sponsored by: PW Technology, USA)*
   PI: Dr. Ganapati V Shanbhag;
   Co-PI: Dr. Sanjeev P Maradur
   Year: 2016-2018

4. Design and development of a catalyst and process for selective methylation of benzene/ toluene to produce *p*-xylene *(Sponsored by: GTC Technology, USA)*

PI: Dr. Ganapati V Shanbhag;
Co-PI: Dr. Sanjeev P Maradur
Year: 2011-2019

5. Catalyst testing and process optimization for Liquid Phase Isomerization (LPI) (Sponsored by: GTC, USA) 2018

PI: Dr. Ganapati V Shanbhag;
Co-PI: Dr. Sanjeev P Maradur

6. Development of novel catalysts for light naphtha valorization
(Sponsored by: Hindustan Petroleum Green Research and Development Centre (HPGRDC), Bengaluru

PI: Dr. Ganapati V Shanbhag;
Co-PI: Dr. Sanjeev P Maradur
Year: 2015-2018

7. Catalyst evaluation studies for methanol reforming for fuel Cell applications *(Sponsored by* Thermax Industries Pune, India)

PI: Dr. Sanjeev P Maradur;
Co-PI: Dr. Ganapati V Shanbhag
Year: 2017-2018

8. Development of Novel Mesoporous Polymer Based Catalysts for Low Temperature Catalytic Applications" Sponsored by Hindustan Petroleum Green R&D Center, Bengaluru

PI: Dr. Sanjeev P Maradur;
Co-PI: Dr. Ganapati V Shanbhag
Year: 2016-2018

11. NATIONAL AND INTERNATIONAL COLLABORATIONS

PPISR has MOU with many institutes for collaborative research like Argonne national laboratory, Chicago, IIT-madaras, Central university Gulbaraga, MSRIT Bengaluru, Genelon institute of life science pvt ltd Bengaluru**,** Nagarjuna College of Engineering and Technology (NCET), Bengaluru , Sir M Visvesvaraya Institute of Technology, Bengaluru **(**SIR MVIT), and Niranthara Scientific Solutions Private Limited ("NSSPL")

The research groups of PPISR frequently collaborate with various national institutes like IISc Bengaluru, JNCSAR Bengaluru, RRI Bengaluru, several IITs, IISERs, MIT manipal, NCL Pune.

The Faculty at PPISR also have international collaborations with various renowned institutions like

- Max Planck Institutes Stuttgart, Germany
- Ulm university, Germany
- Albert Einstein College of Medicine, New York, USA.
- Oak Ridge National Laboratory(ORNL), Tennesse, U.S.A
- Elettra Synchrotron Laboratory,Trieste, Italy
- Australian Nuclear Science and Technology Organization(ANSTO), Sydney
- Global Innovative Center for Advanced Nanomaterials, University of Newcastle, Australia

12. MATERIALS SCIENCE AND CATALYSIS DIVISION

Established in May 2010 by the present Director, Prof. A. B. Halgeri and Prof. K. J. Rao, then Chairman, Executive Committee of AMEF, the department now consists of a core of five faculty members hailing from diverse background as chemistry, industrial chemistry and biochemistry. A new materials synthesis laboratory, with several sophisticated equipment, has been established in the group. Bright students passionate for research were interviewed and inducted into Doctoral Programme in the Department.

Mission of the department:

1. To forge a fruitful academia-industry partnership by innovating, designing and developing novel multifunctional materials that have wide-ranging applications, in catalysis, nanotechnology, new materials design etc.

2. To develop a strong doctoral programme to train students by fostering excellence and original thinking.

The department engages with other national academic institutions through collaborations, education training and outreach activities.
Broad areas of the research: (1) Heterogeneous catalysis (2)Novel micro/mesoporous materials for green chemical processes (3) Biomass conversion to value added products (4) Chemical fixation of CO_2 (5) X-ray crystallographic studies (6) Functional nanomaterials (7) Photocatalytic and photoluminescent materials (8) Mesoporous Polymers (9) Metal-organic frameworks(MOFs)

Academic and sponsored research highlights:

Catalysis Group:
Catalysis is one of the important fields of research in the area of applied chemistry. Catalysts play a vital role in providing society fuels, commodity and fine chemicals, pharmaceuticals, polymers and means for protecting the environment. At PPISR, two research groups are working in the area of heterogeneous catalysis.

Dr. Ganapati Shanbhag's group is involved in frontier research in the area of catalysis such as design of novel catalysts for green chemical processes such as catalytic conversion of CO_2 into value-added chemicals, conversion of biomass byproducts like glycerol and furfural to value-added chemicals, pore engineering of microporous materials for shape selective catalysis etc. The work on mesoporous metal oxides as the novel solid acid catalyst for alcoholysis of furural alcohol and glycerol reaction is under progress. Till 2018, the group has published 23 research articles in internationally reputed journals, co-inventors in 3 patents and two book

chapters. A project on "Chemical fixation of CO_2 by converting into useful chemicals using modified nanoporous catalysts" sponsored by VGST, Govt. of Karnataka has successfully completed two years with two research publications in ChemCatChem (Wiley) journal and Journal of CO_2 utilization (Elsevier). Four students have obtained their PhD degree under Dr. Shanbhag so far. Dr. Ganapati Shanbhag gave an invited talk on his research work at prestigious "3rd International Conference on Emerging Advanced Nanomaterials 2018 (ICEAN-2018)" held in Univesrity of Newcastle, Australia. He received international travel grant from DST for this event. Dr. Shanbhag has been invited to give talks in other prestigious international conferences *viz*. "Carbon Capture and Its Utilization (CCU)" held at CSIR-National Chemical Laboratory, Pune in December 2018 conducted in association with Royal Society of Chemistry and at prestigious 5th Indo-French symposium at NCL, Pune in February 2019. Manjunathan P. received 2nd prize in K V Rao Research Awards for the year of 2017-18 in Chemistry. Consiquently he obtained his PhD degree in July 2018 and became 4th student to obtain PhD from this group. Dr. Manjunathan also won Best Oral Presentation award at CCU conference at NCL. During 2018-2019, 4 sponsored projects are conducted by the Dr. Shanbhag's Group. A new project on "Design and development of a catalyst and process for the conversion aromatics" sponsored by GTC Technology Inc, USA was continued with Dr. Shanbhag as PI and Dr. Maradur Co-PI. "Process development for liquid phase isomerization (LPI)" sponsored by GTC, USA in collaboration with Clariant AG, Switzerland was successfully completed in June 2018. Deepak Novochem Technologies Ltd. sponsored a one year project on "Catalyst and process development for aromatics alkylation to make higher aromatics" in November 2018. A Govt. project sponsored by VGST under CESEM grant on "Chemical fixation of CO_2 by converting into value-added chemicals using metal modified mesoporous silicate catalyst" is under progress. Overall, this year has been quite an eventful for this group in academic and sponsored research programmes.

Dr. Sanjeev Maradur and his group are working on novel mesoporous polymers, supported metal oxides, mesoporous zeolites for catalytic applications. His project on conversion of waste plastic to fuels sponsored by Thermax industries, Pune is successfully completed. A new project sponsored by HP Green R & D Centre on design and development of polymeric materials for catalytic applications was initiated in February 2016 with Dr. Sanjeev Maradur as PI and Dr. Shanbhag as Co-PI. Deepak nitrite sponsored a project on "Design and development of a catalyst and process for regioselective nitration of O-Xylene to 4-NOX" in February 2019. Another project on "Catalyst evaluation studies for methanol reforming for fuel Cell applications" Sponsored by Thermax Industries Pune, India was successfully completed.

Functional Energy Nanomaterials Group:

Dr. Nalinin's group work extensively in key energy areas such as photocatalysis, Photoluminescence, Gas sensing and Ferroelectrics. Research in the group is focussed on the structure-property relationship of functional materials. The group primarily employs low temperature, versatile, simple methods of nanoparticle synthesis coupled with X-ray and Neutron diffraction as tools to envisage a knowledge based design of materials. Current projects include, design of new bismuth based materials for visible light photocatalysis, rare earth complex photoluminescent oxides for theronastic applications, perovskite nanomaterials for low concentration gas sensing at low temperatures and Lead free materials for relaxor ferroelectric and magnetoelectric applications. In the last few years, the group has established many collaborations with various scientists working in many prestigious international as well as national institutes and laboratories such as ORNL, U.S.A, ANSTO, Austrailia, IISc and JNCASR, India. Currently three doctoral students are working in different areas and three sponsored projects are being implemented. This year, the group also has published more than 10 publications in peer reviewed, high impact journals and the students have obtained awards in international and national conferences and workshops.

Materials design group:

Dr. Suresh and his co-workers are involved in the designing of Metal-Organic Frameworks (MOFs) for catalysis, gas sensing, and photocatalysis applications.Crystalline materials like metal-organic frameworks (MOFs) maximise understanding of the link between atomic-scale structure and function and facilitates the explanation of macroscopic events on the basis of interactions occurring at the molecular level. As their names suggest, MOFs are built from the connectivity of organic linker and metal ions/metal clusters, The property that makes these classes of materials distinctly different from others is their "supertunability" i.e., the ability to modulate their properties by modifying the building blocks while maintaining the basic topology.

The group works on the designingof metal-MOF, metal-oxide MOF hybrid materials for catalysis and gas sensing applications. The group currently executing two DST sponsored projects in these areas. The work involves development of new synthetic strategies basing on the principles of chemistry, extensive characterization of materials using PXRD, TEM, BET surface analysis etc. and exploration of synthesized materials for well-aimed applications.

12.1 Faculty Profiles

Dr. A. B. Halgeri

Professor and Director, PPISR
Email: abhalgeri@gmail.com,
director@poornaprajna.org

Homepage:
http://www.ppisr.res.in/faculty/b-halgeri

EDUCATIONAL QUALIFICATIONS:

1. Masters Degree in Chemistry from Karnataka University, Dharwad

2. PhD in Physical Chemistry (Heterogeneous Catalysis) from Bangalore University

3. Post-Doctoral researcher under UNESCO fellowship on Zeolite Catalysis at Department of Tokyo institute of Technology

AREAS OF INTEREST:

Dr. Anand B. Halgeri is currently working as Director of Poornaprajna Institute of Scientific Research and coordinating the entire research activity in Catalysis/ Materials science & Biological sciences. His area of interest includes Nano catalysis, Heterogeneous catalysis, mesoporous materials, novel Zeolites, Solid Acid/ BaseCatalysts, Industrial Refinery/petrochemical processes, adsorption, Eco-friendly processes, and Biodiesel/Biofuel, alternate energy feed stocks etc. He has taken several industrial research projects both from India and abroad in the area of Zeolite Catalysis and Materials Science.

CURRENT ACHIEVEMENTS:

- Prof. Halgeri is actively involved in the industrial projects and, is responsible for getting sponsorships from the companies M/s GTC Technologies, USA, HPCL R & D, and Shell Technology India Pvt Ltd. The process technology for development of catalyst &process for the production of paraxylene which is raw material for polyester industry has been developed in association with GTC and is likely to be commercialized in PetroChina.

Industrial projects successfully completed under his dynamic leadership are as follows:

- Design and development of a catalyst and process for selective methylation of benzene/ toluene to produce *p*-xylene
(Sponsored by: GTC Technology, USA)

- Post-synthesis pore engineering and surface treatment of zeolites and some oxide materials
(Sponsored by: Shell Technology Centre, Bengaluru)

- Development of Zeolite Modified Catalysts for the Hydrocarbon Conversions such as light naphtha aromatization and side chain alkylation of toluene.
(Sponsored by: HPCL R&D Centre, Bengaluru)

ONGOING INDUSTRIAL PROJECTS:

1. **"**Development of a Novel Mesoporous Polymer Based Soild Acid Catalyst for Low Temperature Catalytic Applications" sponsored by HPCL (R&D)
2. "Development of Novel Catalyst for light naptha volarisation" sponsored by HPCL (R&D)
3. "Natural gas conversion to value-added chemicals" sponsored by to M/S. GTC Technology US LLC
4. Catalyst evaluation studies for methanol reforming for fuel Cell applications (Sponsored by Thermax Industries Pune, India)

ONGOING GOVERNMENT AGENCY SPONSORED PROJECTS:

Several projects sponsored by government agencies like DBT, DST, BRNS, DRDO, VGST are being carried out at PPISR.

MAJOR ACHIEVEMENT AT PPISR

During his tenure as the Director, first batch of 10 research scholars have obtained their PhD degrees at PPISR

Successfully completed several industry sponsored project under his leadership.

Under his leadership as Chairman, prestigious 23nd National Symposium on Catalysis (CATSYMP-23) was successfully conducted, during January 17-19, 2018 at Bengaluru.

PUBLICATIONS AND PATENTS

He has published 150 research papers in national and international peer reviewed journals and has also obtained 35 Indian and International patents.

PhDS GUIDED

Three doctorates under his guidance are:

1. Mrs. Swetha Sandesh (Guide)
2. Mr. Vijayakumar M (Co-Guide)
3. Mr. Janardhan HL (Co-Guide)

PREVIOUS R & D ACCOMPLISHMENTS IN INDUSTRY

Dr Halgeri, joined in a newly established Research Centre of the Indian Petrochemicals Corporation Ltd (IPCL), Baroda – Gujarat in 1976. As an Vice President and Head of R&D Division of the Public Sector Indian Petrochemicals Corporation Ltd. Baroda, Gujarat, Dr. Halgeri provided sustained leadership to the large number of scientists engaged in research and Development activities. Later, Dr. Halgeri joined the Research and Development Centre of Reliance Industries Ltd, where he led a team of 150 Scientists and Engineers and coordinated the entire research and development activities on catalysts required for the Petrochemical units and Refineries. He also provided the research support for the Polymer Science and Technology, and Materials Science groups of all the units of Reliance Industries at different locations.

Before joining PPISR, Dr. Halgeri has worked extensively and achieved several milestones in the development and commercialization of catalysts for the petrochemical industry. Dr. Halgeri's contribution in the area of catalysts has helped putting India in the world map of petrochemicals. In recognition of his outstanding contribution, Dr Halgeri has received several National awards and Honors for his achievements in Chemical Technology.

AWARDS AND HONOURS

In recognition of his outstanding contribution in the area of heterogeneous catalysis for over three decades, he has received several National awards and Honors for his achievements in Chemical Technology.

1] I.C.I. India Ltd Award of Indian Institute of Chemical Engineers has been conferred to him for Excellence in process/Product development for para-diethyl benzene

2] Hari Om Ashram Prerit- Prof. S. S. Bhatnagar Endowment Research Award for Excellence in Applied Catalysis

3] Lifetime Achievement Award "Eminent Scientist in Catalysis" by the Catalysis Society of India, Indian Institute of Technology, Madras.

4] Elected as "Fellow of Institute of Chemical Engineer" by Indian Institute of Chemical Engineers, Kolkatta

5] Vividhalaxshi Audyogik Samshodhan Vikas Kendra, Mumbai, VASVIK Industrial National Award in Chemical Sciences and Technology - 2005

6] Prof. K.G. Naik Memorial Gold Award of M.S. University, Baroda – 2007 for outstanding achievements in Chemical Sciences

7] Awarded as "Pride citizen of Baroda" for his significant contribution for Science & Technology from Community Science Centre/Rotary Club of Baroda-2008

8] Life time achievement award by CSI-Bengaluru Chapter for his contribution towards Catalysis research in India during CATSYMP-23 in January 2018.

He has extensively travelled and presented several lectures/papers in International and National conferences. Currently, he has been advisor for many Industrial R&D and also member of Board of studies in Chemical Engineering Departments in many Engineering Colleges.

RAJAPPAN VETRIVEL

Honorary Professor
Materials Science and Catalysis Division
Email: Rajappan.vetrivel@poornaprajna.org

Brief CV:

2007 – 2018: R&D Manager – Shell Technology Centre, Bangalore

2000 – 2007: Team Leader – GE Global Research Centre, Bangalore

1989 – 2000: Scientist – NCL, Pune

1986 – 1988: Research Fellow – University of Keele, Keele, UK

1984 – 1985: Research Officer – IPCL, Vadodara

1979 – 1984: Ph D (Catalysis) – IIT, Madras

1974 – 1979: B Sc & M sc (Chemistry) – Madurai Kamaraj University

Research Expertise:

- "Structure-Property-Performance" correlations in catalyst materials
- Electronic properties of catalyst surfaces
- Modeling and simulation for design of materials for catalytic and related functions
- Materials of interest include catalysts, metal hydrides, zeolites, SWCNT & semi-conductors and devices such as VLSI, Al-CVD, OLED, organic-PV, Nano-PV, PEM based fuel cells, polymer membranes, gas sensors, hydrocarbons and energy materials.

Accomplishments and Recognitions:

- Visiting Associate Professor at Tohoku University, Sendai, Japan from 1993 to 1994 and conducted research under Indo-Japan collaboration program
- Visited University of Cambridge & University College London, UK to perform research studies in Indo-UK collaborative research program
- Visited 'Ecole Nationale Superieure de Chimie', Montpellier, France in 1988 & 1989 for an Indo-French project
- Was conferred the Best Young scientist award – Gold medal (1998) of Catalysis Society of India
- Life member of the Catalysis Society of India, Elected executive committee member and Assistant Editor of Bulletin of the Catalysis Society of India.
- Life member of the Polymer Society of India

- Elected Fellow of the Maharashtra Academy of Sciences
- I supervised 3 research students of NCL, Pune who were awarded Ph D degree by University of Poona, Pune
- I published ~125 research articles in peer reviewed journals
- I have filed 7 global patents and 4 patent applications
- I obtained management recognition awards in the form of company shares for leading R&D projects that led to business benefits

PUBLICATIONS AND PATENTS

He has published 125 research papers in national and international peer reviewed journals and has also obtained Indian and International patents.

R. Vetrivel Et Al, J. Mol. Structure (Theochem), 94, 187 (1983).

R. Vetrivel And Coworkers J. Mol. Catal., 37, 157 (1986).

R. Vetrivel, Et Al, Proc. 9th Int. Cong. Catalysis, Vol. 4,(Eds. M.J. Phillips And M. Ternan), Chemical Institute Of Canada, 1988, P.1766.

R. Vetrivel, Et Al, Proc. R. Soc. London, A417, 81 (1988).

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R. Vetrivel And Coworkers In: Polymer Science - Contemporary Themes, (Ed. S. Sivaram), Tata Mc Graw-Hill Publishing Co Ltd., New Delhi, 1991, P.630. (Proc. Polymers'91 Symp., Pune, India.)

R. Vetrivel, Zeolites, 12, 424 (1992)

R. Vetrivel And Coworkers J. Phys. Chem. 96, 3096 (1992)

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R. Vetrivel And Coworkers, Langmuir, 18, 932 (2002)

R. Vetrivel And Coworkers, Combinatorial Chemistry And High Throughput Screening, 6, 1 (2003)

R. Vetrivel And Coworkers, J. Phys. Chem., B108, 11541 (2004)

R. Vetrivel, And Coworkers, Proc. 10th International Conference On Advanced Materials (Iumrs-Icam 2007) Held In Bangalore, India, Oct. 2007

R. Vetrivel,'Gtl Experience' Proc. 4th R&D Conclave (Organized By Petrotech Society) Held At Goa, India, Jan. 2010

R. Vetrivel, Invited Talk At Jncasr Winter School On "Materials And Processes For Applications In Energy And Environment", Bangalore, Jan. 2015

R. Vetrivel And Coworkers,

'How Supercomputers Help To Overcome The Technical Challenge Of Keeping Satellites Working Smoothly Hundreds Of Kilometres Above Earth?',

Shell Business Innovations; 2016.

Https://Www.Shell.Com/Inside-Energy/Smooth-Moves-In-Space.Html

R. Vetrivel And Coworkers,'Computational Catalysis'

Proc. New Trends in Computational Chemistry for Industrial Applications, Expoquimia, Barcelona, Oct. 2017

Dr. Ganapati V. Shanbhag

Associate professor and HoD

Materials Science & Catalysis Division

Email: shanbhag@poornaprajna.org

Homepage:

http://www.ppisr.res.in/faculty/ganapati-v-shanbhag

BRIEF CV:

- Jan 2018 – till date, Associate Professor, PPISR, Bengaluru, India
- 2010 – 2017: Asst. Professor, PPISR, Bengaluru, India
- 2008 – 2010: Research Scientist, Dept. of Chemistry, Korea Advanced Institute of Science and technology (KAIST), South Korea
- 2002 – 2008: Ph.D. CSIR-National Chemical Laboratory, Pune India
- 2000 – 2001: Research Associate, ICI India Ltd (MNC), Mumbai, India
- 1999 – 2000: Lecturer, M.M Arts & Science College, Sirsi, Karnataka, India
- 1999: M.Sc. Organic Chemistry, Karnatak University, Dharwad, India

RESEARCH INTERESTS:

1. Novel catalytic materials

There are many reactions for which existing catalysts have some drawbacks and could not give good efficiency for required products. Also, there are many reactions for which homogeneous catalysts are used till today and need to be replaced with heterogeneous catalysts. Catalysis research is never stagnant and requires constant efforts to find new catalysts better than existing ones. New materials always open up a lot of research to study their unknown properties.

2. Chemical fixation of CO_2 by converting into valuable chemicals.

Industrial and automobile effluent gas, CO_2 conversion to hydrocarbons over catalysts has been shown very little research and development attention so far, as other technologies has been much cheaper and efficient in yielding hydrocarbons. However, nowadays, with the increasing awareness of the impact CO_2 is having on the environment,a lot of attention is being directed at the methods to mitigate the effects CO_2 as a greenhouse gas. Electricity generation from coal flue gas from chemical industries and running automobiles contribute to a great extent in

generating CO_2. Hence it is necessary to convert CO_2 from industrial flue gas into valuable chemicals instead of leaving it into atmosphere. However, CO_2 being an inert gas, its activation and conversion into valuable chemicals is a challenge and require a design of catalyst to make these processes feasible.

3. Catalyst design for biomass conversion

The research in the present decade is mainly dedicated to "energy" because of the concerns over diminishing fossil fuels like LPG, petrol and diesel. A lot of efforts are going on to make new biofuels from renewable sources such as non-edible vegetable oils, wet biomass and wood based biomass. Biodiesel synthesized from catalytic transesterification of vegetable oilwas already tested to be fit to use as a blend with diesel. Biomass processing with multiple steps like hydropyrolysis and gasificationyields mixture of hydrocarbons and oxygenated compounds which upon refining can yield biofuels with desired quality. However, easier said than done, it is a challenge to design catalysts to selectively produce the desired biofuels with high efficiency.

4. Light Alkane activation and functionalization

Light alkanes are cheap and abundant chemicals mainly obtained from petroleum refinery which tend to be resistant to many forms of activation. Hence catalysts play an important role in converting them into valuable products. Important processes like cracking, aromatization, ammoxidation and oxidation are some examples of chemical transformation of alkanes depending on the desired end products.

Following are the applications of the products obtained by the activation of Light alkanes.

In chemical industries, aromatics i.e., Benzene, toluene, ethylbenzene & xylenes (BTEX) are important feedstocks for a large number of intermediates used in the production of synthetic fibers, resins, synthetic rubber, explosives, pesticides, detergent, dyes, intermediates, etc. Cracking of lighter alkanes targeting light olefins like propylene is in great demand in the manufacture of Polypropylene, acrylic polymers, acrylonitrile, poly(propenonitrile). Nitriles derivatives obtained from ammoxidation finds its uses in various medical and industrial application.

RECOGNISTIONS/ACHIEVEMENTS:

- **Award for Research Publications** (ARP) was awarded to Dr. Shanbhag for the year 2016-17 for best publications during last 3 years by VGST, Govt of Karnataka. It contains Rs. 25,000/- + Citation.
- Dr. Ganapati Shanbhag worked as **Co-convener and Chairman of Technical Committee** for 23rd National symposium on Catalysis

(CATSYMP-23) held during January 17-19, 2018 at Royal Orchid Convention Centre, Bengaluru.

- Invited by Jain University, Bengaluru to become **External Member of the Board of Studies** for MSc from April 2018.
- **Chemical Today** magazine published an interview of Dr. Shanbhag in June 2016 issue.
- Received a **Meritorious Award** for Excellence in Research from AMEF during Founder's day July 6, 2012 in recognition of contribution towards research and development at PPISR.
- Received '**plaques**' as a Principal Investigator of the sponsored project from **GTC Technology Inc. USA** in 2012, 2014 and 2015 in recognition of the milestones achieved by the group in developing a modified zeolite catalyst for aromatics technology.
- **Editorial board member** of the journal "**Journal of Catalyst and Catalysis.**"
- Member of the **Syllabus revision committee for Chemistry** for Siddaganga Institute of Technology (SIT), Tumkur.
- **Referee for international journals** *viz.* Chemical Communicaions (RSC), Applied Catalysis A (Elsevier), Catalysis Science and Technology (RSC), Catalysis Communications (Elsevier) and Journal of Chemical Sciences (Elsevier), Springer Plus, Energy Technology (Wiley).
- **Resource person** for Refresher Course Programme for PU college Lecturers sponsored by VGST, Govt of Karnataka.
- **Co-inventor** in the 2 World **patent (PCT)**applications filed by HPCL R & D Centre, Bengaluru evolved as a result of a collaborative project.
- **Nine Best oral/poster presentation awards** to the group for the research papers presented at National symposiums/workshops,

1) Kuvempu University on "Social Relevance of Chemical Sciences" in March 2011 (student: Mrs. SwethaSandesh); 2) Manipal Institute of Technology , "National Symposium on Chemistry and Humanity" in Manipal, July, 2011 (Student: Mr. Janardhan H L); 3) National Workshop on Catalysis, CSIR-NEERI, Nagpur, Maharashtra on 4-5, Feb 2014 (Student: Mr. VijaykumarMarakatti). Marakatti), 4)17th National Workshop on on Challenges in Catalysis Science and Technology organized by Catalysis Society of India June 2016 at CSIR-IICT, Hyderabad (Student: Manjunathan), 5) Research Colloquium-2016 held at MAHE, Manipal on April 4, 2016 (Manjunathan), 6) Best Oral presentation award at 23rd National symposium on Catalysis held during January 17-19, 2018, Bengaluru (Student: Mr. Manjunathan P. 7) Best Poster presentation award at 23rd National symposium on Catalysis held during January 17-19, 2018, Bengaluru (Student: Sujith S.). 8) Best Oral presentation to Mr. Manjunathan P. K V Rao Research Awards for the year of 2017-18 in Chemistry 9) Dr. Manjunathan P. won Best Oral presenter award at "Carbon

Capture and its Utilization conference" held at CSIR-NCL, Pune conducted on December 14-15, 2018

STUDENTS

PhD students

1 Mr. Manjunathan P
2 Mr. Nagendra Kulal
3 Ms. Vaishnavi B J

Project Fellows

4 Mr. Manjunath Doddamani
5 Mr. Sujith S
6 Mr. Neehar P.
7 Mr. Rahul Ravindran

Project Fellows

8 Mr. Pandurang Dalavi
9 Mr. Subramanya
10 Mr. Madhav Nayak
11 Ms. Nimisha Simon

Past students

Doctoral students

1. Vijaykumar Marakatti (Present: Marie Skłodowska-Curie Fellow, Universite catholique de louvain (UCL) Belgium)
2. Janardhan H L (Present: Research Associate, HP Green R&D Centre, HPCL, Bengaluru)
3. Swetha Sandesh (Present: CEO, Nirathara Scientific Solutions Pvt Ltd)
4. Manjunathan P. (Present: Post Doctoral Fellow, KRICT, South Korea)

M. Tech. project students

5. Satish Burla (Present: Scientist, SABIC, Bengaluru)
6. Prashant Kumar (Present: Research Engineer, SABIC, Bengaluru)
7. Girish Kamath (Present: Doctoral student, at Univ. of Saskatchewan, Canada)

NATIONAL AND INTERNATIONAL COLLABORATORS

1. Dr. Ding ZhongYi, Technology Manager, PWT Inc, USA
2. Prof. Ajayan Vinu, University of Newcastle, Australia
3. Dr. Raman Ravishankar, Deputy General Manager, HP Green R & D Centre, Bengaluru
4. Dr. G. Valavarasu Deputy General Manager, HP Green R & D Centre, Bengaluru
5. Prof. Shubhangi Umbarkar, Sr. Scientist, CSIR-NCL, Pune.
6. Prof. Rajendra Srivastava, Asst. Professor, IIT-Ropar, Punjab
7. Prof. A. Sakthivel, Central University of Kerala, Kasargod.

RESEARCH

SPONSORED PROJECTS:

1. **Design and development of a catalyst and process for the hydrocarbon conversions**

(Sponsored by: ***GTC Technology, USA)****($1,80, 000/ Year = ~**Rs. 1.2 Crores**)April 2017 to June 2019*

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

Project fellows: Manjunath Doddamani, Sujith S. Neehar P, Rahul Ravindran and Pandurang Dalavi, Subramanya and Madhav Nayak

The design and development of second regeneration catalyst for toluene methylation process has been initiated. For this, pore engineering of zeolite with novel techniques were adopted to improve shape selectivity for desired para isomer. Zeolite catalysts treated with different pore modifiers were prepared and tested for this reaction to obtain high selectivity for para-xylene.

The first generation TM catalyst has been further tested to achieve high toluene conversion of >40% per pass with mixed xylene selectivity of >80% in a two series reactor set up and under high throughput conditions. The reaction was conducted for 50-100 h each cycle and regenerated in-situ to make it ready for next cycle. Few catalysts were initially tested and then with one selected catalyst long time on stream studies and several regenerations and catalytic cycles were conducted. Overall, 8 regenerations and about 1000 h time on stream run were conducted. The catalyst withstood the successive regenerations and recycles testings and high temperature conditions and did not lose the activity after 1000 h run.

Status: In progress

2. **Process development for liquid phase isomerization (LPI) of xylenes to selectively produce p-xylene**

(Sponsored by: ***GTC Technology, USA in collaboration with Clariant, Switzerland)***

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

Project fellows: Manjunath Doddamani, Sujith S. Neehar P, Rahul Ravindran and Pandurang Dalavi

Liquid phase isomerization of xylenes at high pressure and low temperature condition was studied extensively with commercial Clariant catalysts. Initially, several catalysts were screened under same conditions and a best catalyst was selected which gave desired performance. This catalyst was then studied in detail with a long time on stream studies and process optimization. Overall, more than 1000 hrs time on stream run was conducted for a selected catalyst with multiple regeneration steps. It is seen that the catalyst gave similar performance even after 1000 h run and repeated regeneration.

Status: Completed

3. **Aromatization of Light Naphtha over Non-Zeolitic Catalysts**
   (Collaboration work with HP Green R & D Centre)
   Principal Investigator: Dr. Ganapati V Shanbhag
   Project fellow: Ms. Vaishnavi B J, Sujith S.

   Light naphtha is a fraction obtained in petroleum refining which has low value as a fuel and required to be converted into valuable chemical by processes such as aromatization, isomerisation and cracking. Aromatization of light naphtha was primarily focussed so far in literature on MFI based zeolites with mostly n-hexane as model compound. Metal modified zeolite based catalysts although give high conversions, they have a disadvantage of producing equally high amount of cracking products. The purpose of this work is to develop non-zeolitic catalyst that can produce aromatics with high selectivity and less cracking products.
   In this study, several non-zeolitic solid acid catalysts were tested for aromatization. Selected catalysts which gave better performance were then studied in detail.
   Status: Manuscript under preparation

4. **Catalyst and process development for aromatics alkylation to make higher aromatics**
   (Sponsored by Deepak Novochem Technologies Ltd., Pune) from November 2018-October 2019)
   Principal Investigator: Dr. Ganapati V Shanbhag
   Co-Investigator: Dr. Sanjeev P Maradur
   Project fellows: Dr. Manjunathan, Mr. Neehar P. and Ms. Nimisha Simon

   The project was initiated in November 2018 by recruiting the project fellows and purchasing required chemicals and glasswares. A fixed bed down-flow quartz reactor was set up to conduct aromatic alkylation. After some initial runs to optimize the set up, mass balance etc, the catalyst screening was started initially with catalysts in pure form with pellet particles and meanwhile catalysts were prepared in extrudate form. The catalysts were modified to achieve targeted conversion and product selectivity. A good mass balance was obtained for the reactions and all the analytical procedures were established. Further work is under progress.
   The different zeolite catalysts were screened for the C9+ aromatics synthesis from alkylation of aromatics like xylene in fixed-bed reactor in continuous mode operation. A good conversion os ~70% with about 35% selectivity for the desired products were achieved. Further catalyst screening in single and series reactor set up is under progress.
   Status: Ongoing

5. **Identification and tuning of active sites in selected mixed metal oxide catalysts for cyclic carbonate synthesis from epoxides and CO_2**
   Sponsored project CESEM, VGST, Govt. of Karnataka

Principal Investigator: Dr. Ganapati V Shanbhag
Project fellow: Mr. Nagendra Kulal

Mn-Ba oxide and Sn-Ni oxides were further characterized to understand the structure activity correlation for cyclic carbonate synthesis from methanol and CO_2. FT-IR spectra of the Mn-Ba(4.3:1) and Sn-Ni(1.5:1) catalysts calcined at different temperatures showed a broad band at 3430 cm^{-1} is assigned to O-H stretching vibration and peak at 1630 cm^{-1} is assigned to bending vibration of O-H. For Mn-Ba(4.3:1) catalyst, as the calcination temperature increased, intensity of O-H vibration decreased till 600 °C then remained almost constant, whereas for Sn-Ni(1.5:1) catalyst, the intensities of O-H vibrations did not change after 500 °C. This indicates that 400 °C calcined catalyst still has considerable amount of O-H from metal hydroxide precursors and decreased with increase in calcination due to dehydroxylation. After certain calcination temperature as mentioned above, there was a little change in intensities of the O-H vibrations. This remaining O-H groups could be solely due to Brönsted acidity generated by the coordinative unsaturation of metals. Physical mixture of NiO and SnO_2 as well as Mn_2O_3 and BaO gave lower activity compared to their respective mixed oxide

Status: Completed, manuscript under revision

6. Synthesis of cyclic urea from amine and CO_2 using novel heterogeneous catalysts

(Sponsored by: Vision Group on Science & Technology, Govt. of Karnataka, 2015-2020)
Center of Excellence in Science Engineering and Medicine (CESEM), ***60 Lakhs/ 3 years***
Principal Investigator: Dr. Ganapati V Shanbhag
Project fellow: Mr. Nagendra Kulal
Internship student: Mr. Crowny John, Christ University, Bengaluru

The synthesis of cyclic ureas using CO_2 has recently gained interest in view of the utilization of a greenhouse gas as well as their wide variety of applications as intermediates of pharmaceuticals, cosmetics, pesticides and urethanes. A novel metal and base functionalized catalyst was designed for this reaction which gave more than 95 % conversion and 97% selectivity for cyclic urea under optimized conditions. Further work on catalyst characterization and activity studies are in progress.

Efficient and greener preparation of catalyst for the direct synthesis of 1, 3-imidazolidone from ethylediamine and CO_2 is mainly focus on development of stable, active and selective catalyst. In this work, metal oxide on basic support as catalyst which is inexpensive and nontoxic, were prepared by simple wet impregnation method. Tuning of active sites by the incorporation of metal and basicity into a support which enhanced the catalytic activity compared with

individual metal oxide and basic support. Catalyst was characterized by XRD, TPD TPR, N_2 Sorption, SEM and TEM to know the physicochemical and surface chemistry.

Status: Completed, manuscript under preparation

7. Direct synthesis of dimethyl carbonate (DMC) from methanol and CO_2

Sponsored project CESEM, VGST, Govt. of Karnataka
Principal Investigator: Dr. Ganapati V Shanbhag
Project fellow: Mr. Nagendra Kulal

Dimethyl carbonate (DMC) has drawn much attention in recent years as an environmentally friendly versatile intermediate. It has been used as a good solvent, an alkylation agent, and a substitute for highly toxic phosgene and dimethyl sulfate in many chemical processes. In addition, it is expected to replace the gasoline oxygenate methyl tert.butyl ether (MTBE), because of its high oxygen content, low toxicity, and rapid biodegradability. DMC has been produced by the reaction of methanol with phosgene in a concentrated sodium hydroxide solution. However, owing to the high toxicity and the severe corrosivity of phosgene, this process has been abandoned gradually. Currently, DMC is produced mainly by oxidative carbonylation of methanol (non-phosgene route). The synthesis can be carried out in both liquid- and gas-phases. However, both routes use poisonous gas carbon monoxide and there is the possibility of an explosion. Recently, direct synthesis of DMC from CO_2 and CH_3OH has been reported as a most attractive route due to the low-cost of CO_2 and the environmentally benign process. However, DMC yield in this route is relatively low due to the fact that CO_2 is thermodynamically stable and kinetically inert and due to the deactivation of catalysts induced by water formation in the reaction process.
Initial catalyst preparation and testing for this reaction under batch process has been initiated.

Status: Under progress

8. Investigation on tuning structural properties of tin phosphate and its application as solid acid catalyst for the synthesis of alkyl levulinates and nopol

Principal Investigator: Dr. Ganapati V Shanbhag
Project fellow: Dr. Manjunathan P.

To clarify the nature of active sites in SnPO-P123 responsible for alcoholysis and Prins cyclization reactions, the reaction was carried out with the catalyst which was pretreated with basic 2,6-lutidine. It is known that 2,6-lutidine selectively interacts with Brønsted acid sites but not with Lewis acid sites due to steric hindrance caused by its methyl groups. In case of Prins reaction, 2,6-lutidine-treated-SnPO-P123 catalyst gave 49% β-pinene conversion lower than

that for untreated SnPO-P123 (87%). To further understand the role of specific active sites, the catalytic performance was normalized by subtracting the conversion obtained with catalyst from that of without a catalyst. Then the contribution from Brønsted and Lewis acid sites towards conversion was calculated separately. Notably, it shows 29% β-pinene conversion for Lewis acid site and 40% for Brønsted acid site upon normalization with blank run. Therefore, it confirms that both the Lewis (Sn^{4+}) and Brønsted acid sites (P-OH) in SnPO-P123 catalyst are responsible for this reaction but the majority contribution is from Brønsted acid sites. Hence, based on these results, a plausible reaction mechanism was proposed for both the reactions.
Status: Completed, manuscript under revision

9. Novel bifunctional bimetal spinel structured material as an efficient catalyst for the synthesis of glycerol carbonate *via* carbonylation of glycerol with urea

Principal Investigator: Dr. Ganapati V Shanbhag
Project fellow: Mr. Manjunathan P.
In order to confirm there is no leaching of metal during the reaction, AAS and XRD analysis were performed. AAS analysis reveals that there is no presence of active metal in the reaction medium. The other possibility of leached metal is to form the metal-glycerolate species and this can be confirmed by X-ray diffraction. Therefore, few experiments on carbonylation of glycerol with urea were carried out using bimetal spinel structured material and its corresponding oxides. This shows the formation of metal-glycerolate by using metal oxide as a catalyst, whereas the metal-glycerolate was absent in bimetal oxide and confirms there is no leaching and catalytic material is stable during the reaction. Catalytic activity studies are completed and further catalyst characterization and DFT studies for this work is under progress.

Status: Under Progress

10. Synthesis of β-amino alcohols by aminolysis of epoxides using novel mesoporous metal oxide catalyst

Principal Investigator: Dr. Ganapati V Shanbhag
Research Scholar: Mr. Manjunathan P.
Internship student: Mr. Sachin Kumar, Government Science College

Aminolysis of epoxides yields β -amino alcohols which are versatile intermediates for the synthesis of various biologically active natural products, unnatural amino acids, b-blockers, insecticidal agents, chiral auxiliaries and oxazolines. Oxycontin, Coregand Toprol-XL are a few examples of active pharmaceutical ingredients (APIs) that contain a b-amino alcohol unit in their structure. Among several synthetic strategies, the most straightforward approach for the synthesis of β-amino alcohols is the direct reaction of epoxide with an excess amount of amine at elevated temperatures and in the presence of solvents.

A series of meso-MO_2-T-*x* catalyst calcined at temperatures ranging from 300 to 500 °C bearing different amount of acidic sites were used to study the effect of acidity towards the epoxide aminolysis with aniline. The epoxide conversion increased appreciably from 75.8 to 76.2% upon increasing the calcination temperature of meso-MO_2-T*x* from 300 to 350 °C. The enhanced catalytic performance of meso- MO_2-T-350 was mainly attributed to the presence of greater amount of acidic sites compared to other catalysts. Therefore, meso- MO_2-T-350 catalyst was selected as the best catalyst for further studies.

Status: Manuscript is under preparation

11. Synthesis of glycerol carbonate by transesterification of glycerol using solid base catalyst

Research Scholar: Mr. Manjunathan P.
Internship student: Ms. Varsha P., Christ University, Bengaluru

Glycerol carbonate finds direct application in as biobased solvent, as electrolyte in lithium ion batteries, curing agent, as liquid membrane in gas separation, blowing agent, detergent, and in cosmetics. In this work, main aim is to design a solid base catalyst to achieve high yield of glycerol carbonate and with catalyst possessing good stability. It is synthesized from carbonylation of glycerol with dimethyl carbonate under liquid phase batch conditions. Different solid base catalysts namley CaSn, MgSn, SrSn and BaSn mixed metal oxide were prepared using co-precipitation method and followed by calcination at 600 °C. These materials were employed as catalysts for glyceol carbonate synthesis. Among the different mixed oxide catalysts screened, the best catalyst was further studied in detail and prepared by different methods by varying precursors and reagents to optimize the catalyst recipe as well as understanding the structure and its correlation with catalytic activity. The main problem with the catalyst was leaching of active sites and reaction was catalyzed by homogeneous leached sites due to the formation of soluble metal-glycerolate species.

Status: Completed

12. The effect of porosity, acidity and crystallite size of zeolite ZSM-5 catalyst for alcoholysis of furfuryl alcohol to produce butyl levulinates.

Principal Investigator: Dr. Ganapati V Shanbhag
Research fellow: Ms. Vaishnavi B J

Among biomass sugar-derived chemicals, alkyl levulinates have gained specific attention due to their unique properties such as high lubricity, fash point stability, non-toxic nature, and finer flow properties under cold conditions. These potential characteristics make it one of the important value added chemicals especially as fuel additives in transportation fuels. Furthermore, alkyl levulinates are used to synthesize drug and chemical intermediates, and flavors and

fragrances are used in solvent and plasticizer industries. Initial catalyt screening of zeolite ZSM-5 based catalyst for alcoholysis of furfural alcohol to alkyl levulinate is conducted. The zeolite with different Si/Al ratio, crystallite size are being characterized to derive the structural activity correlation.
Status: Work in progress

EVENTS AND ACHIEVEMENTS

The industry project on "Process development for liquid phase isomerization (LPI) of xylenes to selectively produce p-xylene" sponsored by GTC Technology Inc in collaboration with Clariant Switzerland was successfully completed.

PUBLICATIONS:

Book Chapter:

"Application of tin oxide based materials in catalysis"
Ganapati Shanbhag and Manjunathan P
Book Title: "Tin Oxide Materials--Synthesis, Properties, and Applications"
Elsevier Publisher, 2019 (By invitation)
Status: Accepted, **In Press**

B. Papers Presented in conferences:

Best presentation awards:

1) Mr. Manjunathan P. received 2nd prize in K V Rao Research Awards for the year of 2017-18 in Chemistry competing with South Indian researchers in Chemistry (includes 5 states, Karnataka, Tamil Nadu, Andhra Pradesh, Telangana and Kerala) held at Hyderabad, India on 14th April 2018.

2) Dr. Manjunathan P. won Best Oral presenter award at "Carbon Capture and its Utilization conference" held at CSIR-NCL, Pune conducted on December 14-15, 2018.

Invited talks at conferences and workshops

1) Dr. Ganapati Shanbhag gave an invited talk on his research work at prestigious "3rd International Conference on Emerging Advanced Nanomaterials 2018 (ICEAN-2018)" held in the Newcastle Exhibition and Convention Center, Newcastle, NSW, Australia from October 30th to November 2nd 2018. This conference covered frontier topics like nanostructured materials, energy storage & conversion (batteries, capacitors, etc), nanoporous materials, heterogeneous catalysts, biomedical devices, environmental applications, drug delivery & developments etc. There were over 600 participants from 22 countries from various universities and institutes. Dr. Shanbhag received International Travel Grant SERB, DST, Govt. of India to travel to Australia to attend this conference. He also visited Universiy of Newcastle

and established a collaboration with Prof. Ajayan Vinu, Director of Global Innovative Center for Advanced Nanomaterials (GICAN).

2) Dr. Ganapati Shanbhag gave an invited talk on his research work titled "Novel mesoporous tin phosphate/oxide as catalyst for valorization of biomass derivatives" at *prestigious* *5th Indo-French symposium* at National Chemical Laboratory (NCL), Pune on Feb 26-March 1, 2019. It was a bilateral 5th Indo-French symposium on "Functionalized Materials for Sustainable Catalytic and Related Applications" MATSUCAT-2019 under the auspices of the CSIR, New Delhi and the CNRS, France within the International Associate Laboratories between CSIR-NCL and Unite de Catalyse et de Chimie du Solide (UCCS), and University of Strasbourg, France.
3) Dr. Ganapati Shanbhag delivered an invited talk on "Tuning properties of mixed metal oxide catalysts for direct transformation of CO_2 into cyclic carbonate and dialkylurea" at international conference on "Carbon Capture and Its Utilization" held on 14-15 December 2018 at the CSIR-National Chemical Laboratory, Pune conducted in association with Royal Society of Chemistry.
4) Dr. Ganapati Shanbhag delivered an invited lecture at KSTA sponsored workshop at Christ University, Bengaluru on 27th and 28th November, 2018 with a theme "Conceptual and Practical Advances in Materials Chemistry".
5) Dr. Ganapati Shanbhag delived an invited talk at Poornaprajna College, Udupi on December 31, 2018 on the topic "Catalysis and its role in green synthesis of fuels and chemicals; Present challenges" to undergraduate Chemistry students.
6) 1) Dr. Ganapati Shanbhag delivered an invited lecture at Faculty Development Programme on "Functional Materials for Industrial Applications" at Department of Chemistry, Ramaiah Institute of Technology, Bengaluru on July 26th, 2018.

Other Presentations in Conferences:

7) Mr. Nagendra Kulal presented his work by poster on "Tuning active sites in Ni-Sn mixed oxide catalyst for direct transformation of CO_2 into dialkylurea" at international conference on "Carbon Capture and Its Utilization" at NCL, Pune on December 14-15, 2018.
8) Mr. Nagendra Kulal delivered an oral presentation titled "Ni-Sn mixed oxide catalyst for the synthesis of substituted urea from carbonylation of dialkylurea with CO_2" in National Conference on Advances in Chemical Sciences on November 2-3, 2018 in MAHE, Manipal.

PhD defence Viva and award:

Ph.D. defence Viva of Mr. Manjunathan P. was held on 21st August 2018 at 10:00 A.M. at Poornaprajna Auditorium, PPISR Devanahalli. The title of his thesis is: "Designing Heterogeneous Catalysts for the Conversion of Glycerol & Furfuryl Alcohol into Value-Added Chemicals". Dr. C. V. Rode, Senior Scientist (G), Chemical Engineering & Process Development Division, CSIR-National Chemical

Laboratory (NCL), Pune was external examiner appointed by MAHE, Manipal. PhD Guide, Dr. Ganapati Shanbhag and Co-guide Dr. S. P. Mardur were internal examiners. The examiners and audience asked several questions which Mr. Manjunathan answered and defended his work satisfactorily.

Manjunathan P. received his PhD degree at 26th Convocation ceremony at MAHE, Manipal on November 16, 2018.

PhD Registration:

The PhD registration seminar of Ms. Vaishnavi B. J. was conducted on 31st December 2018, at MAHE, Manipal in front of the review committee appointed by the University. Her PhD guide, Dr. Ganapati Shanbhag was also present in this meeting. The committee members approved her PhD synopsis after some minor corrections.

International Travel Grant:

Dr. Ganapati Shanbhag has been invited to give a talk on his research work at prestigious "3rd International Conference on Emerging Advanced Nanomaterials 2018 (ICEAN-2018)" to be held in the Newcastle Exhibition and Convention Center, Newcastle, NSW, Australia from October 30th to November 2nd 2018. Consequently, he received International Travel Grant SERB, DST, Govt. of India to travel to Australia and give invited talk at the conference.

C. Review Meetings

1. HPCL Team of Mr. Gandham SriGanesh, Executive Director, Dr. N. V. Choudhary, Emeritus Scientist, Dr. G. Valavarasu, Dy. Gen. Manager and Mr. Bennet visited PPISR for final project review meeting on July 20, 2018 at PPISR. Dr. A. B. Halgeri presided over the meeting. PI of the project Dr. Shanbhag presented the highlights and achievements in the two-years work. HPCL team expressed their satisfaction with the progress made by PPISR and happy that all the milestones were achieved. Further discussions are initiated for the new collaborative project proposal with HPCL.
2. Dr. Ganapati Shanbhag visited Deepak Novochem Technologies Pvt. Ltd at Pune for a project review meeting on March 1, 2019 and presented the results obtained so far on the ongoing DNTL sponsored project. Mr. Shreekrishna Sawant, CEO and Dr. Anand Hunoor, Executive Director were present in the meeting. They gave several suggestions to improve the performance of the catalyst and also expressed their satisfaction for the progress made so far in the project.

D. DAC Meetings

1. The third six-month Doctoral Advisory Committee meeting of Mr. Nagendra Kulal, was conducted on July 28, 2018 in Sadashivnagar Campus. Mr. Nagendra Kulal presented his research progress to the DAC members, Prof. Y.

S. Bhat, Prof. Nagaraju and Dr. P. Manikandan on July 28, 2018. Dr. Ganapati Shanbhag, PhD Guide was present and Dr. A. B. Halgeri, Director and Chairman of the committee conducted the DAC meeting. Experts expressed their satisfaction on the progress made and gave several suggestions to improve the quality of the research work. Six-month report and the proceedings of the meeting have been prepared and submitted to MAHE, Manipal

2. The pre-PhD Doctoral Advisory Committee meeting for Mrs. Vaishnavi B. J. was conducted on October 24, 2018, in Sadashivnagar Campus. I presented her synopsis to the DAC members, Prof. Y. S. Bhat, Prof. Nagaraju, and Dr. R. Vetrivel. Dr. Ganapati Shanbhag, Ph.D. Guide was present and Dr. A. B. Halgeri, Director and Chairman of the committee conducted the DAC meeting. Proceedings of the meeting have been prepared and submitted to MAHE, Manipal.
3. The pre-PhD Doctoral Advisory Committee meeting for Nagendra Kulal was conducted on January 12, 2019 in Sadashivnagar Campus. He presented the six month progress to the DAC members, Dr. P. Manikandan, Prof. Y. S. Bhat, Prof. Nagaraju, and Dr. R. Vetrivel. Dr. Ganapati Shanbhag, Ph.D. Guide was present and Dr. A. B. Halgeri, Director and Chairman of the committee conducted the DAC meeting. Proceedings of the meeting have been prepared and submitted to MAHE, Manipal.

New recruitments:

1. Mr. K. S. Subramanya joined the catalysis group as Research Fellow to work in GTC sponsored project. He did his MSc from Karnatak University, Dharwad with Organic Chemistry Specialization in 2016 and then worked as Scientific Analyst in a company before joining PPISR.
2. Mr. Madhav Nayak joined the catalysis group as Research Fellow to work in GTC sponsored project. He did his MSc from Mangalore University, Mangalore with Organic Chemistry Specialization in 2016 and then worked as Research Associate in Syngene International Ltd, Bangalore. from July 2016 to March 2018 before joining PPISR.
3. Ms. Nimisha Simon joined PPISR as Research Engineer to work in Deepak Novochem sponsored project. She did her B. Tech. in Chemical Engineering at Dayanand College of Engineering, Bengaluru in 2018.

Dr. Nalini G Sundaram

Associate Professor
Email: nalini@poornaprajna.org
Homepage:
http://www.ppisr.res.in/nalinis.html

Brief Curriculum vitae

- 2017-present: Associate Professor, PPISR,Bengaluru,India
- 2010-2017: Asst. Professor, PPISR, Bengaluru, India.
- 2005-2008: Postdoctoral Researcher , Dept. of Physics,University of California, Santa Cruz, USA.
- 2004-2005: Postdoctoral Reseacher, Los Alamos National Laboratory, New Mexico and Stanford Synchrotron Laboratory,Stanford, U.S.A
- 1997-2003: Ph.D. Solid State Chemistry ,Indian Institute of Science, Bengaluru, India,2003

Research Areas

- Oxide nanoparticles, Nanocomposites and Thick films selective Gas Sensors
- Rare Earth Photoluminescent nano-oxides for Theronastic applications
- Ceramic Nanomaterials Photocatalysts for dye degradation and organic reactions
- Design and Structure of Lead free Ferroic Materials
- Structure-Property Relationships in Functional energy nanomaterials
- Synthesis, structural studies, polymorphism, local structure and phase transitions in multifunctional materials using Single Crystal, Powder X-ray as well as Neutron diffraction techniques

Awards and Scholarship

1. Awarded a project by DST, India for three years under the SERC- Fast Track Scheme For Young Scientists (FAST)
2. Senior Research Fellowship from Council of Scientific and Industrial Research (CSIR), Government of India
3. Recipient of the Joshi award for securing first rank in M.Sc. (Physical Chemistry)

Sponsored Projects

Starter grant of $1000 under the **ICDD** (International Centre for Diffraction Data)Grant-In-Aidprogram for the year 2016-2017.

- Phase Transitions in $BiMWO_6$ (M=Ce,fe,Cr) Smart Functional Nanomaterials by UGC-DAE CSR Mumbai Centre, India for three years (2016-2019)
- "Design and development of lanthanum based nanoparticles for Thick film gas Sensors.": Sponsored by DST-India, Under Extra Mural Research grant (April 2015-April 2018)
- Influence of Electron Beam Irradiation on the Crystal Structure and Photoluminescence of Rare Earth doped Tungstate Nanophosphors: Sponsored by **BRNS, DAE**, India for three years (April 2013-Apr 2017)

Publications 2019-2019

1. Archana K. Munirathnappa, Joerg C. Neuefeind, Prema kumarYanda, A. Sundaresan, I.V Kityk[d], K.Ozga, J.Jedryka, Poornesh P and **Nalini G. Sundaram,** Average Structure, Local Structure, Photoluminescence and NLO properties of Scheelite type $NaCe(WO_4)_2$, **Cryst. Growth Des.**(Under revision)
2. 2. Pradeep P. Shanbogh, Vikash Chandra Petwal, Jishnu Dwivedi, Ashok Rao, and **Nalini G. Sundaram**, High Energy Electron Beam Induced Evolution of Secondary Phase and Enhanced Photocatalytic Activity in Monoclinic BiEuWO6 Nanoparticles, **J. Phys. Chem. C**, Just Accepted Manuscript DOI: 10.1021/acs.jpcc.8b12368
3. 3. Archana K Munirathnappa, Debasmita Dwibedi, James R Hester, Prabeer Barpanda, Diptikanta Swain, Chandrabhas Narayana, and **Nalini G. Sundaram**, "In-Situ Neutron Diffraction Studies of LiCe(WO4)2 Polymorphs: Phase Transition and Structure-Property Correlation", ***J. Phys. Chem. C***, 2019, 123, 2, 1041-1049
4. Pradeep P. Shanbogh , Rajamani Raghunathan, Diptikanta Swain , Mikhail Feygenson, Joerg Neuefeind, Jasper Plaisier, Chandrabhas Narayana, Ashok Rao and **Nalini G. Sundaram** "Impact of Average, Local and Electronic Structure on Visible Light Photocatalysis in Novel BiREWO6 (RE= Eu & Tb) Nanomaterials." ***ACS Appl. Mater. Interfaces*****,** 2018, *10* (42), pp 35876–35887
5. 5. Marilyn Esclance DMello, **Nalini G. Sundaram**, Akash Singh, Abhishek K. Singh and Suresh Babu Kalidindi, "An amine functionalized zirconium metal–organic framework as an effective chemiresistive sensor", ***Chem. Commun.***, 2019, Advance Article , 2019,55, 349-352 .
6. M. E. DMello, **N. G. Sundaram**, S. B. Kalidindi, "Assembly of ZIF- 67 Metal–Organic Framework over Tin Oxide Nanoparticles for Synergistic Chemiresistive CO2 Gas Sensing", ***Chem. Eur. J.*** 2018, **Volume24, Issue37** Pages 9220-9223
7. Distinct Phase Formation Of $BiREWO_6$ (RE = La-Yb) Nanoparticles By A One Step Hydrothermal Synthesis And Their Photocatalytic Applications. Pradeep P. Shanbogh, Diptikanta Swain, Chandrabhas Narayana, Ashok

Rao and **Nalini G. Sundaram, Cryst. Growth Des.,** 2018, 18 (4), pp 1935–1939 as a communication

8. High Surface Area SnO2-Ta2O5 Composite for Visible Light Driven Photocatalytic Degradation of an Organic Dye", Bharath Velaga[1], Pradeep P. Shanbogh, Diptikanta Swain, Chandrabhas Narayana and **Nalini G. Sundaram,** Photochemistry and Photobiology *DOI: 10.1111/php.12896*
9. "Enhanced red luminescence and improved crystallinity in Enhanced Red Luminescence and Improved Crystallinity in$NaEu(WO_4)_2$phosphors: an electron beam irradiation study", Archana K. Munirathnappa, Vikash C. Petwal, Jishnu Dwivedi,a and **Nalini G. Sundaram**,*New J. Chem.*, 42, 2726-2732, 2018
10. Effect of Solvent on the Red Luminescence of Novel Lanthanide NaEu(WO4)2 Nanophosphor for Theranostic Applications", Archana K. Munirathnappa, Ananda K, A.K Sinha and **Nalini G. Sundaram**. *Crystal Growth and Design* ,vol. 18, no. 1, pp. 253-263, 2018.

Total Number of Publications in National and International Journals: 32

Research Group

1. Mr. Pradeep Shanbogh (Thesis submitted)

Research Area:Rare earth doped Complex Bismuth Oxide Nanoparticles for Photoluminescent and Photocatalytic Applications

2. Ms. Archana K.M (CSIR-SRF)

Research Area:Complex Oxide Materials and Nanocomposites for PL and Gas sensor applications

3.Ms. Chethana Aranthady (JRF Supported by DST and UGC-DAE India)

Research Area:Design of Complex oxide nanomaterials for Selective Gas Sensing and Ferroic Applications

Group Alumni

(i) Former Ph.D. Students

1. Dr. Swetha S. M. (completed Ph.D. in 2014): presently post-doc at Seoul National University, Korea
2. Dr. Srinidhi R. (Completed Ph.D. in 2014): presently post-doc at CeNSE, IISc)

(ii) Former Post Doctoral Researcher

1. Dr. Sowmya Palimar, presently working at IISER, Pune, India

(iii) Former M. Tech and Summer Students

1. Mr. Bharath, M.Tech, MIT, Manipal (Currently Ph.D. student at IIT Guwahati)
2. Mrs. Uma. C.N. M. Tech Dayanand Sagar College, Bengaluru
3. Ms. Srilakshmi Prabhu, B.Sc. Student, Poornaprajna College, Udupi
4. Ms. Najiya K.P.P., M. Tech, Pondicherry University (Currently at NIIST,Trivandrum)
5. Ms. Shuba, M.Sc. SDM College, Ujire

Teaching Experience

- Workshops with Hands-on Demonstration on the Rietveld method has been conducted in MRC, IISc and CMRIT, Whitfield.
- Dr. Nalini presently teaches three courses for the doctoral students in PPISR. She is also the coordinator for PP21 course
- Taught a basic X-ray diffraction to Undergraduate students at University of California at Santa Cruz, CA, U.S.A
- Teaching Assistant at SSCU, IISc Bengaluru for the crystallography course for freshman doctoral students by Professor Guru Row

International and National Collaborators

- Dr. Mikhail Feygenson, JCNS, Germany
- Dr. Joerg Neuefeind, ORNL, U.S.A
- Professor. Shivashankar, CeNSE, IISc
- Professor Chandrabhas Narayana ,CPMU, JNCASR
- Professor Sundaresan, CPMU, JNCASR
- Dr. Ashfia Huq, Apple Research Centre, U.S.A
- Dr. James Hester, ANSTO, Australia
- Dr. Andre Lausi from Elettra, Trieste, Italy
- Dr. Abhishek Mishra, UPES, Dehradun
- Dr. Diptikanta Swain, SSCU, IISc
- Dr. Rajamani, UGC-DAE, Indore Centre
- Dr. Prabeer Barpanda,MRC, IISc, Bangalore

Membership of Professional bodies*:*

1. Member of National crystallographic Association
2. Neutron Scattering Society of India
3. Catalysts Society of India

Current Research Projects

A. Photocatalysis: Semiconductor photocatalysis has received much attention during last few decades as a promising solution for both energy generation and environmental problems because it represents an easy way to utilize clean solar energy abundantly available everywhere in the world. Semiconductor photocatalysis is initiated by electron-hole pairs after bandgap excitation. When a photocatalyst is illuminated by light with energy equal to or greater than band-gap energy, the valence band electrons can be excited to the conduction band, leaving a positive hole in the valence band. The excited electron-hole pairs can recombine, releasing the input energy as heat, with no chemical effect. However, if the electrons (and holes) migrate to the surface of the semiconductor without recombination, they can participate in various oxidation and reduction reactions with adsorbed species such as water, oxygen, and other organic or inorganic species. Potential applications of photocatalysis are found mainly in four aspects a) Photocatalytic degradation of organic pollutants, b) Photoc atalytic water splitting

to produce H_2 and O_2, c) Photocatalytic reduction of CO_2. d) Photocatalytic synthesis for organic substances. These oxidation and reduction reactions are the basic mechanisms of photocatalytic water-air remediation and photocatalytic hydrogen production, respectively.

1. Average, Local and Band Structure of Rare earth Substituted Bi_2WO_6 (*RE* = Nd, Eu, Tb) Nanoparticles: Implications on their Photocatalytic Activity

Aruvillius phases with layered perovskites are shown to be good photocatalysts and better luminescent materials. Bi_2WO_6 is the basic structure in the layered perovskite structure, which exhibits polymorphism, hence crystallographically also very interesting to explore the structure-property relationship. Nanoparticles of rare earth ion substituted Bi_2WO_6 were synthesized by varying temperature, pH and composition. The obtained nanoparticles were characterized by PXRD, PL and photocatalytic activity of the materials are being studied

B. Photoluminescent Nanomaterials for Solid State Lighting and Theronastic Applications

Alkali rare earth double tungstates with general formula $ARE(WO_4)_2$ (A=alkali metal ion, RE= rare earth ions) are promising materials for optoelectronics, solid state lighting and in stimulated Raman scatterin shift due to their unique optical, elastic and magnetic properties[1]. However, luminescent properties heavily rely on the crystal chemistry of host material i.e., local environment of an activator ion. Crystallographic features of these materials are isostructural to the tetragonal Scheelite structure[2]. It is found that the substitution of a pair of A^+ and RE^{3+} ion in the place of Ca^{2+} could results in crystallographic changes such as distortion in crystal structure, lowering of the parent structure and phase transitions[3]. These could eventually influence physical properties such as luminescence as a function of crystal structure[4]. Nowadays most of the research is focused on rare earth doped upconverison materials because of their potential uses in *in-vitro* and *in-vivo* applications as drug delivery systems In recently times especially ytterbium and erbium doped oxides, fluorides, sulphides and molybdates are used since the electronic energy levels of Er^{3+} and Yb^{3+} are more suitable for green emission under IR excitation[5]

1. Design, Crystal structure and Photoluminescence of Lithium Rare Earth Tungstate Nanoparticle Polumorphs (RE=La,Ce,DyYb)

The alkali rare earth double tungstate materials are found to be multifunctional used as solid state luminescent hosts and undergo high temperature polymorphic phase transition that results in a different luminescence properties. First time polymorphism observed in these materials by different synthesis methods. These materials show PL in red and green region. These are promising potential for up conversion materials. They are a very important class of compounds for both solid state lighting devices as well as biological applications.Currently, tetragonal and monoclinic polymorphs of some rare earth tungstate nanoparticles have been

synthesized by conventional hydrothermal and solution combustion method Photoluminescent measurements of these materials was carried out and found that both compounds show good emission in the visible region.

2. Upconversion fluorescence in Nano $NaLa(WO_4)_2$: Yb^{3+}/Er^{3+} phosphor for in-vitro applications

This project deals with the application of upconverison fluorescence properties of $NaRE(WO_4)_2$ in biomedical applications. These materials are unique as they can be excited in the lower energy IR range to obtain emission in a variety of wavelengths in the higher energy visible region. As IR radiation does not cause tissue damage, they have lot of potential to be used as probes for theranostic applications. Hence, we are interested in exploring their unique fluorescence properties for bioimaging and cell tracing applications. Thus we employed facile hydrothermal method to design rare earth substituted double tungstates with an activator and an emitter.

C. Gas Sensors

Design of Lanthanum based Perovskite Nanoparticles for the Development of Thick Film Gas Sensor

Lanthanum (La) based perovskite nanoparticles have been designed and developedas selective and sensitive thick film gas sensors to detect toxic and flammable gases. The work involves investigation of the effect of substitution and particle size on the crystal structure of the nanoparticles and then to obtain good quality thick films from the particles in order to study their sensing properties to different gases such as sulphure dioxide acetone, ammonia, hydrogen sulphide, hydrocarbons and L.P.G. Sulphur dioxide (SO_2) is a highly toxic gas which is released during various reactions in chemical and petrochemical industries. This gas posions the victim by inhalation through lungs and the threshold limit of this gas is 5 ppm. Thus there is a great demand to develop low concentration SO_2 gas sensor. To establish selectivity further gas sensing study will be performed with other gases. These materials showed a significantly good response to SO_2 gas at a lower temperature with remarkably good response and recovery time, whereas at this temperature a significantly low response was seen for higher ppm of other gases such as methane

1. Design of Transition Metal Oxide -SnO_2 Based Nanocomposites for Highly Selective Gas Sensors

Tin oxide has been proven to be a highly gas sensitive material for detection of both reducing and oxidizing gases. However it has a few disadvantages such as low selectivity, low stability and higher operating temperature. Hence our approach is to couple n-type semiconducting SnO_2 to V_2O_5, Nb_2O_5 and Ta_2O_5 to derive a nanocrystalline composite as a selective gas sensing material. SnO_2 was prepared by conventional different surfactant assisted hydrothermal and Co-precipitation methods.

D. Ferroic Materials

In recent years much research is focused on obtaining nanomaterials that exhibit multifunctional applications. For example, focus is on the relaxor ferroic as well as magnetoelectric effect exhibited by materials. In the magnetoeelectric materials control of electric polarization can be achieved by a magnetic field and magnetization by electric field. This opens up many new applications such as magnetic/ferroelectric data storage, magnetocapacitive devices, magnetic sensors, non-volatile memories. Many of these materials have layered structures that can be tuned by substitution to obtain the application

1. Design of Bismuth based Nanomaterials for Magnetoelectric Properties:Oxide materials belonging to the Aurivillius family or the Aurivillius-Sillen phase of oxides has gained significant attention due to their unique layered structure. Among these the isostructural Bi_2WO_6 and Bi_2MoO_6 are the simplest (n= 1) members of the large family of layered perovskite related (Aurivillius phases). The structure of these isostructural materials consist of alternating Bi_2O_2 sheets and perovskite-like layers of corner linked BO_6 octahedra (B=W.Mo). Substitution to this layered material with a magnetic ion can alter the crystal structure resulting in magnetoelectric materials.

2. Structural Analysis of Lead Free Relaxor Dielectrics with TiO_2 Rutile Structure

Multiferroic oxides have wide range of applications as sensors, transducers and other switching devices Eg:Novel relaxor ferroic oxides, $FeTiTaO_6$, $FeTiNbO_6$. Low-temperature dielectric measurements depict anomalous dielectric relaxations with frequency dispersion in these materials. To investigate the dielectric anomalies a series of solid solutions of $FeTiTa_xNb_{1-x}O$ using high temperature sold state reactions was synthesized and low temperature X-ray data from 20K to 300K were collected.The dielectric anomalies reported are clearly seen in the variations in cell parameter and volume of the unit cell with temperature

Awards and Achievements:

- Mr. Pradeep presented his Doctoral Thesis colloquium on 10th of January 2019 and Submitted his Thesis on 2nd May 2019
- Ms. Archana was awarded the **CSIR-Senior Research Fellowship(SRF)** from Govt. of India
- Ms. Chethana's proposal titled "Design of Perovskite thin films for gas sensing applications" has been accepted under the Indian Nano User's program at CENSe, IISc
- Ms. Archana K.M. was awarded the **best poster award** for her research work titled "Design of Alkali Rare Earth Double Tungstates for Theranostic, Photoluminescence and Electrode Applications" in Manipal Research Colloqium-2018, at MAHE Manipal on 4th April, 2018

Research Highlights

- Dr. Nalini Sundaram was invited to deliver a lecture for a workshop on **"X-ray Crystallography"** on March 16 2019 at the Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, sponsored by DST and RSC, India Chapter
- Dr. Nalini Sundaram was invited to deliver a lecture in the Winter School on "Synchrotron Techniques in Materials Science" Held at the S.N.Bose National Centre for Basic Sciences from October 25-31 2018
- . Ms. Archana's presented an oral titled"**Average and local structure of $NaCe(WO_4)_2$: A Structure-Property Correlation**" was selected for oral presentation at the ADD2019 (School And Conference on Diffraction Data in Real Space) at ILL (Institut Laue-Langevin) Grenoble, France in April 2019. Her travel was supported by DST-SERB
- Dr. Nalini was invited to deliver a lecture titled "Exploiting Functional Nanomaterials for Environmental and Biomedical Applications" *at the FDP on "Functional Materials for Industrial Applications (FMIA-2018)" organized at MSRIT on 25 July 2018*
- *D*r. Nalini was invited to deliver a talk on "Principles and Applications of UV-Visible Spectroscopy in Materials Science" at Maharani Science College, Bangalore =
- Dr. Nalini was invited to conduct hands on training on "Crystal Structure determination using Rietveld refinements method" at Dayanand Sagar University, Bengaluru, in September 2018. Ms.Archana assisted in the same
- Dr. Nalini is the Coordinator of **PPISR's outreach program** for Poornaprajna School students . The motto of the program was "**Today's Science for Tomorrow's Scientists**" where IX standard students of five PP high schools participated

Dr. Sanjeev P. Maradur

Assistant Professor

E-mail: sanjeevpm@poornaprajna.org

BRIEF CV:

- 2012-Present: Asst. Professor, PPISR, Bangalore, India
- 2011-2012: Postdoctoral Research Associate, Dept. of Chemistry, University of Oklahoma, USA
- 2010-2011: Postdoctoral Student, Alan MacDiarmid Energy Research Institute (AMERI), Chonnam National University, Gwangju, South Korea
- 2009-2010: Postdoctoral Scientist, Dept. of Chemistry, Korea Advanced Institute of Science and technology (KAIST), Daejeon, South Korea
- 2007-2009: Research Scientist, Jubilant Life Sciences Ltd, Noida, India
- 2006-2007: Senior Research Fellow, Dept. of chemistry, IIT-Bombay, Mumbai, India
- 2003-2006: Ph.D. Dept. of Chemistry, Shivaji University Kolhapur, India

ACHIEVEMENTS/RECOGNISTIONS/AWARDS/MEMBERSHIP:

1. Received Seed Money for Young Scientist Research Program Award from Vision Group on Science and Technology, Govt of Karnataka in 2014.
2. Received a plaque from GTC Technology Inc. USA in 2014& 2015 in recognition of the milestones achieved by the group in developing a modified zeolite catalyst for aromatics technology.
3. Co-inventor in 2 Korean patents on a). Preparation of novel mesoporous polymer and b). Low cost carbon-fiber technology with two different research groups of South Korea.
4. Life member of International Zeolite Association (IZA) and Catalysis Society of India (CSI) and member of American Chemical Society.

PROFESSIONAL EXPERIENCE

1. Materials Science Division, Poornaprajna Institute of Scientific Research, Bangalore (Dec 2012-present)
   Designation: Assistant Professor

2. Department of Chemistry, University of Oklahoma, Norman, USA (Dec 2011-Nov 2012)
   Designation: Postdoctoral Research Associate

   Mentor : **Prof. Dr. Kenneth. M. Nicholas**

   Deoxydehydration of glycols to alkenes: Catalysis by molybdenum complexes: development of non destructive and cost effective catalytic process for the production of olefins from biomass derived polyols.

3. Alan MacDiarmid Energy Research Institute (AMERI), Chonnam National University,Gwangju, South Korea (Dec. 2010-Nov.2011)
   Designation: Postdoctoral Student

   Mentor : **Prof. Dr. K. S. Yang**

   Development of lignin based carbon fibers: Utilization of lignin for manufacture of carbon nanofibers for use in energy applications and high performance materials (Technology development).

4. Korea Advanced Institute of Science & Technology, Daejeon, S.Korea (Jul.2009-Nov.2010)
   Center for Functional Nanomaterials, Department of Chemistry

   Designation: Postdoctoral Scientist

   Mentor : **Prof. Dr. Ryong. Ryoo**

   Developing green chemical processes utilizing mesoporous/nanoporous materials as catalysts for cleaner organic synthesis/oxidations/C-C bond forming reactions.

5. Jubilant Life Sciences Ltd, India (Feb. 2007 –Feb. 2009)
Designation: Research Scientist

Department: Advanced Intermediated and Vitamins

Entrusted with R&D of fundamentals for future process in fine tuning the heterogeneous catalytic processes. Deftly carry out literature search for optimization of synthetic methodology and design schemes for possible execution in the area of catalysis either fix bed/fluidized bed or batch processes.

Projects Handled

1. Liquid phase oxidation of 3-picoline to niacin
2. Vapor phase heterogeneous catalysis for air oxidation of 3-picoline to niacin
3. Process improvement of vapor phase heterogeneous catalysis for the synthesis of pyridine and pyridine derivatives using zeolitic silica-alumina materials
4. Process development of a batch process for the hydration of nitriles to amides targeting niacin amide as product

7.**INDIAN INSTITUTE OF TECHNOLOGY-BOMBAY (JUL. 2006 - JAN. 2007)**

Designation: Senior Research Fellow

Department: Chemistry

Worked on a project, TS-1 catalysis for the hydroxylation of phenol to hydroquinone and heteropoly acid immobilized mesoporous MCM-41, materials as solid acid catalyst.

8. Graduate Research Fellow (Jul. 2003 - Oct. 2006)

Shivaji University Kolhapur, India

Department: **Chemistry**

Advisor: **Prof. G. S. Gokavi**

Gained experience in dealing with synthetic methodologies and development of new catalytic methodologies for cleaner organic synthesis. Research focused on the utilization of polyoxometalates/heteropoly acids as homogeneous catalysis for functional group transformations/ synthesis.

Current Research Interests:

Nanoporous Materials:

Nanoporous materials have gained scientific and technological importance because of the presence of their pore structures of tunable dimensions at nanometer scales. Over the last few decades, there has been an ever increasing interest and research effort in the synthesis, characterization, functionalization of nanoporous materials. The challenges in research include the fundamental understanding of structure-property relations and tailoring of nanostructures for specific properties and applications.

The main research focus of our group is the synthesis and characterization of nanostructured catalysts for various applications. Among the priorities are the development of materials with organic framework, search for new and improvement of existing catalytic systems, and studies of intimate mechanisms of heterogeneous reactions and reactant-to-surface reactions, identification of active sites.

Heterogenization of homogeneous catalysis & its application on various chemical processes:

Development of new, highly efficient heterogenized catalysts is an active and important area in fine chemical synthesis. Homogeneous catalysis though has witnessed significant growth in the last few decades in terms of high selectivity, TON and TOF's, however the success in catalyst and process development has not been in parallel by similar growth on industrial scale. Supports play a significant role in such systems. The micro environment around the catalyst active site will be the deciding factors in achieving high conversions with high selectivity. Our research group is working on heterogenization of homogeneous catalysts onto supports such as zeolites, nanoporoous materials like silica and polymers and their catalysis for fine chemicals production.

STUDENTS

	PhD students
1	Sathyapal Churipard. R.
2	Kempanna S. Kanakikodi
3	Manjunathan P (Joint Student with Dr Shanbhag)
4	Arpana Hegde

M.Tech. project students

1.Manish Kumar, Chem Engg Dept, MAHE, Manipal (Present: PhD Scholar, NIT-Trichy)

2. Sharath Ravi Chem Engg Dept, MAHE, Manipal (Present: Research Engineer, Shell Technology, Bengaluru)

Summer Internship Students

1. Ms. Nileena Jose**,** M.Sc Project, ST.ALOYSIUS COLLEGE (AUTONOMOUS), Mangalore From May-Jul 2017.
2. Mr. Abdul Mueed Moulana & Aditya Sharma, B. Tech Petroleum Engg , Presidency University, Bengaluru Industrial Practice Course Project, From June-Aug 2017.
3. Ms. Komala Y**,** M.Sc Project, Government Science College (Autonomous), Bengaluru (May-Jul 2018).
4. Mr. Mohammed Touheed V I & Mr. Mohammed Farhan Jameel, B. Tech Petroleum Engg , Presidency University, Bengaluru Industrial Practice Course Project, From June-Aug 2018

NATIONAL AND INTERNATIONAL COLLABORATORS

1. Dr. Ding ZhongYi, Technology Manager, PWT Inc, USA
2. Dr. Raman Ravishankar, Chief Manager, HP Green R & D Center, Bengaluru
3. Dr. Nagesh Kini, Senior Manager, R&D, Thermax Industries Ltd., Pune
4. Dr Jyoti Roy Choudhary, Department of Chemisty, BMS Institute of Technology, Bengaluru.
5. Dr. Hemandra. C. Pahcholi, Head R&D, Deepak Nitrite Ltd. Vadodara, Gujarat

RESEARCH

SPONSORED PROJECTS:

1. **Design and development of a catalyst and process for regioselective nitration of O-Xylene to , 4-nitro-o-xylene (4-NOX)**
   (Sponsored by **Deepak Nitrite Ltd, Vadodara, India)**
   PI: **Dr. Sanjeev P Maradur**; Co-PI: Dr. Ganapati V Shanbhag
   Project Fellow: Arpana Hegde
   Date: 2019-2020
2. **Catalyst evaluation studies for methanol reforming for fuel Cell applications** *(Sponsored by* **Thermax Industries Pune, India)**
   PI: **Dr. Sanjeev P Maradur**; Co-PI: Dr. Ganapati V Shanbhag
   Project Fellow: Mr. Kempanna S. Kanakikodi and Jemin Joy
   Date: 2017-2018
3. **Development of Novel Mesoporous Polymer Based Catalysts for Low Temperature Catalytic Applications"** Sponsored by **Hindustan Petroleum Green R&D Center, Bangalore**
   PI: **Dr. Sanjeev P Maradur**; Co-PI: Dr. Ganapati V Shanbhag
   Project Fellows: Sathyapal Churipard. R and Mr. Kempanna S. Kanakikodi
   Date: 2016-2018
4. **Design and development of a catalyst and process for C1-C3 hydrocarbon conversion to olefins and aromatics** *(Sponsored by:* ***PW Technology, USA****)*
   PI: Dr. Ganapati V Shanbhag; Co-PI: **Dr. Sanjeev P Maradur**
   Project fellows: Mr. Santosh Kumar, Mr. Saikiran, Mr. Manjunath D., Mr. Mahesh Kumar, Ms. Anusha R; Date: 2016-2017
5. **Design and development of a catalyst and process for selective methylation of benzene/ toluene to produce *p*-xylene**
   (Sponsored by: ***GTC Technology, USA****)*
   PI: Dr. Ganapati V Shanbhag; Co-PI: **Dr. Sanjeev P Maradur**
   Research Fellows: Mr. Santosh Kumar, Mr. Saikiran and Mr. Kempanna
   Date: 2011-2019
6. **Conversion of Waste Plastics into Fuels"** Short Term Project Sponsored by Thermax Industries Ltd, Pune
   PI: **Dr. Sanjeev P Maradur**; Co-PI: Dr. Ganapati V Shanbhag
   Project Fellow: Manish Kumar
   Date: 2015

Project Proposal in Pipeline

1) Selective Hydrogen Production FOR FUEL Cell Applications: Design And Development Of A Novel Non-Precious Metal Based Catalyst Through Methanol Reforming

(Possible Sponsorship by: ***VGST, Govt of Karnataka 2018****)*

The main objective of this proposal is the selective production of hydrogen through selective methanol reforming over a novel non-precious metal based catalyst for methanol based Fuel Cell Applications.

2) Design and Development of Catalyst and Process for C-H Activation of Methane to Acetic Acid through Halogen Mediated Route

(Possible Sponsorship by: ***DST Core Research Grant 2018****)*

Acetic acid is one of the most important chemicals and its current global production is about 14 million metric tons of acetic acid in 2017. More than 60 % of total acetic acid is being produced by Monsanto process which is based on iodide-promoted rhodium catalyst. The major bottle neck in the methanol carbonylation process we envision is the price of methanol will be a deciding factor for economics of the process. Although there is no economical alternative process available to replace Monsanto process, an altenative route of utilizing methane via halide mediated carbonylation route to acetic acid might become economically attractive as methane is one of the most abundant natural gases and thereby avoiding the methane to syn-gas, then syn-gas to methanol and methanol carbonylation to acetic acid.

In the proposed research project, we would like to continue further investigations on activation of methane through halogen mediated route for the synthesis of acetic acid which will be entirely a unique process which will reduce the dependence on methanol for the purpose. Catalyst and process development will be undertaken and also scale up studies will be attempted based on the outcome of the project.

ACADEMIC PROJECTS:

1. **Peroxotungstate supported mesoporous polymer as catalyst for the oxidation of alcohols by hydrogen peroxide**

   PI: Dr. Sanjeev P. Maradur;

   Research Student: Sathyapal Churipard. R

   In this project we have synthesized peroxotungstate supported polymer catalysts and used it for oxidation reaction. Tungsten based catalysts are well known for oxidation reactions. So we have heterogenized the peroxotungstate complex on mesoporous polymer and used it for oxidation reactions. Initially mesoporous divinylbenzene-co-vinyl benzyl chloride co polymer containing 20 mol% of vinyl benzyl chloride (VBC) was synthesised using free radical polymerization technique, it was functionalized with amines and subsequently it was ion exchanged with prepared peroxotungstate complex to get PW4 supported DVB/VBC copolymer catalyst.

2. **Oxidation of cyclohehene to adipic acid**

PI: Dr. Sanjeev P. Maradur;

Research Students: Sathyapal Churipard. R

Adipic acid is industrially important compounds and they rarely occur in nature, adipic acid was synthesised industrially by the oxidation of mixture containing cyclohexanol and cyclohexanone collectively called KA oil,(ketone-alcohol oil) using nitric acid but this was leading to lot of N_2O production, to avoid production of toxic N_2O adipic acid is synthesised using H_2O_2 as oxidant in presence of various catalyst. This is an ecofriendly method for the adipic acid production, various oxidants like oxygen, H_2O_2, TBHP etc can be used but using H_2O_2 as oxidant gives water as by product and this is environmentaly benign. We are developing a heterogeneous catalyst for the adipic acid production using environmentally beningn oxidant hydrogen peroxide.

3. **Room temperature tetrahydropyranilation of alcohols using acid functionalized mesoporous polymers**

   PI: Dr. Sanjeev P. Maradur;

   Research Students: Sathyapal Churipard. R, Kempanna S. Kanakikodi.

   The utilization of protecting groups is inevitable in synthetic organic chemistry. The chemoselective transformation of a particular functional group in presence of various other functional groups is a challenging task for an organic chemist and this could be accomplished with the help of protecting groups. Owing to its stability and chemical compatibility with various reaction conditions, tetrahydropyran (THP) is most widely used protecting group for the protection of alcohols. Heterogeneous catalysts such as ion exchange resins, natural clays, zeolites etc have been studied for tetrahydropyranylation. But it suffers limitations such as longer reaction time and lower catalytic activity. There is still scope for development of efficient protocol for tetrahydropyranylation under mild reaction conditions with shorter reaction times. Hence, we have used the acid functionalized mesoporous polymers (MP-SO_3H) to resolve the diffusion restriction of bulky substrates so that reaction occurs at faster rate under mild reaction conditions.

4. **Tuning Hydrophobicity and Acidity in Porous Organic Polymer for the Etherification of Glycerol to Potential Fuel Additives**

   PI: Dr. Sanjeev P. Maradur;

   Research Students: Kempanna S. Kanakikodi, Sathyapal Churipard. R.

5. **Synthesis and characterization of mesoporous polymeric catalyst and testing it as a novel catalyst for the synthesis of tert-butylated phenols**

   PI: Dr. Sanjeev P. Maradur;

   Project fellow: Kempanna S. Kanakikodi, Sathyapal Churipard. R.

   To accomplish organic transformations such as isomerization, esterification, alkylation, acylation etc, acid catalysis plays an important role. To turn demerits of homogeneous catalysis into advanages heterogeneous catalysts came into existence. The alkylation of phenol by TBA has got tremendus

research interest due to wide spread applications of the end products. Among solid acid catalysts employed for this transformation, cation-exchanged resins demonstrate the good performance, but ion exchange resins are thermally unstable at higher temperature. Zeolites have high acidity, high thermal stability and easy separation from reaction products however, these microporous materials possess small pore size (>02 nm), which severely limits the formation of butylated products like 2,4-DTBP. The kinetic parameters of the DAPs (di-alkylated phenols) limits the applicability of zeolite catalysts.

6. **Sustainable Approach for the Selective Synthesis of Alkyl Methyl Carbonates from Dimethyl Carbonate by Sulfonated Polymer Under Mild Conditions**
   PI: Dr. Sanjeev P. Maradur;
   Research Students: Kempanna S. Kanakikodi, Sathyapal Churipard. R.
7. **Synthesis of Alkyl Levulinates from Furfuryl Alcohol Using Sulfonic Acid Functionalized Mesoporous Polymer**
   Principal Investigator: Dr. Sanjeev P. Maradur
   Research Students: Mr. Sathyapal and Mr. Manjunathan

Furfurylalcohol (FA) is one of the important furan derivatives, industrially produced via hydrogenation of furfural derived from thehydrolysis and dehydration of xylan contained in lignocellulosic biomass.Furfural has an annual production volume of more than 200,000 tones, 65% of furfural is converted to FA by hydrogenation. The development of a feasible and competitive pathwayto reform and upgrade FA is therefore highly desirable. The value generations of furanic biofuels are determined by the methods of transformation of furfural into different biofuels such as 2-methylfuran, 2-methyltetrahydrofuran, alkyl levulinate etc.

An atom-economic and convenient method for the synthesis of high value-added alkyl levulinates can be accomplished via alcoholysis of FA in the presence of acid catalysts. Various solid acid catalyst systems were successively examined for the alcoholysis of FA to alkyl levulinates. Although these solid acid catalysts were effective and easily recovered from the reaction products, the deactivation of recovered catalysts in recycling runs is usually obvious if they go untreated before reuse due to the adsorption of formed carbonaceous products on the solid acid surface and the gradual loss of acid sites. Our current research is focused on direct conversion of furfural to value added products using sulfonic acid functionalized mesoporous polymers.

RESEARCH HIGHLIGHTS

A. Published papers (2018-19)

1. "Catalytic tertiary butylation of phenol over sulfonated mesoporous polymer catalyst (MP-SO_3H): Exceptional selectivity towards 2,4-di-*t*-Butylphenol" Kempanna S. Kanakikodi, Sathyapal R Churipard, AB Halgeri, Sanjeev P Maradur. Microporous and Mesoporous Materials, 286(2019) 133-140.
2. "Exploring the Brønsted Acidity of UiO-66 (Zr, Ce, Hf) Metal-Organic Frameworks for Efficient Solketal Synthesis from Glycerol Acetalization" Vasudeva Rao Bakuru, Sathyapal R. Churipard, Sanjeev P. Maradur and Suresh Babu Kalidindi. Dalton Trans., 2019,48, 843-847

B. Papers presented in Conferences

1. Mr. Kempanna S. Kankikodi presented a poster in Manipal Research Colloquium on Ph.D thesis entitled **"**Designing Functionalized Mesoporous Materials for Catalytic Conversion of Biomass Platform Chemicals to Value Added Products**"** organized by Manipal Academy of Higher Education on March 31st, 2019

C. Review meetings:

Project Review Meetings

1) Final technical review meeting of HPCL sponsored project was held on 20th July 2018 at PPISR campus. Mr. G. Shri Ganesh (Exe. Director) Dr. N. V. Choudhary (Emeritus Scientist), Dr. Valavarasu (DGM), Mr. Benedict from HPCL and Dr Maradur, Dr Shanbhag and Dr Halgeri were present during the meeting. Dr Maradur made presentation of the two years research work carried out and the milestones achieved in the sponsored project.
2) Dr. Valavarasu (DGM) and Dr Sudsharan Reddy HPCL Scientists visited PPISR Campus on 24th September 2018 for Revalidation and closure process of the sponsored project on Mesoporous Polymers. Dr Maradur and his group demonstrated experiments before the HPCL Team.

a. Other Highlights

1. Dr. Maradur' project proposal entitled "Design and Development of Catalyst and Process for C-H Activation of Methane to Acetic Acid through Halogen Mediated Route" was shortlisted and called for presentation before the technical committee. Dr. Maradur made a presentation on 7th January 2019 at IIT-Bombay before the committee. Results are awaited.
2. A new industry sponsored project from Deepak Nitrite entitled "*Design and development of a catalyst and process for regioselective nitration of o-Xylene to 4-nitro-o-xylene (4-NOX) "* has been initiated from 1st March 2019.
3. Mr. Sathyapal has got the prestigious CSIR Senior Research Fellowship starting from April 2019.

Dr. Suresh Babu Kalidindi

DST-INSPIRE faculty
/Assistant Professor
E-mail:sureshk@poornaprajna.org
Homepage:
www.ppisr.res.in/faculty/
suresh- babu-k

Brief Curriculum vitae

- Aug 2015-present: DST-INSPIRE Faculty/Assistant Professor. PPISR, Bangalore.
- Sept 2013-July 2015: Postdoctoral Research Associate, University of Liverpool, United Kingdom.
- Aug 2011-Sept 2013: Alexander von Humboldt Fellow, Max Planck Institute for Intelligent Systems, Stuttgart and Ruhr University, Bochum, Germany.
- May 2010-July 2011: RD-IFSC Post-doctoral Fellow, Ruhr University, Bochum. Germany.
- Aug 2005-July 2010: Ph. D, Indian institute of science, Bangalore.

Research Areas

The material design group@PPISR is actively involved in the development of a new class of nanostructured hybrid materials through the intermingling of reticular chemistry and nanotechnology.

- Metal-organic frameworks (MOFs)
- Nanostructured hybrid materials
- Metal/Metal oxide nanoparticles
- Synergetic Catalysis
- Gas sensing

Awards

- **2016**"Early career research Award" from Department of science and technology, Government of India
- **2015**"DST-INSPIRE Faculty Award"from Department of science and technology, Government of India
- **2011-2013** "Alexander von Humboldt Fellowship" from Alexander von Humboldtfoundation, Germany government
- **2010-2011** "Post-doctoral fellowship" from Research Department-Interfacial Systems Chemistry, Ruhr University, Bochum

- **2009-2010** "Best Ph. D thesis award- Prof. S. Soundarajan Medal" from Indian Institute of Science (IISc), Bangalore**.**
- **2007-08** "Vasudevamurthy-Soundarajan prize" for best seminar during the academic year from Department of Inorganic Physical Chemistry, Indian Institute of Science (IISc), Bangalore

Sponsored Projects at PPISR (Academic and Industry)

1. Design and Development Stable Metal Organic Frameworks with Multiple Functional Sites for Catalysis

Principal Investigator: Dr. Suresh B. Kalidindi
Project fellow: Ms. Marilyn E Dmello
Funding agency: DST (2015-2020)

2. Transformative Crystalline Hybrid Porous Materials: Chemical Synthesis and Applications Principal Investigator: Dr. Suresh B. Kalidindi
Project fellow: Mr. B. Vasudeva rao
Funding agency: DST (2016-2019)

Research Group

1. B. Vasudeva Rao
   Research Area: Metal-organic frameworks and catalysis
2. Marilyn E Dmello
   Research Area: Metal-organic frameworks and gas sensing

Publications 2018-2019

Total Number of Publications in National and International Journals: 5

1) Bakuru, V. R.; DMello, M. E.; Kalidindi, S.B.* "Metal- organic frameworks for hydrogen energy applications: Advances and Challenges" ChemPhyChem, **2019**, 20, 1177-1215..

2) Bakuru, V. R.; Churipard, S. R.; Maradur, S. P.; Kalidindi, S.B.***** "Exploring the Brønsted Acidity of UiO-66 (Zr, Ce, Hf) Metal-Organic Frameworks for Efficient Solketal Synthesis from Glycerol Acetalization", *Dalton transactions*, **2019**, *48*, 843–847.

3) DMello, M. E.; Sundaram, N. G.; Singh, A.; Singh, A. K.; Kalidindi, S.B.***** "Amine Functionalized Zirconium Metal-Organic Framework as an Effective Chemiresistive Sensor for Acidic Gases" *Chem. Comm.* **2019**, *55*, 349–352.

4) Bakuru, V. R.; Velaga, B.; Peela, N. R.; Kalidindi, S.B.***** "Hybridization of Pd Nanoparticles with UiO- 66(Hf) Metal- Organic Framework and the Effect of Nanostructure on the Catalytic Properties" *Chem. Eur. J.* **2018**, 24, 15978–15982.

5) DMello, M. E.; Sundaram, N. G.; Kalidindi, S.B.***** "Assembly of ZIF- 67 Metal–Organic Framework over Tin Oxide Nanoparticles for Synergistic Chemiresistive CO_2 Gas Sensing"
Chem. Eur. J. **2018**, 24, 9220-9223

International and National Collaborators

1) **Dr. Michael Hirscher**

Max-Planck-Institut für Intelligente Systemeehemals Max-Planck, Heisenbergstrasse 3, D-70569 Stuttgart, Germany

2) **Radim Beránek**

Deputy Head Albert-Einstein-Allee 47 89081 Ulm, Germany

3) **Prof. Dr. Roland A. Fischer**

Technical University of Munich (TUM), Chair of Inorganic and Metal-Organic Chemistry Lichtenbergstrasse 4, Garching, Germany

4) **Prof. Balaji R. Jagirdar**

Professor, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore-560012, India

Current Research Project Details (Academic and Industry)

1. Cooperative Hydrodeoxygenation of Vanillin over Pd Nanoparticles Covered with UiO-66(Hf) Metal-Organic Framework

Principal Investigator: Dr. Suresh Babu Kalidindi

Student: B. Vasudeva rao

Conversion of vanillin a biomass based platform molecule into 2-methoxy-4-methyl phenol involves hydrogenation of aldehyde followed by deoxygenation.

Pd@UiO-66(Hf) and Pd/UiO-66(Hf) bifunctional catalysts have been synthesized and were tested in the hydrodeoxygenation of vanillin. Compared to Pd@UiO-66(Hf), the vanillin conversions were found to be far low over Pd/UiO-66(Hf) under same reaction conditions. Even after 120 min reaction time, only ~55% vanillin conversion was achieved. Also, the structure of the catalyst has pronounced influence on the distribution of the products. Over Pd@UiO-66(Hf), 2-methoxy-4-methylphenol is the dominate product at both low and high conversions. On the other hand, over Pd/UiO-66(Hf) till 60 min(~45% conversion) of reaction time the intermediate vanillin alcohol is the major product. The observed striking differences in the catalytic performances between core-shell and support catalysts are ascribed to the differently distributed metal and acidic sites. In the first instance, vanillin should pass through the UiO-66 pores and get converts into intermediate vanillin alcohol by hydrogenation over Pd active sites and further this intermediate converted into 2-methoxy-4-methylphenol owing to close proximity of Pd active sites and Brønsted acidic sites in the Pd-UiO-66(Hf) core-shell. In case of Pd/UiO-66(Hf), since Pd active sites are exposed on the surface of UiO-66, vanillin directly hydrogenated to vanillin alcohol with maximum selectivity from beginning of the reaction time and finally at 2h the selectivity of 2-methoxy-4-methylphenol is 91.3% and vanillin alcohol is 8.7 %.

2. Semi-hydrogenation of Alkynes into Alkenes through Hydrogen Transfer from Ammonia Borane

Principal Investigator: Dr. Suresh Babu Kalidindi, Student: B. Vasudeva rao

Semi-hydrogenation of alkynes to alkenes is one of the preferred reactions in chemical industry process. Generally, alkenes formed from alkynes via hydrogenation path using molecular hydrogen which is unsafe to handing at harsh reaction conditions. In this regard, hydrogen transfer reactions playing vital role in

the among hydrogenation processes due to easy to handle and safer. Certainly, ammonia borane(NH3BH3) received great attention as hydrogen storage material(19.4 wt%). Since, AB considered as polarized complex compound, it can transfer the hydrogen to unsaturated C≡C bond of alkynes via concerted mechanism. With this concept, we initially selected semi-hydrogenation of phenylacetelyne (PA) as model reaction and carried reaction at 110°C for 1h using AB as a hydrogen source. The analysis of final products suggests that only styrene (selectivity>99%) was formed over the ethyl benzene.

Additionally, we studied Pd supported UiO-66(Hf) material to increase the rate of reaction. With supported catalyst reaction is fast and occurs within 30 min at optimized conditions. In this case also, we observed styrene selectivity of >99.

3. Hybrids of Metal and 2D Redox active conductive MOFs for the development of hydrogen sensors.

Principal Investigator: Dr. Suresh Babu Kalidindi, Student: Marilyn DMello

2D materials that behave as conductors can find application in resistance-based sensing. They can offer different properties not seen in 3D materials. Through metal-ion ligand couples and their inner-sphere redox reactions, remarkable electronic structures and reactive properties can be explored for chemiresistive sensing. In an attempt, to extend our sensing studies, we turned our attention to 2D conductive MOFs. A layered 2D-conductive Cr-MOF was successfully synthesized, characterized by powder XRD and N2 sorption studies and explored for chemiresistive gas sensing. Here the electrical conductivity operates through 2D hopping-based transport mechanism. These properties are induced by the redox-activity of the pyrazine ligand, which leads to a smearing of the Cr 3d and pyrazine π states. Pd nanoparticles were deposited on this MOF which acted as good hydrogen sensor.

Research Highlights

- Dr. Suresh Babu Kalidindi has visited(01/06/2018 to 31/08/2018) Germany as visiting scientist at University of Ulm(Prof. Radim Berneck group) under Alexander von Humboldt Foundation renewed program.
- Ms. Marilyn Attended2 weeks training workshop at Indian Institute of Science- Indian Nanoelectronics Users Program(INUP) Hands on Training workshop in gas sensors (12- 22nd February 2019).

13. BIOLOGICAL SCIENCES DIVISION

13.1 Mission and research progress

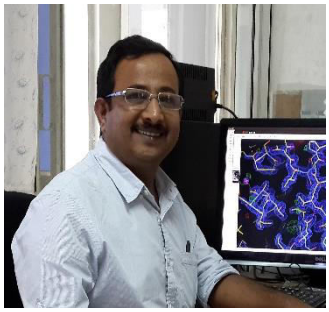
The mission of the Biological Sciences division is to be part of the solution for socially relevant medical problems which could eventually lead to allevating the standard of health in our country. In accordance with this mission, we have identified thrust areas like Cancer immunotherapy, novel antibiotics against purine and pyrimidine pathways in disease causing microorganisms, use of active biomolecules from endophytic fungi against diabetes, bioremediation using fungal enzymes. To address these challenging issues, we are continually adding pieces of research infrastructure and now possess facilities which are and not limited to gene cloning, protein expression, refolding, purification and crystallization of biomolecules. Facilities for the isolation of endophytic fungi, molecular identification, bulk extraction of secondary metabolites and their respective assay's have also been upgraded. The research activities in the department are supported by PPISR and as well as grants from government funding agencies such as Department of Biotechnology (DBT), Board for Research in Nuclear Science (BRNS), Vision Group On Science and Technology (VGST) and Department of Science and Technology (DST).

The biological sciences division offers Ph.D. programmes in Structural biology, Biochemistry and Microbiology. The structural biology group headed by Dr. Udupi A. Ramagopal works on structure-based rational modification of T-cell co-stimulatory molecules to generate lead molecules for autoimmune disorders and cancer. Enzymes having biological and therapeutic importance like enzymes involved in purine metabolism, methyltranseferases implicated in antibiotic resistance are also of interest. The microbiology group headed by Dr. Ananda K., mainly focuses on finding natural inhibitors from medicinal plants and their endophytic fungi, for the enzymes involved in carbohydrates metabolism and insulin for treating diabetes. Dr. Ananda's group are also interested in laccase enzymes and their role in bioremediation. Three students obtained their PhD degree from Biological Science division and there are five more are registered for PhD under Manipal Academy of Higher Education (MAHE), Manipal.

Major Areas of Research

1. Modification of T-cell costimulatory molecules to generate lead biologics to treat autoimmunedisorders and cancer.
2. Structural and functional studies of enzymes involved in purine metabolism.
3. Natural inhibitors from plant and endophytic fungi for treating diabetes.
4. Laccase from fungi for bioremediation of textile and pharmaceutical wastes.
5. Modification of therapeutic protein for their novel applications

13.2 Faculty profiles



Dr. Udupi A. Ramagopal

Associate Professor
Dean-Academics
udupi.ramagopal@poornaprajna.org
http://www.ppisr.res.in/faculty/udupi-ramagopal

Brief CV

- Associate Professor (2014 to 2018) and Dean Academics (Current), Poornaprajna Institute of Scientific Research, Bangalore, India.
- Associate Professor (2-14-2018) and Ramalingaswami Fellow (2014 – 2016) – Department of Biotechnology), 2011-2016.
- Assistant Professor (Ramalingaswami Fellow - DBT), 2011 – 2013, Poornaprajna Institute of Scientific Research, Bangalore, India.
- Visiting Faculty, 2011 – Present: Albert Einstein College Of Medicine, New York, USA. http://www.einstein.yu.edu/home/faculty/profile.asp?id=9276
- 2009-2011: Instructor (Faculty), Albert Einstein College Of Medicine, New York, USA.
- 2005-2009: Associate of Biochemistry (Faculty), Albert Einstein College Of Medicine, New York, USA.
- 2003-2005: Senior Research Associate, Department of Biochemistry, Albert Einstein College Of Medicine, New York, USA.
- 2001-2003: Visiting Fellow, National Institute of Health, USA.
- 2001: PhD, Department of Physics, Indian Institute of Science, Bangalore, India.

Awards and Recognitions/Achievements

1. Ramalingswami fellow, DBT, India (2011 - 2016).
2. Best thesis “Kumari L. A. Meera Award and a Gold Medal”, 2001, IISc, India.
3. Visiting Fellow (2001 – 2003, NIH, USA).
4. Visiting Faculty (Albert Einstein College of Medicine, 2011 – current).

5. Invited Instructor (2003-2010) at RapiData, a comprehensive course offered at Brookhaven National Laboratory for budding crystallographers around the world (http://www.bnl.gov/rapidata/).

6. Proposal reviewer: Macromolecular Crystallography, APS, Argonne National Laboratory.

7. Served in the "User Executive Committee 2002-2003" of National Synchrotron Light Source, Brookhaven National Laboratory, USA.

8. Jeffery Award (poster award - IUCr 2002, co-author).

9. Contributed ~ 250 protein structures to World Wide Protein Data Bank (wwPDB).

10. Referee for Acta-D, Protein Science, BioChem Journal, Nature Scientific Reports and other International Journals.

11. Doctoral Advisory committee member for students registered under MAHE, Manipal

12. Scientific Advisor “Genelon Life Science Ltd.”, Yelahanka, Bangalore

13. Started the Biological Science Division at PPISR where Biology was a new word.

14. Collaborated/collaborating with pharmaceutical industries working towards novel biologics for auto-immunity and cancer.

15. Coauthored publications with Prof. James Allison, Nobel Laureate in Physiology and medicine -2018.

NATIONAL AND INTERNATIONAL COLLABORATORS

Prof. Steven C. Almo, Albert Einstein College of Medicine, New York, USA.
Prof. Ramakumar S., Indian Institute of Science, Bengaluru, India
Prof. Udaykumar Ranga, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.
Prof. Hemalatha Balaram, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.
Dr. Dibyendu Samanta, Indian Institute of Technology, Kharagpur, India
Dr. Natesh Ramanathan, Indian Institute of Science Research and Education, Thiruvananthapuram, India.

RESEARCH INTEREST:

(1) Modification of immune checkpoint blockade receptors for cancer immunotherapy.
(2) Structural and functional characterization of phosphoribosyltransferases from pathogenic bacteria.
(3) Structural and functional characterization of antibiotic resistance conferring

methyltransferases from *Mycobacterium Tuberculosis*.

(4) *De novo* structure determination of proteins and methodology development.

Lab Members/Mentoring Experience:

Students:

Dr. Pavithra G. C. (degree awarded).

Ms. Swetha Lankipalli (graduate student, Registered under MAHE, Manipal)

Mr. Shankar Kundapura (graduate student, Registered under MAHE, Manipal)

Post-Doctoral Fellows.

Dr. Raghurama Hegde 2011-2018 (Ph. D., IISc, Bangalore, currently working at Elletra, Trieste, Italy)

Dr. Debayan Day (PhD. D.IISc, Bangalore, worked as a DBT-Research Associate and currently working at Emory University, USA, (debayan.dey@emory.edu)

Past Experience:

I have co-mentored several students and post-doctoral fellows on the structural-immunology projects at Albert Einstein College of Medicine, including

Students:

Dr. Erhu Cao (Julius Marmar Award for best thesis, currently faculty at University of Utah, erhu.cao@biochem.utah.edu).

Dr. Rotem Rubinstein (Julius Marmar Award for best thesis, *rotem.rubinstein*@phd.einstein.yu.edu)

Dr. Dibyendu Samanta (Post-Doctoral Fellow, Albert Einstein College of Medicine), currently faculty at IIT Kharagpur, India.

M. Sc. and M. Tech. Project Students.

Mr. Saurav Kampa (Presently Scientist at Indian Immunological Limited, Hyderabad, India)

Recent publications:(2013-2019, *corresponding author)

1. Shankar V Kundapura and **Ramagopal UA***, **2019,** Away from CDRs: The CC′ loop of IgV domains of the immune checkpoint receptors play a key role in receptor:ligand affinity modulation (Submitted and on BioRxiv, doi: https://doi.org/10.1101/656462.
2. Liu. W, Garrett S, Fedorov E, Ramagopal UA, Garforth S, BonannoJB, AlmoSC, **2019,** Structural basis of CD160:HVEM recognition. In press (Structure- Cell press)
3. Pavithra GC and **Ramagopal UA***, **2018**, Crystal structures of APRT from *Francisella tularensis*: An N-H···N hydrogen bond imparts adenine specificity in adenine phosporibosyltransferases. FEBS, DOI:10.1111/febs.14481.
4. Ghosh A, **Ramagopal UA**, Bonanno JB, Brenowitz MD, Almo SC. **2018,** Structures of the L27 domain of Disc Large homolog 1 protein illustrate a self-assembly module, Biochemistry. ***Biochemistry***, 57 (8), pp 1293–1305.
5. Raghurama P. Hegde, Pavithra G. C., Debayan Dey, Ramakumar S, **Ramagopal UA***, **2017**, " Can the propensity of protein crystallization be increased by using systematic screening with metals?, Invited

review/perspective with our experiments and database analysis, ***Protein Science*****,** 26(9), 1704-1713.

6. **Ramagopal UA**, Liu W, Garrett S, Yan Q, Srinivasan M, Wong S, Bell A, Mankikar S, Vangipuram R, Deshpande S, Korman A, Almo, SC. **2017**, Structural basis for cancer immunotherapy by the first-in-class checkpoint inhibitor Ipilimumab. ***Proc. Nat. Acad. Sci. (USA)***, 114(21), E4223-E4232. (This article is highligted in "In this Issue" section of PNAS). **Comments and media coverage:** http://www.deccanherald.com/content/623201/bodys-battle-against-cancer.html and https://medicalxpress.com/news/2017-05-cancer-immunotherapy-drugs-x-ray-crystallography.html and https://immuno-oncologynews.com/2017/06/06/insights-into-yervoy-and-target-molecule-may-improve-immunotherapies/ and https://www.natureindex.com/article/10.1073/pnas.1617941114 and http://cancerimmunolres.aacrjournals.org/content/5/7/515.

7. Raghurama P. Hegde, Fedorov, A.A., Sauder, J.M., Burley, S.K., Almo, S.C. & **Ramagopal UA***, **2017**, The hidden treasure in your data: phasing with unexpected weak anomalous scatterers from routine data sets., ***Acta Cryst F,*** *73*, 184-195.
8. Samanta D, Guo H, Rubinstein R, **Ramagopal UA***, Almo SC, **2017**, Biochemical and Structural studies reveal a canonical mode of molecular recognition between immune receptor TIGIT and nectin-2, ***Molecular Immunology*** 81, 151-159.
9. Lázár-Molnár E, Scandiuzzi L, Basu I, Quinn T, Sylvestre E, Palmieri E, **Ramagopal UA**, Nathenson SG, Guha C, Almo SC. **2017,** Structure-guided development of a high-affinity human Programmed Cell Death-1: Implications for tumor immunotherapy. ***EBioMedicine***, 17:30-44.
10. Liu W, **Ramagopal UA**, Cheng H, Bonanno JB, Toro R, Bhosle R, Zhan C, Almo SC.**2016,** Crystal Structure of the Complex of Human FasL and Its Decoy Receptor DcR3. ***Structure (Cell Press),***24(11), 2016-2023.

Grants:

1. Ramalingaswami Fellowship titled "Co-stimulatory molecules: Biology and therapeutic intervention", Department of Biotechnology (DBT), New Delhi, India.
2. Design of modified B7-1 (CD-80) and B7-2 (CD86) molecules to create potential reagents for cancer and auto-immune disorders", Vision Group on Science and Technology (VGST), Karnataka.
3. Structural and evolutionary investigations on antibiotic resistance conferring rRNA methyltransferases for designing novel strategies of drug development, Department of Science and Technology, India.
4. Structure based rational design of PD-1 mutants to create lead molecules for cancer immunotherapy, Bristor Mayers Sqibb, USA.

Current Research Projects:

Structural Studies of Purine Phosphoribosyltransferases from Pathogenic Bacteria

Primary Investigator: Dr. Ramagopal U. A.

Research Student: Mrs. Pavithra G. C.

Nucleotides are critical for every aspect of cellular life. There are two pathways for the synthesis of nucleotides: the *de novo* and the salvage pathways. Purine PRTases are enzymes involved in purine salvage pathway, catalyzes a reaction between purines bases into respective nucleotides with the help of PRPP. In this project, we have chosen to study purine PRTases from three pathogenic bacteria such as *Y. pseudotuberculosis, H. pylori* and *F. tularensis* that are known to cause Far East scarlet-like fever, gastritis/duodenal cancer and tularemia respectively. This project resulted in few publications and a thesis that describes structural and functional understanding of four novel structures, they are an APRT and an XGPRT from Yersinia species and an APRT and a HPRT from F. tularensis. In total, this work describes 12 crystal structures in their apo form as well as with substrate(s) and product.

Rational modification of immune checkpoint receptors of PD-1 pathway for cancer immunotherapy

Antibodies targeting negative regulators of immune checkpoints have shown unprecedented and durable response against variety of malignancies. While the concept of blocking the negative regulators of immune checkpoints using mAbs appears to be an outstanding approach, their limited effect and several drawbacks such as resistance, poor solid tumor penetration and so on, calls for the rational design of next generation of therapeutics. Soluble isoforms of negative regulators of immune checkpoints are expressed naturally and are shown to regulate immune response, suggesting the soluble version of these molecules and affinity-modified versions of these self-molecules could be effective lead molecules for immunotherapy. In this project, we propose to produce rationally designed and minimally modified soluble version of PD-1 (Programmed Death -1; an inhibitory receptor on T-cells).

Design of modified B7-1 (CD-80) and B7-2(CD86) molecules to create potential reagents for cancer and auto-immune disorders.

The knowledge gained from the structures of immune receptors involved in the CD28:B7 pathway, including the structure of congnate receptor-ligand coplexes will be exploted to design decoy B7's (B7-1 and B7-2) that can effectively differentiate CTLA-4 from CD28. Efficacy of the modified B7 molecules to bind to their cognate receptors will be assessed using biophysical methods including X-ray crystallography. The results are expected to provide lead molecules that are effective against auto-immune disorder or cancer

Structural study of a putative rRNA methyltransferase from *Sinorhizobium meliloti*

Ribosomal RNA (rRNA) methyltransferases play crucial role in many cellular processes and are implicated in antibiotic resistance in many antibiotic producing strains. These methyltransferases modify the rRNA associated with ribosomes and hence the antibiotic binding site. We are pursuing structural studies of a putative rRNA methyltransferases (Mtase) from the *Mycobacterium Tuberculosis* and from the soil bacterium S*inorhizobium meliloti*. The study is expected to provide better insights on mechanism of antibiotic resistance and also gives clues to design the so called "antibiotic resistance breakers".

Other activities/achievements:

Dr. Ramagopal's proposal "Structure based rational design of PD-1 mutants to create lead molecules for cancer immunotherapy", is approved by **Bristol Myers Squibb, USA.**

Dr. Ramagopal's proposal for the experiment at **Elettra Synchrotron Facility, Trieste, Italy, was approved by DST grant administered by IISc.,** and he visited the facility and conducted the experiment at Elettra, from Dec 4-8th, 2018.

Mr. Shankar Kundapura presented a poster titled "The CC′ loop of immunoglobulin V domain: from a bystander to an active determinant of receptor-ligand interactions" in the 46th National Seminar on Crystallography at NIMHANS, Bangalore. This poster was awarded the **best poster award** among 110 posters present in the conference.

Dr. Ramagopal was invited to conduct practical sessions on "structural solution and refinement of macromolecular structures" in the workshop/meeting "**Practical Protein Crystallography at Indus-2 Synchrotron**", March 27-28, 2018, RRCAT, Indore, India.

Dr. Ramagopal delivered an invited talk in the workshop **"CCP4 Crystallography School and Workshop conducted by CCP4 consortium, UK"** tilled " From data processing to structure refinement and beyond" 22-Oct-2018 to 26-Oct-2018, held at IMTEC, Chadigarh, India and helped the students in week long workshop on practical aspects of macromolecular crystallography.

Dr. Ramagopal delivered an invited talk titled "From structure to function: Defining the substrate specificity of purine phosphoribosyltransferases" at the **46th National Seminar on Crystallography**, 27th to 29th June 2018, held at NIMHANS, Bangalore and delivered invited talk.

Ms. Pavithra delivered an **invited talk** titled "Structural studies of APRTs from pathogenic bacteria reveals an N-H…N hydrogen bond imparts adenine specificity" at the **46th National Seminar on Crystallography**, 27th to 29th June 2018, held at NIMHANS, Bangalore.

Dr. Raghurama Hegde delivered an **invited talk** titled "Systematic screening with metals as a novel strategy for protein crystallization" at the **46th National Seminar on Crystallography**, 27th to 29th June held at NIMHANS, Bangalore.

Dr. Ramagopal was invited to give a talk in the workshop "Physics of living matter and medical equipment" held at St Aloysius college, 18th and 19th of December 2018.

Dr. Raghurama Hegde participated as a judge, for debates presented by pre-university students as part of the State Level NCET Science Fest 2018 held at the Nagarjuna College of Engineering and Technology, Bengaluru, on 16th November 2018.

Mr. Shankar V. Kundapura delivered a talk on "Immunotherapy" at Poornaprajna College, Udupi on 7-8th December 2018.

Dr. Ramagopal delivered an invited talk at Government Science College on "Checkpoint Blockade Cancer Immunotherpy.

Dr. Ramagopal visited TDU, Bengaluru to inaugurate a workshop titled "Genomics and Transcriptomics" on 01 April 2019.

Dr. Ramagopal together with the director visited Jyothi Institute of Technology and gave a talk on overview of activities in Biological Science Division, PPISR.

Dr. Raghurama Hegde accepted the senior postdoctoral fellowship position at Elettra, Trieste, Italy

Dr. Ananda K

Associate Professor
Biological Sciences
E-mail: ananda @poornaprajna.org
ananda@ppisr.res.in

BRIEF CV:

2018- Onwards: Associate Professor, PPISR, Bangalore

2011-2017: Assistant Professor, PPISR, Bangalore, India

2010-2011: Faculty Fellow, PPISR, Bangalore, India

2004-2010: Post-Doctoral Fellow, Albert Einstein College of Medicine, NY, USA

2004-2004: Lecturer, P A College of Engineering, Mangalore, India

2003-2004: Project Associate, IWST, Bangalore, India

1999-2003: Administrative Supervisor, KSRTC, Govt. of Karnataka, India

1996-2001: PhD, Mangalore University, Mangalore, India.

1995-1996: Project Assistant, College of Fisheries, Mangalore, India

1993-1995: MSc, Biosciences, Mangalore University, Mangalore, India

Training of Students:

PhD Awarded	: 02
MSc Project completed	: 03
BSc/BE Project completed	: 07
BSc Inspire students	: 03
PhD students working	: 03

RESEARCH INTERESTS:

1. **Natural Enzyme Inhibitors for controlling type 2 diabetes:**

   Natural inhibitors for glucosidase enzymes located in the small intestinal region are isolated from the medicinal plants and from their endophytic fungi. The inhibitors extracted using different solvents were tested for inhibition of alpha glucosidase enzyme, the active extracts will be purified and identified using the advanced techniques. Similarly, extractions made from the endophytic fungi (isolated from the same plant) are tested as above. The endophytic fungus which shows best inhibition for AG enzyme is grown in large scale for the isolation of inhibitors. We are trying to sequence

the human gene for AG enzyme and want to test these inhibitors, this may provide us the information how these natural inhibitors can work with human enzyme in-vitro. The final goal of this project is to get a natural inhibitor for controlling type-2 diabetes.

2. **Laccase producing endophytic fungi and applications of fungal laccase**
   Fungi are well known for their role in degrading diverse group of complex molecules found in nature. There are group of ligninase enzymes responsible for the breakdown of natural lignin, cellulose or hemcellulose are also involved in degrading phenolic and polyphenolic compounds released from various industrial and anthropogenic activities. In this area, we are studying degradation of synthetic dyes using one of ligninases, the laccase enzyme from endophytic fungi as well as enzymes from known white rot fungi. The role of electron beam radiation and gamma radiation was also studied to improve the rate of bodegradation by endophytic fungi. The enzyme degraded dye was analysed for identification of its degraded products and phytotoxicity and agriculturally important microbial toxicity of degraded compounds.

3. **Modification of Insulin molecule to improve its half-life and other therapeutic properties**
   In this project we are trying to modify unique amino acids by PEGylation and bio-conjugation methods to increase the half life of the insulin. Using the bioinformatics tool and phylogenetic analysis of proteins related to insulin found some interesting mutations and these might lead to novel insulin molecules. Possibly, the new modified insulin molecules would bring out the novelty for the future therapeutic applications. The modified therapeutic molecules will be characterised for their biophysical, biochemical properties and analysed for structural and functional behaviours before using in clinical test.

RECOGNISTIONS/ACHIEVEMENTS:

PhD Co-coordinator at PPISR for MAHE, Manipal
Life Member of Mycological Society of India
Life member of Association of Microbiologist of India
Postdoctoral Senate member in Faculty Senate, Quality of Life Committee and of Committee on Committees of Albert Einstein College of Medicine 2007-2009.
Working experience as Administrative supervisor in KSRTC, Karnataka, India.1998-2003
President of Mangalore university researcher's forum (MURF) during the period of Ph.D. for a year.
Member of New York academy of science, NY, USA.2006-2008
Member of Protein Society, San Diego. USA 2006.

STUDENTS

PhD students

3. Ms. Kavitha K N
4. Mr.Kirana M P
5. Ms. Shrilakshmi S

Project Fellows

1. Anusha , B.E

Past PhD students

1. Dr. Pavithra N.
2. Dr.Sathish L.

RESEARCH

SPONSORED PROJECTS:

1. "α-amylase and α-glucosidase inhibitors from endophytic fungi for treating Type 2 diabetes" funded by VGST-Karnataka for the year 2016-17 for 3 years (Rs.30 lakhs).

ACADEMIC PROJECTS:

1. Effect of electron beam and Gamma radiation on endophytic fungi producing laccase enzyme. PI:Dr.Ananda, K. ; Research Scholar: Ms.Kavitha KN
2. Enzymatic degradation of chloramphenicol by laccase from *Trametes hirsute*. PI: Dr. Ananda K.; Research scholar: Ms. Kavitha K N
3. Alpha glucosidase enzyme inhibitors from *Simarouba glauca* and from its endophytic fungi. PI: Dr. Ananda K, Reseach Scholar: Mr. Kiran M P
4. Alphaglucosidase enyme inhibitors from *Ensete superbum* for the treatement of diabetes. PI: Dr.Ananda K. ; Research Scholar: Mr.Kirana M. P.
5. Site specific modification of insulin for increasing its half-life and pharmacological properties. PI: Dr. Ananda K.; Research Scholar: Ms. Shrilakshmi S
6. Rational modification of insulin driven by evolution and chemistry to produce novel insulin analogues PI: Dr. Ananda K. Research Scholar: Ms.Shrilakshmi S
7. Evaluation of α-glucosidase enzyme inhibitors and nutritional value of edible fruit seeds project report. Student: Shreya.H, B.E. Biotechnology, PES University, Bangalore

RESEARCH HIGHLIGHTS:

A. Published papers:

1. Kavitha Keshava Navada and **Ananda Kulal**, (2019). Enzymatic degradation of chloramphenicol by laccase from Trametes hirsuta and comparison among mediators," International Biodeterioration & Biodegradation **138**, 63-69.
2. Nagaraja, Akshatha, Yashoda Malgar Puttaiahgowda, **Ananda Kulal**, Ajithkumar Manayan Parambil, and Thivaharan Varadavenkatesan. **(2019)**

"Synthesis, Characterization, and Fabrication of Hydrophilic Antimicrobial Polymer Thin Film Coatings." *Macromolecular Research*: 1-9.

3. Jalageri, Manohara Dhulappa, Yashoda Malgar Puttaiahgowda, Ajithkumar Manayan Parambil, and **Ananda Kulal**. (**2019)**"Design of multifunctionalized piperazine polymer and its activity toward pathogenic microorganisms." *Journal of Applied Polymer Science*: 47521.
4. Sunil Kumar, A., J. Kudva, B.R. Bharath, **K. Ananda**, R. Sadashiva, S. Madan Kumar, B.C. Revanasiddappa, V. Kumar, P.D. Rekha, and D. Naral. **2019**. Synthesis, structural, biological and in silico studies of new 5-arylidene-4-thiazolidinone derivatives as possible anticancer, antimicrobial and antitubercular agents. *New Journal of Chemistry* 43:1597-1610.
5. Kolangare, Irfana Moideen, Arun Mohan Isloor, Zulhairun Abdul Karim, **Ananda Kulal**, Ahmad Fauzi Ismail, and Abdullah Mohamed Asiri. **(2018**) "Antibiofouling hollow-fiber membranes for dye rejection by embedding chitosan and silver-loaded chitosan nanoparticles." *Environmental Chemistry Letters*: 1-7.
6. Bharadwaj, S.S., B. Poojary, S.K.M. Nandish, J. Kengaiah, **M.P. Kirana**, M.K. Shankar, A.J. Das**, Ananda Kulal**, and D. Sannaningaiah**.(2018**). Efficient Synthesis and in Silico Studies of the Benzimidazole Hybrid Scaffold with the Quinolinyloxadiazole Skeleton with Potential α-Glucosidase Inhibitory, Anticoagulant, and Antiplatelet Activities for Type-II Diabetes Mellitus Management and Treating Thrombotic Disorders. *ACS Omega 3:12562-12574.*
7. Kavitha Keshava Navada, Ganesh Sanjeev and **Ananda Kulal (2018**). Enhanced biodegradation and kinetics of anthraquinone dye by laccase from an electron beam irradiated endophytic fungus. *International Biodeterioration & Biodegradation, 132*, 241-250.

B. Papers presented in conferences:

1. Gave an oral presentation on title “Alpha glucosidase inhibitors isolated from medicinal plants for treating type 2 diabetes” in the International conference on “Current concepts on the role of Indian medicine and phytoceuticals in maintenance of health” at 39th Annual Summit of IABMS 2018, Chikka Aluvara Campus, Mangalore University during 15-17 November 2018 and got **‘Best Oral Presentation Award’**.
2. Presented a poster in the one-day conference “Recent advances in Biochemistry” organized by St. Aloysius college, Mangalore on 23rd February 2019 and won the “**Best Poster Presentation Award**”

Research Collaboration

1. Dr. Arun M Isloor, Associate Professor, NITK, Surathkal
2. Genelon Institute of Life sciences, Yelahanka, Bangalore.
3. Dr. Yashoda M P and Dr. Danya Sanil, from MAHE, Manipal.
4. Dr. Boja Poojari, Mangalore University, Mangalore

14. THEORETICAL SCIENCES DIVISION

14.1 Mission and research progress

Theoretical sciences division works on major goals; the scientific understanding of the mathematical structure and conceptual theme underlying the physical laws and the emergence of this macroscopic world from these laws. The broad areas are many-body and mesoscopic physics, nanoscience, quantum information theory, quantum foundations and Solar physics.

Two new students have joined the group, Mr. Y. R. Karthik and Mr. M. Vinod Rao, working under Dr. Sujit Sarkar and Dr. R. Srikanth, respectively, with the former student having just registered for his PhD. Mr Kartik, funded under a DST-SERB project, will work on the physics of geodesics applied to topological states in quantum matter, while Mr. Vinod, funded under a DRDO project, will be involved in the feasibility analysis of semi-counterfactual cryptography. Our first PhD student, Ms (Dr.) Akshata Shenoy-Hejmadi (PhD, IISc, 2015), our second student was Dr S. Omkar (PhD, MU, 2016), and our third student, Dr. S. Aravinda, are currently doing their postdocs in the country or abroad.

The Doctoral Advisory Committee (DAC) has been constituted for our PhD student Mr Y R Karthik: Prof. C. Sivaram (IIA, Bengaluru) and Prof. B. S. Ramachandra.

We hope to conduct the DAC meeting for Mr N. Vinod Rao shortly.

Mission & Goals

- Exploring various topological aspects of light-matter interactions and many-body physics: the interplay of topology and interactions in light-matter systems.
- Understanding the nature of the quantum state through quantum cryptography and communication, rather than a specific ontological framework.
- Exploring practical issues pertaining to quantum information processing, among them quantum cryptography and quantum noise.
- Identifying patterns in Solar surface phenomena and their connection to terrestrial weather.

Glimpses of Current Research

- Topological phase for interacting light-matter physics and relativistic physics for condensed matter system
- Relaxing the no-signaling principle in generalized probability theories.
- Physics of edge states for topological insulator and interacting light-matter system.
- Bridging the generalized probability theories and device independence in the context of mistrustful cryptography.
- Semiotic approach to the problem of free will.
- Bell-Kochen-Specker theorem for identity in quantum mechanics.
- Superlocality and superunsteerability in quantum mechanics.
- Rotational Effects on Supergranulation.

14.2 Faculty Profiles

Dr. Sujit Sarkar

Associate Professor

E-mails: sujit@poornaprajna.org
sujit.tifr@gmail.com

http://www.ppisr.res.in/faculty/sujit-sarkar

BRIEF CV:

- Associate Professor, PPISR: Jan 2018--present
- Assistant Professor, PPISR: 2007 -- 2017
- Faculty Fellow, PPISR: 2005 -- 2007
- IISc Physics Department (year 1997-1998)
- Bar-Ilan University, Physics Department (year 1999-2000)
- Max-Planck Institute, Germany as a Guest Scientist (year 2000-2002)
- The Weizmann Institute of Science (year 2002-2005).
- Visiting Scientist Positions: Tata Institute of Fundamental Research (Mumbai) National Centre for Theoretical Science (NCTS, Taiwan), Karl-shrue Institute of Technology, Germany.

RESEARCH INTERESTS:

(1). Quantum Many Body Physics and Quantum Field Theoretical Studies of Quantum Condensed Matter System.
(2). Cavity Quantum Electrodynamics.
(3). Non-equilibrium Statistical Physics.
(4). Quantum Phase Transition and Topological Quantum Phase Transition
(5). Geometric Structure of Space-Time and Quantum Geometrical Tensor.

RECOGNITIONS/ACHIEVEMENTS:

Seminars, Lectures, Workshops and Conferences:

(1). International Conference on "Non-comutative Geometry and Quantum State" at S. N. Bose Centre, Kolkata, November 2018.

(2). Seminar given in International Centre of Theoretical Science on "Conformal-Field Theory Study for the Topological State of Matter", 15th February 2019, in Indian Statistical Physics Community Meeting.

(3). "Bangalore Statistical Physics School" at the ICTS, June (2018).

(4). “Workshop on Exactly Integrable System” at the ICTS, July (2018).

(5). “Discussions Meeting on Topology” at ICTS, June (2018).

Students Poster Presentations:

All of them have presented poster

(1) “Workshop on Non-Hermitian Physics” at the ICTS, June (2018).
(2)“Workshop on Differential Geometry” at the ICTS, June (2018).
(3)“Bangalore Statistical Physics Meeting” at the ICTS, February (2019).
(4)Distinguished Lecture by F. D. M. Haldane (Nobel Prize-2016), January (2019).

STUDENTS

Current PhD students

1. Mr. Rahul Sharma (JRF Student)
2. Mr. Ranjith Kumar R (JRF Student)
3. Mr. Y. R. Kartik (JRF Student)

RESEARCH

Current Academic Projects:

1) 2nd DST PROJECT: Topological States of Superconducting Nanowires and interacting light-matter systems at nano scales.
Principal Investigator: Sujit Sarkar
Project Students: Mr. Rahul Sharma (JRF Student), Mr. Ranjith Kumar R (JRF student).

1) A Brief Summary of the Project:

(1). The Physics of different physical systems at nanoscale are interesting in their own right. This research project has few scientific objectives for answering fundamental questions currently debated in the literature on the topological properties in superconducting nanowire and interacting light-matter physics.
(2). The description of topological excitations like quantum phase slip center in disordered superconducting nanowire and the appearance of Berezinskii-Kosterlitz-Thouless transition in interacting light-matter physics are among the most important problems of topological quantum phase transition.
(3). Find the relation between the topological invariant number and the physical quantity of the system.
(4). The objective of this project is to find the answers of these questions *and if possible the interrelations between them.*

Research Highlights:

1). Physics of Majorana modes in interacting helical liquid, Sarkar S, Nature Sci.Rep. 6, 30569 doi:10.1038/srep30569 (2016) (Nature Publication Group).

2). Topological Quantum Phase Transition and Local Topological Order of Light in a One-Dimensional Array of Nonlinear Cavities. Sarkar S, Nature Sci. Rep. 7, 41598 (2017) (Nature Publication Group) doi:10.1038/srep41598 (2017).

3). Quantization of geometric phase with integer and fractional topological characterization in a quantum Ising chain with long-range interaction. Sarkar S, Nature Sci. Rep. 8, 5864 (2018) (Nature Publication Group). DOI:10.1038/s41598-018-24136-1.

4). Characterization of Majorana-Ising phase transition in a helical liquid system, Journal of Magnetism and Magnetic Materials 475 (2019) 257–263.
(In collaboration with S. N. Bose Centre)

Scientific Collaboration:
(1). Prof. C. D. Hu (The National Taiwan University).
(2). Prof. Masaki Tesuzaka (Tokyo, Japan).
(3). Prof. Igor Goryni (Karlshrue, Germany).
(4). Prof. M. Kumar (S. N. Bose Centre).

Dr. R. Srikanth

Associate Professor

E-mail:srik@poornaprajna.org
Homepage:
http://www.ppisr.res.in/faculty/r-srikanth

BRIEF CV:

- Associate Professor, PPISR: Jan 2018--present
- Assistant Professor, PPISR: 2010 -- 2017
- Faculty Fellow, PPISR: 2006 -- 2010
- RA, Raman Research Institute, Bengaluru: 2003--2006
- RA, CTS, IISc, Bengaluru: 2001--2003
- RA, IIA, Bengaluru: 2000--2001

RESEARCH INTERESTS:

1. **Quantum information theory:** Quantum non-Markovianity in quantum channels, rmeasures of (non-)Markovian channels, counterfactual quantum digital signature; quantum differential phase cryptography.

2. Foundations of quantum mechanics: Causality, computational speedup and steering in multipartite systems as studied in generalized probability theories.

3. Solar physics: Solar supergranulation, Rotational Effects on Supergranulation, and Fractal Dimension of Supergranulation.

4. Cognition: Free will, consciousness, Identity and individuation; quantum cognition, decision making.

RECOGNITIONS/ACHIEVEMENTS:

- Various invited talks and lectures. Most recently:
  - “Quantum information theory: an invitation” presented at "Advanced Workshop 2019 on Quantum Computer Science", CFRCE, Bengaluru, Mar 2-3, 2019

- "Quantum computation and quantum error correction" Presented at "Quantum Information & Computation" at St. Philomena's College, Mysore Aug 18-20, 2018,

- Invited talk: Operationally Lorentz-covariant extensions of quantum mechanics,International Conference on Quantum Foundations 2015, National Institute of Technology, Patna, November 30 -- December 4, 2015.

- Editor (Quanta, quanta.ws)
- Reviewer (Phys Rev A, Physical Rev Lett., Quantum Information Processing, Physica Scripta, Int. J. Theoretical Physics, Quanta, etc.)

STUDENTS

Current PhD students

1. U. Shrikant
2. N. Vinod Rao
3. G. M. Sowmya (part-time, jointly with Prof U. Paniveni, shortly registering VTU)
4. G. Rajni (part-time, jointly with Prof U. Paniveni, shortly registering VTU)
5. M. Yamuna (part-time, jointly with Prof U. Paniveni)

Past PhD students

1. S. Omkar (2016)
2. S. Aravinda (2017)

PUBLICATIONS (in peer-reviewed international journals) : 8 papers

RESEARCH

CURRENT ACADEMIC PROJECTS:

1. Feasibility study of a practical Realization of a protocol for semi-counterfactual quantum key distribution (QKD)

Principal Investigator: Dr. R. Srikanth
Project fellow: Mr N. Vinod Rao
Funding Agency: DRDO, India

2. Computational speedup in quantum mechanics and generalized probabilistic theories"

Principal Investigator: Dr. R. Srikanth
Student: U. Shrikant
Funding agency: DST-SERB, India

3. Center for Excellence in quantum cryptography

Principal Investigator: Prof Anirban Pathak
Co-Investigator: Dr. R. Srikanth
Funding Agency: QuST (DST)

Current projects:

Measure of positive and not completely positive single-qubit Pauli maps: The time evolution of an initially uncorrelated system is governed by a completely positive (CP) map. More generally, the system may contain initial (quantum) correlations with an environment, in which case the system evolves according to a not-completely positive (NCP) map. It is an interesting question what the relative

measure is for these two types of maps within the set of positive maps. After indicating the scope of the full problem of computing the true volume for generic maps acting on a qubit, we study the case of Pauli channels in an abstract space whose elements represent an equivalence class of maps that are identical up to a non-Pauli unitary. In this space, we show that the volume of NCP maps is twice that of CP maps.

1. Maximally nonlocal subspaces: A nonlocal subspace HNS is a subspace within the Hilbert space Hn of a multi-particle system such that every state ψ∈HNS violates a given Bell inequality B. Subspace HNS is maximally nonlocal if each such state ψ violates B to its algebraic maximum. We propose ways by which states with a stabilizer structure of graph states can be used to construct maximally nonlocal subspaces, essentially as a degenerate eigenspace of Bell operators derived from the stabilizer generators. Two cryptographic applications-- to quantum information splitting and quantum subspace certification-- are discussed.
2. Non-Markovian dephasing and depolarizing channels: We introduce a method to construct non-Markovian variants of completely positive (CP) dynamical maps, particularly, qubit Pauli channels. We identify non-Markovianity with the breakdown in CP-divisibility of the map, i.e., appearance of a not-completely-positive (NCP) intermediate map. In particular, we consider the case of non-Markovian dephasing in detail. The eigenvalues of the Choi matrix of the intermediate map crossover at a point which corresponds to a singularity in the canonical decoherence rate of the corresponding master equation, and thus to a momentary non-invertibility of the map. Thereafter, the rate becomes negative, indicating non-Markovianity. We quantify the non-Markovianity by two methods, one based on CP-divisibility (Hall et al., PRA 89, 042120, 2014), which doesn't require optimization but requires normalization to handle the singularity, and another method, based on distinguishability (Breuer et al. PRL 103, 210401, 2009), which requires optimization but is insensitive to the singularity.
3. Non-Markovian evolution: a quantum walk perspective: Quantum non-Markovianity of a quantum noisy channel manifests typically as information backflow, characterized by the departure of the intermediate map from complete positivity, though we indicate certain noisy channels that don't exhibit this behavior. In complex systems, non-Markovianity becomes more involved on account of subsystem dynamics. Here we study various facets of non-Markovian evolution, in the context of coined quantum walks, with particular stress on disambiguating the internal vs. environmental contributions to non-Markovian backflow. For the above problem of disambiguation, we present a general power-spectral technique based on a distinguishability measure such as trace-distance or correlation measure such as mutual information. We also study various facets of quantum correlations in the transition from quantum to classical random walks, under the considered non-Markovian noise models. The potential for the

application of this analysis to the quantum statistical dynamics of complex systems is indicated.

4. Operational nonclassicality of local multipartite correlations in the limited-dimensional simulation scenario: Recently, the quantumness of local correlations arising from separable states in the context of a Bell scenario has been studied and linked with superlocality [Phys. Rev. A {\bf 95}, 032120 (2017)]. Here we investigate the quantumness of unsteerable correlations in the context of a given steering scenario. Generalizing the concept of superlocality, we define as \textit{super-correlation}, the requirement for a larger dimension of the preshared randomness to simulate the correlations than that of the quantum states that generate them. Since unsteerable states form a subset of Bell local states, it is an interesting question whether certain unsteerable states can be super-correlated. Here, we answer this question in the affirmative. In particular, the quantumness of certain unsteerable correlations can be pointed out by the notion of \textit{super-unsteerability}, the requirement for a larger dimension of the classical variable that the steering party has to preshare with the trusted party for simulating the correlations than that of the quantum states which reproduce them. This provides a generalized approach to quantify the quantumness of unsteerable correlations in convex operational theories.
5. Operational characterization of quantumness of unsteerable bipartite states: For a bipartite local quantum correlation, superlocality refers to the requirement for a larger dimension of the random variable in the classical simulation protocol than that of the quantum states that generate the correlations. In this work, we consider the classical simulation of local tripartite quantum correlations P among three parties A,B and C. If at least one of the bipartitions (A|BC), (B|AC) and (C|AB) is superlocal, then P is said to be absolutely superlocal, whereas if all three bipartitions are superlocal, then P is said to be genuinely superlocal. We present specific examples of genuine superlocality for tripartite correlations derived from three-qubit states. It is argued that genuine quantumness as captured by the notion of genuine discord is necessary for demonstrating genuine superlocality. Finally, the notions of absolute and genuine superlocality are also defined for multipartite correlations.

15. PUBLICATIONS/ PATENTS [2018-2019]

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2. DMello, M. E.; Sundaram, N. G.; Singh, A.; Singh, A. K.; Kalidindi, S.B. (2019). "Amine Functionalized Zirconium Metal-Organic Framework as an Effective Chemiresistive Sensor for Acidic Gases" **Chem. Commun.** 55, 349—352,
3. Kavitha Keshava Navada, and Ananda Kulal (2019). Enzymatic degradation of chloramphenicol by laccase from *Trametes hirsuta* and comparison among mediators. **International Biodeterioration & Biodegradation** *138: 63-69.*
4. Bakuru, V. R.; Velaga, B.; Peela, N. R.; Kalidindi, S.B. (2018) "Hybridization of Pd Nanoparticles with UiO-66 (Hf) Metal Organic Framework and the Effect of Nanostructure on the Catalytic Properties" **Chem. Eur**. **J**., DOI: 10.1002/chem.201803200
5. Pradeep P. Shanbogh, Vikash Chandra Petwal, Jishnu Dwivedi, Ashok Rao, and Nalini G. Sundaram, (2019),High Energy Electron Beam Induced Evolution of Secondary Phase and Enhanced Photocatalytic Activity in Monoclinic BiEuWO6 Nanoparticles, **J. Phys. Chem. C**, Just Accepted Manuscript DOI: 10.1021/acs.jpcc.8b12368
6. 3. Archana K Munirathnappa, Debasmita Dwibedi, James R Hester, Prabeer Barpanda, Diptikanta Swain, Chandrabhas Narayana, and Nalini G. Sundaram, (2019), "In-Situ Neutron Diffraction Studies of LiCe(WO4)2 Polymorphs: Phase Transition and Structure-Property Correlation", **J. Phys. Chem. C**, 123, 2, 1041-1049
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8. Pradeep P. Shanbogh , Rajamani Raghunathan, Diptikanta Swain , Mikhail Feygenson, Joerg Neuefeind, Jasper Plaisier, Chandrabhas Narayana, Ashok Rao and Nalini G. Sundaram (2018). Impact of Average, Local and Electronic Structure on Visible Light Photocatalysis in Novel BiREWO6 (RE= Eu & Tb) Nanomaterials." **ACS Appl. Mater. Interfaces**, *10* (42), pp 35876–35887
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10. Pradeep Kumar, Subhashish Banerjee, R. Srikanth (2018). Vinayak Jagadish, Francesco Petruccione. Non-Markovian evolution: a quantum walk perspective. **Open Systems & Information Dynamics** 25, 1850014.
11. Jebaratnam, C., Das, D., Goswami, S., Srikanth, R. and Majumdar, A.S., (2018). Operational nonclassicality of local multipartite correlations in the

limited-dimensional simulation scenario. **Journal of Physics A: Mathematical and Theoretical**, *51*(36), p.365304.

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23. Bharath Velaga, Pradeep P. Shanbogh, Diptikanta Swain, Chandrabhas Narayana and Nalini G.Sundaram (2018). High Surface Area SnO2-Ta2O5 Composite for Visible Light Driven PhotocatalyticDegradation of an **Organic Dye.** ***Photochemistry & Photobiology,*** Wiley publications, D*OI:10.1111/php.12896.,2018*

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28. Srikanth, R. (2018). Quantum bit commitment and the reality of the quantum state. ***Foundations Of Physics,*** 48, 92-109*;* Posted on arXiv physics archive:https://arxiv.org/abs/1708.04964.

16. NEW RESEARCH STUDENTS AND Ph.D REGISTRANTS

16.1 Junior Research Fellows Registered for PhD

In the year 2018-2019, the following research students working at PPISR have registered for their PhD at MAHE, Manipal

(i) Ms. Vaishnavi B. J. , under the guidance of Dr. Ganapati Shanbhag , Materials Science and Catalysis Division

(ii) Mr. Vinod N. under the guidance of Dr. Srikanth R , Theoretical Sciences Division.

(iii) Ms. Chethana under the guidance of Dr. Nalini G Sundaram, Materials Science and Catalysis Division

16.2 New Research Fellows/Engineers

- Mr. K. S. Subramanya has joined PPISR as a Research Fellow to work on the industry sponsored project under the guidance of Dr. Ganapati V Shanbhag.
- Ms. Arpana Hegde has joined PPISR as a Research Fellow to work under the guidance of Dr. Sanjeev P Maradur
- Mr. Madhav Nayak joined as Research Fellow to work on the project sponsored by GTC Technology, USA. under the guidance of Dr. Ganapati V Shanbhag
- Ms. Nimisha Simon joined as a Research Engineer to work on the project sponsored by Deepak Novochem Technologies, Ltd, under the guidance of Dr. Ganapati V Shanbhag

17. HIGHLIGHTS OF RESEARCH ACTIVITIES

17.1 ACHIEVEMENTS

1. Mr. Manjunathan P. received his PhD degree at 26th Convocation ceremony at MAHE, Manipal on November 16, 2018 for his research on "Designing Heterogeneous Catalysts for the Conversion of Glycerol & Furfuryl Alcohol into Value-Added Chemicals". He conducted under Dr. Ganapati Shanbhag who was guide and Dr. Sanjeev .P.Maradur as his co-guide, in the Materials Science and Catalysis Division, PPISR, Bengaluru

2. Mrs. Pavithra G C. submitted her thesis on "Structural studies of purine phosphoribosyltransferases from pathogenic bacteria" to MAHE, Manipal for the award of PhD degree in February 2019. She conducted her research under the guidance of Dr. Ramagopal

3. Mr. Pradeep P Shanbogh, working as CSIR-SRF under the Guidance of Dr. Nalini G Sundaram and Co-Guide as Prof. Ashok Rao, MIT, Manipal, submitted his thesis titled "Semiconducting Oxide Nanoparticles: Band Gap Engineering, Photocatalysis and Photoluminescence Studies" on May 3rd, 2019

4. Dr. Shanbhag received International Travel Grant from SERB, DST, Govt. of India to travel to Australia to give an invited talk on his research work at prestigious "3rd International Conference on Emerging Advanced Nanomaterials 2018 (ICEAN-2018)" held in the Newcastle Exhibition and Convention Center, Newcastle, NSW, Australia from October 30th to November 2nd 2018. He also visited University of Newcastle and established collaboration with Prof. Ajayan Vinu, Director of Global Innovative Center for Advanced Nanomaterials (GICAN).

5. Dr. Suresh K Babu received Alexander von Humboldt fellowship under renewed research stay program to visit Germany.

6. Dr. Udupi A Ramagopal received DST Grant for his proposal for the experiment at Elettra Synchrotron Facility, Trieste, Italy and he visited the facility and conducted the experiment at Elettra, from December 4-8th, 2018.

7. Ms. Swetha's abstract has been selected for a poster presentation at the European Molecular Biology Organization (EMBO) workshop on "Antibodies and Complement: Effector functions, therapies and technologies" to be held at Girona, Spain in June 2018. She has also been awarded a travel grant by EMBO

8. Ms. Archana's abstract titled "Average and local structure of $NaCe(WO_4)_2$: A Structure-Property Correlation" was selected for oral presentation at the ADD2019 (School And Conference on Diffraction Data in Real Space) at ILL

(Institut Laue-Langevin) Grenoble, France. Her travel was supported by DST-SERB

9. Ms. Archana and Mr. Satyapal from the Materials Science and Catalysis Division of PPISR have been awarded Senior Research Fellowships (SRF) from Council of Scientific and Industrial Research, (CSIR) Govt. of India

10. An US Patent has been granted for the collaborative research programme on "A process for the preparation of isomers of xylene" sponsored by HPCL R&D Centre, Bengaluru, in which Faculty Members of PPISR in Catalysis group are Co-Inventors.

11. Ms.Archana was awarded the best poster prize for her poster presentation was given on title "Design of Alkali Rare Earth Double Tungstates for Theranostic, Photoluminescence and Electrode Applications" at Manipal Research Colloquium-2018, MAHE, and Manipal in April 2018

12. Dr. Manjunathan P. won Best Oral presenter award at "Carbon Capture and its Utilization conference" held at CSIR-NCL, Pune conducted in December 2018.

13. Mr. Kirana M won Best Oral Presentation Award in the International conference on "Current concepts on the role of Indian medicine and phytoceuticals in maintenance of health" at 39th Annual Summit of IABMS 2018, Chikka Aluvara Campus, Mangalore University during 15-17 November 2018.

14. Mr. Shankar V. Kundapura won best poster presentation award in the 46th National Seminar on Crystallography at NIMHANS, Bengaluru. This poster was awarded the best poster award among 110 posters present ed in the conference.

15. Dr. Suresh Babu Kalidindi's article on Metal–Organic Frameworks for Hydrogen Energy Applications: Advances and ChallengesAuthors: B. Vasudeva rao, Marilyn Esclance DMello, and Suresh Babu Kalidindi* Wiley Publications (Invited article special issue on hydrogen energy)

16. Ms. Shrilakshmi S presented a poster in the one-day conference "Recent advances in Biochemistry" organized by St. Aloysius college, Mangalore on 23rd February 2019 and won the best poster presentation award.

17. In 2018-19 alone, the Institute has published 23 research papers in all areas of sciences and in overall, PPISR has crossed 239 publications in peer reviewed high impact factor international journals

17.2 CONFERENCES/SEMINARS/WORKSHOPS

1. Dr. Ganapati Shanbhag delivered an invited talk on “Tuning properties of mixed metal oxide catalysts for direct transformation of CO_2 into cyclic carbonate and dialkylurea” at international conference on "Carbon Capture and Its Utilization" held on 14-15 December 2018 at the CSIR-National Chemical Laboratory, Pune conducted in association with Royal Society of Chemistry.
2. Dr. Ganapati Shanbhag gave an invited talk at “3rd International Conference on Emerging Advanced Nanomaterials (ICEAN-2018)” at University of Newcastle, Australia during Oct 30–Nov 2, 2018 on the topic “Novel mesoporous tin oxide and phosphate as catalysts for the conversion of biomass derivatives into value-added chemicals”.
3. Dr. Nalini Sundaram was invited to deliver a lecture in the Winter School on “Synchrotron Techniques in Materials Science” Held at the S.N.Bose National Centre for Basic Sciences from October 25-31 2018

4. Dr. Ramagopal presented a talk titled "Check-point blockade cancer immunotherapy“ at the Industry and Academia Interaction Programme” held at the Government Science College, Bengaluru on 4 April, 2018. At the same programme, Raghurama P Hegde presented a talk titled “From A Gene to A Crystal Structure: An Overview of Protein Crystallography”
5. Dr. Ganapati Shanbhag gave an invited lecture on “Catalysts and their applications in biomassconversion into energy and chemicals” during 2-day “Industry Academia Interation Programme” atGovernment Science College, Bengaluru on 3-4, April, 2018.
6. Dr. Sanjeev Maradur gave an invited talk on *“Porous Polymers as Platforms for Green Chemical Synthesis and Enviornmental Applications”* on 3rd April 2018 at Industry-Academic interaction workshop, PG Department of Chemistry, Government Science College, Bengaluru
7. Dr. Ramagopal delivered first talk in the workshop “CCP4 Crystallography School and Workshop: From data processing to structure refinement and beyond” 22-Oct-2018 to 26-Oct-2018, held at IMTEC, Chandigarh, India and helped students on practical aspects of macromolecular crystallography.
8. Dr. Ramagopal was invited to give a talk in the workshop “Physics of living matter and medical equipment” held at St Aloysius college, 18th and 19th of December 2018.
9. Ramagopal’s delivered a talk titled “Macromolecular crystallography and its impact on biology” at PES University, Bengaluru on 26th April 2018
10. Dr. Nalini Sundaram was invited to deliver a talk on “Rietveld Refinement” for the workshop on PXRD in Pharmaceutical and Materials Industry conducted as a satellite meeting of the National Seminar on Crystallography(NSC-46) held at NIMHANS, Bengaluru on 25 June 2018
11. Dr. Nalini was invited to deliver a lecture titled “Exploiting Functional Nanomaterials for Environmental and Biomedical Applications” *at the FDP on*

"Functional Materials for Industrial Applications (FMIA-2018)" organised at MSRIT on 25 July 2018

12. Dr. Ganapati Shanbhag delivered an invited lecture at Faculty Development Programme on "Functional Materials for Industrial Applications" at Department of Chemistry, Ramaiah Institute of Technology, Bengaluru on July 26th, 2018
13. Dr. Ganapati Shanbhag delivered an invited lecture at KSTA sponsored workshop at Christ University, Bengaluru on 27th and 28th November, 2018 with a theme "Conceptual and Practical Advances in Materials Chemistry".
14. Dr. Ganapati Shanbhag delivered an invited talk at Poornaprajna College, Udupi on December 31, 2018 on the topic "Catalysis and its role in green synthesis of fuels and chemicals; Present challenges" to undergraduate Chemistry students.
15. Dr. Nalini was invited to conduct hands on training on "Crystal Structure determination using Rietveld refinements method" at Dayanand Sagar University, Bengaluru, in September 2018. Ms. Archana assisted with the hands-on training.
16. Ms. Archana delivered on "An Overview of Nanoscale Materials and Their Significance" as part of the outreach activity for the 10th standard Students of Poornaprajna School at Sadashiva Nagar on 14th January-2019.
17. MsArchana volunteered to help make a working model based on title "Hybrid Hydro-Solar Plant for Renewable Energy" for class 8th Students of "Vihaan Public School" on behalf of Interschool Science Forum on 18th Janauary-2019 as part of the outreach activity
18. Dr. Nalini Sundaram was invited to deliver a lecture for a workshop on "X-ray Crystallography" on March 16th 2019 at the Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore, sponsored by DST and RSC, India Chapter
19. Mr. Kempanna presented a poster at the Manipal Research Colloquium 2019 from 31 st March to 4 th April 2019 in MAHE Campus "Organised by Manipal Academy of Higher Education".
20. Ms. Shrilakshmi S presented a poster in the one-day conference "Recent advances in Biochemistry" organized by St. Aloysius college, Mangalore on 23rd February 2019 and won the best poster presentation award. Also, she presented a talk on her PhD work at PPISR in the alumnae association of the St. Aloysius college, Mangalore
21. Mr. Kirana M.P. participated in two weeks on hand workshop on "Multi-omics applications in medicinal plant research" organized at Trans Disciplinary University (TDU), Bengaluru during February 11-22, 2019.
22. Dr. Sujit Sarkar's group attended the "Indian Statistical Physics Community Meeting" at ICTS, Bangalore from 14th to 16th February'19.
23. Dr. Raghurama Hegde accepted the senior postdoctoral fellowship position at Elettra, Trieste, Italy.
24. Dr. Srikanth conducted 3 meetings of the Center for Excellence in Quantum Information, Machine Learning and Artificial Intelligence with the Director, Dr Vetrivel and Mr Karthik Joshi for the use of machine learning for predicting crude oil prices.

25. Dr. Raghurama Hegde accepted the senior postdoctoral fellowship position at Elettra, Trieste, Italy

26. Dr. Srikanth conducted 3 meetings of the Center for Excellence in Quantum Information, Machine Learning and Artificial Intelligence with the Director, Dr Vetrivel and Mr Karthik Joshi for the use of machine learning for predicting crude oil prices.

27. Dr. Srikant drafted an MoU for Center for Foundational Study, via a trust called “Center for Integrative Studies in Science and Philosophy” (CISSP)

28. Dr. Srikanth signed an MoU with QuNu Labs, who wished to interact with one of our PhD students for studying the security of their QKD product. We discussed a potentially realizable venture called “Quantum ATMs” with them, which has the potential to be patented and have considerable financial implications.

18. INVITED LECTURES

1. Dr. C V Rode, Senior Scientist, CSIR-National Chemical Laboratory (NCL), Pune gave an invited lecture on "Multifunctional Catalysis for Bio-refinery Applications" on August 21, 2018.
2. Prof. Umesh V Waghmare, Professor from TSU, JNCASR, Bengaluru gave a talk on "Functional Properties of Materials at Nano-scale: First-principles Theory on September 21, 2018.
3. Prof. S.Venkatraman Manager, Duracell, R&D Division, Bengaluru gave an invited lecture on "The humble battery-why the sudden attention & demand" on September 25, 2018
4. Dr. Manjunath Ramarao, Group Director and Head, Discovery Biology and Translational Sciences at Bristol-Myers Squibb Bengaluru Area, India gave a talk on "Novel Drug Discovery" on November 5, 2018.
5. Prof. Yashonath Subramanian, SSU Division, IISc, Bengaluru gave a Lecture on the title "Dance of Atoms and Molecules: Molecular Dynamics" on November 21, 2018.
6. Dr. Swetha Bhat, Seoul National University, South Korea gave a talk on "Fabrication of hetero-junction photo-anodes for photo-electrochemical applications" on December 24, 2018
7. Dr. Omkar Srikrishna, Seoul National University, South Korea gave a talk on Topological Fault Tolerant quantum computation using hybrid entangled states" on December 24, 2018
8. Prof. N. D. Hari Dass, TIFR Hyderabad and former Director, PPISR delivered a lecture on Time in classical and quantum physics on February 2, 2019.

9. Dr. Rani Jha, Scientist, National Chemical Laboratory, Pune and gave a talk on "Designing for Sustainability: Novel Solvent Systems" on March 14, 2019

19. IN-HOUSE SEMINARS

1. Title: Klein Paradox and its Applications
Speaker: Mr. Rahul Sharma, Theoretical Physics Division, PPISR
Date: 06.04.2018

2.Title: Quantum non-Markovianity: characterization and quantification
Speaker: Mr. Srikant Utagi, Theoretical Sciences Division, PPISR
Date: 18.04.2018

3. Title: Geometric phase and topological phase transitions in interacting light-matter physics
Speaker: Prof. Sujith Sarkar, Theoretical Sciences Division, PPISR
Date: 01.06.2018

4.Title: Catalytic Activation and functionalization of light alkanes
Speaker: Ms. Vaishnavi B. J., Materials Science Division, PPISR
Date: 27.04.2019

5.Title: Bloch States, Energy Bands and The Theory of Solids
Speaker: Mr. Y. R. Kartik, Theoretical Sciences
Date: 25.05.2018

6.Title: Rare Earth Upconversion Nanophosphors for Theranostic Applications: Perspectives and Challenges
Speaker: Dr. Nalini Sundaram, Materials Science Division, PPISR
Date: 01.06.2018

7.Title: Photocatalysis for sustainable energy and environmental applications
Speaker: Ms. Chethana. A, Materials Science Division, PPISR
Date:31.08.2018

8. Title: An Introduction to Quantum Digital Signatures
Speaker: Mr. Vinod N, Theoretical Physics Division, PPISR
Date: 06.04.2018

9.Title: The Methane Chemistry, C1 to Cn
Speaker: Mr. Kempanna K. Materials Science Division Materials Science Division, PPISR
Date:07.09.2018

10.Title: Phylogenetic, sequence and structural analysis of proteins of Insulin super family
Speaker: Ms. Shrilakshmi S., Biological Sciences Division, PPISR
Date: 21-0.9-2018

11.Title: Cooperativity in Heterogeneous Catalysis for Exceptional Catalytic Activity
Speaker: Mr. Sathyapal R Churipard, Materials Science Division,
Date: 02.10.2018

12.Title: Advances in catalysis for making synthetic gasoline, diesel and methanol via Fischer-Tropsch method
Speaker: Mr. Nagendra Kulal, Materials Science Division,
Date: 12.10.2018

13.Title: Proton-Conducting Metal-organic Frameworks for Fuel Cell Applications
Speaker: Dr. Suresh Babu Kalidindi, Materials Science Division,
Date: 25.10.2018

14.Title: An Overview of Electrochemical and Optical Biosensors
Speaker: Ms. Archana K. M., Materials Science Division
Date: 04.01.2019

15.Title: Why we Renormalize the Nature?
Speaker : Mr. Ranjith Kumar R, Theoretical Science Division
Date : 01.02.2019

16. Title: An Animal Cell Culture: Modern technology in advanced research
Speaker: Dr. Ananda Kulal,
Date: January 25, 2019, Friday

17. Title: Homogeneous Catalysis: New Paradigms and Importance in Present Day Research
Speaker: Dr. Ganapati Shanbhag
Date: February 8, 2019

18. Title: How to break RSA cryptosystem?
Speaker: Mr. Shrikant Utagi
Guide: Dr. Srikanth R.
Date: 15.02.2019.

19. Title: Water: The mysterious molecule
Speaker: Dr. Udupi Ramagopal
Date: February 22, 2019, Friday

20. EVENTS AND MEETINGS

20.1. Founder's Day Celebrations

PPISR celebrates Founder's Day in the memory of HH Sri Vibhudesha Theeratha Swamiji on the first week of July every year. Founder's Day-2018, was celebrated with two-day scientific session on July 5th and 6th, 2018. Prof. Ramaswamy. S, Founding Dean of InStem, Co-Founder and First CEO of Centre for Cellular and Molecular Platforms, National Centre for Biological Sciences, Bengaluru was the chief guest and inaugurated the Founder's Day at the Bidalur Campus on 5th July, 2018. In his inaugural address, he discussed about the "Curiosity and Science-Fish and Cockroach Stories". Further, we had technical lectures on Biological Sciences by Dr.Goutam Soni, Raman Research Institute, Bengaluru on the title "Role of Nanotechnology in Structure-function Relationship in Biology" and another interesting lecture was on "Plant Specialized Metabolism: Understanding and Metabolic Engineering" given by Dr. Dinesh Nagegowda, Scientist, Central Institute of Medicinal and Aromatic Plants, Research Centre Bengaluru.

Later on the day, there were two interesting talks in the area of Theoretical physics by Prof. Bala Iyer, International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru, who spoke on "From Gravitational Wave Detection to Multi-Messenger Astronomy". Followed by a lecture on " Fielding Particles" by Prof.Raghavendra from Sri Dharmasthala Manjunatheshwara College, Ujire.

On July 6th, 2018, there were technical talks in the Materials Science area, Prof. Shivaprasad Math, Director, Karnataka State Higher Education Academy, Dharwad & Professor, International Centre for Materials Science, JNCASR, Bengaluru gave a first talk of the day on a title "Multi-manifestations in nano-structured GaN", followed by Prof. Ravishankar, FRSc, FASc, Professor, Materials Research Centre, IISc, Bengaluru who gave a talk on "Some Insights into Nucleation and Growth of Nanostructures and Hybrids" and Dr. G. Satyanarayana, Senior Vice President & Head ,Polymer Research & Technology Group, Shilpa Medicare Limited gave a talk on "Recent Advances in Polymeric Materials".

The valedictory function of Founder's Day was celebrated in the afternoon of July 6th, 2018. Prof. M. R. S. Rao, Former President, JNCASR, Bengaluru and SERB Distinguished Fellow, was the Chief Guest and he delivered the valedictory address. Dr. Anand B Halgeri, Director of PPISR, Dr. K Srihari, Honorary Secretary for AMEF and AMEC and Sri. P. Sreenivasa Rao, Financial Advisor of PPISR/AMEF were also present on the dais on this function. In this occasion three PhD students, Mr. Shankar Kundapura, Biological Science division, Mr. Vasudeva Rao, Materials Science division and Mr. Ranjit S, Theoretical Sciences division have received best seminar presentation awards. At the end of the program, the prizes for the winners of various sports and games competition were distributed by the dignitaries on this occasion.

20.2. HH Sri Vibudhesha Teertha Swamiji Second Memorial Endowment Lecture

The second endowment lecture series in memory of founder chairman HH Sir Sri Vibudesha Teertha Swamiji was organized at the Bidalur campus. This lecture series had been initiated in 2017 with the idea of recognizing and appreciating highly accomplished Indian scientists. Therefore it was appropriate that, Prof. G.U. Kulkarni, Director, CNSMS, Bangalore, who has made many important contributions in the area of Materials sciences gave the second endowment lecture. The programme began with the welcome address by the Director, , followed by lighting of the lamp. Then, Prof. K. Srihari, Hon. Secretary of AMEC and AMEF gave a brief idea about the vision and mission of HH Sri Vibudhesha Teertha Swamiji to encourage basic and applied research in India for the betterment of Indian science and society. Later, in his talk titled " Nobler than Normal: New Crystal Forms of Gold ", Prof. Kulkarni explained in depth the seredipitious discovery of a new form of gold by his group. He also discussed how this new type of gold had better properties which could be applied in many areas Considering the general audience, Dr. Kulkarni made his talk as simple as possible. He also presented many cutting-edge experiments carried out in his laboratory. The talk was followed by benediction from the present chairman HH Sri Vishwapriya Teertha Swamiji. The function was attended by the invited guests from PPE schools, Trustee members and others.

20.3 Organisation of State Level Workshop at the Poornaprajna College and Post Graduate Centre, Udupi

Two days State Level Workshop on " Recent Advances in Scientific Research: A Glimpse" was organised in association with Poornaprajna College and Post Graduate Centre, Udupi for the Science students during December 7-8, 2018. Chairman of Admar Mutt Education Foundation, His Holiness Sri Vishwapriya Theertha Swamiji inaugurated the workshop with his blessings. The Guests of the inauguration, Dr. G S Chandrashekhar, Hon. Secretary, PCMC and Dr. Anand B Halgeri, Director, PPISR addressed the participants in their inaugural talks. A team of faculty and students represented PPISR in the workshop by delivering lectures on various topics. In the Materials Science Dr. Suresh K. Babu gave a talk on "Metal-organic frameworks: Materials with enormous surface areas", Dr. Sanjeev P. Maradur delivered a talk on "Advances in Polymer Research Related to Water, Energy and Environmental Applications" and Dr. P. Manjunathan's talk was on "Heterogeneous Catalysis: Introduction and its importance in present day research".

On the second day of the workshop in the area of Biological Sciences Dr. Ananda K, gave his first talk on "Novel lead molecules for the treatment of diabetes: Efforts from PPISR" and later on gave a second talk on "Endophytic fungi as a source of bioactive compounds for medicinal applications". Mr. Shankar Kundapura gave a talk on "Immunotherapy: Priming our immune system to treat cancer and

autoimmune disorders". In the area of Physics, Mr. Shrikanth Utagi gave a talk on "Quantum Weirdness: From uncertainty to entanglement", Mr. Rahul Sharma gave a talk on " Tunneling Paradox" and a third talk was given by Mr. Karthik Y.R. on a title "Mathematical mapping in the physical system". Each session had an interesting discussion in the respective topics as this workshop was conducted with an objective to kindle the science curiosity in undergraduates.
On December 8, 2018 afternoon, the workshop was closed with a valedictory function. Dr. B.S.Sherigar, former Vice Chancellor of Kuvempu University, was the Chief Guest for this function. Sri. Pradeep Kumar, Hon. Treasurer, PCMC; Dr.Ananda K, PPISR; Dr.B.Jagadeesh Shetty, Principal PPC, Dr.A.P.Bhat, PPC and Sri. Srikantha M., PPC were also present on this valedictory function. Sri.Srikantha M from PPC and Dr.Ananda K from PPISR were prepared and executed the whole workshop program.

20.4 State Level Science Fest 2018

A state level Science fest 2018 was organised on November 16, 2018 in association with Nagarjuna College of Engineering and Technology (NCET), Chikkaballapur. The NCET Science Fest -2018 was organised with the objective to bring out the hidden talents in young science students and to provide them a platform to showcase their Scientific ideas and creativity. Dr.A.B.Halgeri, Director, PPISR was the Chief Guest of the function, who inaugurated and addressed the participants. In his inaugural address he said that the Science and Technology have major role in overall development of the country. Bengaluru is known as a hub of IT-BT and this is one of the great platforms for the students from this area to showcase their talents.

All the faculty from PPISR rendered their experience in evaluating different types of competitions such as Science Project Exhibition, Science and Technology quiz, Tech Talk and Debate. Management and faculty from NCET hosted the program with all the pre-requisite preparations and made a very successful Science Fest-2018.

20.5 Meeting on Causally Open Systems

As part of activity under the aegis of the Center for Foundational Study (CFS), PPISR, a one-day meeting was held on July 21, 2018, on the broad theme of "causally open systems" covering from a physics perspective topics such as decoherence, causality, entropy, but also including more open-ended subjects such as free will, consciousness & its relation to artificial intelligence, and the description of the interface between consciousness and the material world. The overarching purpose was to bridge modern science and ancient philosophical insights into the nature of reality, in a way envisioned by Their Holinesses, the.

Founder Swamiji Shri Vibudhesha Theertha Swamiji, Shri Vishwapriya Theertha Swamiji and Shri Eeshapriya Theertha Swamiji, and with active encouragement of

the Director, PPISR, Prof. A. B. Halgeri. The conveners were Prof. Udupi Ramagopal, Prof. Sujit Sarkar and Prof R. Srikanth.

The meeting was commenced by an invocation of Shri Bharat Mata by our PhD student Mr Y. R. Karthik and anchored by our former student, Dr. S. Aravinda. Prof Nithin Nagaraj (NIAS, Bangalore) spoke on "Causality Testing - Practical Approaches & Challenges", Prof. Vivek Narayanan (Rochester Institute of Technology, USA) spoke on "Consciousness in the Universe and Copernican principle of mediocrity", while Prof. R. Srikanth (PPISR) addressed the audience on the subject of "A Semiotic Approach to Causality and Consciousness in Vedantic Philosophy". The meeting was well attended, with all students of the Theoretical Sciences group participating, and a few others, including Mr Sundar, an independent tech consultant.

20.6 Research Review Meeting

Professor. V. Nagaraja, President, JNCASR, Bengaluru after becoming AMEF trustee member, wanted to interact with all the faculty and was interested to know about the research activities undertaken by PPISR. All the faculty members presented their ongoing research programs and their future plans to Prof. Nagaraja on 13.10.2018. He evaluated all the proposals presented by the faculty and discussed critically with each and gave his comments. There was a very fruitful discussions with lots of constructive inputs from the new Trustee for the scientific growth of the Institute. He also gave valuable suggestions to each faculty, how to go about the proposed future projects. Dr.A.B. Halgeri, Director of PPISR presided over the meeting.

20.7 Outreach Programmes for PP School Students

The outreach programme for all the Poornaprajna schools of Bangalore was organised at PPISR for the sixth consecutive year. All the class IX students from the five PP schools in and around Bangalore participated in the programme which was from 5th March to 9th March, 2019. This program has been designed to give high school students an opportunity to take a tour of the research facilities established at PPISR and experience research activities undertaken by current Ph.D students. The objective was to inspire high school students to pursue higher studies and further research in fundamental and applied sciences. As this year is the international year of the periodic table, in chemistry, reaction that highlight the characteristic to each block of elements, like flame test for ‘s’ block elements, complex formation of d block elements etc. were demonstrated by research scholars to the students. In biology, transpiration process in plants, microbial cell viability, visialization of dNA etc, were some of the experiments shown. In physics, a medley of lectures on planets, measures used and intereference experiments were performed. The students were also given a glimpse of the various sophisticated equipment in the materials as well as the biology

laboratories. Finally, a valedictory session which consisted of discussions about the experiments with the students as well as obtaining feed back about the programme was held at the end of each day. Teachers from all the PP schools expressed their satisfaction with the periodic table experiments, interference and DNA experiments as they felt that it would make it easier for them to introduce these concepts in the X standard next year.

20.8 Science Day celebration:

Science Day celebration was organized at PPISR on Feb 28, 2019 to commemorate the invention of the Raman Effect by the great Indian physicist Sir Chandrasekhara Venkata Raman. The activity involved a morning session talk by renowned scientist, Prof N. Mukunda (Retd. Center for Theoretical Studies, IISc), on "Science and the Human Predicament" followed, by two moderated debates on "Artificial intelligence: boon or bane? & Human cloning: pros (therapeutic) vs cons", which aim to reassess the role of science and technology in our daily life:

20.9 Teacher's Day Celebrations

In commemoration of Teacher's Day on September 5th, a programme was organized by the students of the institute to honour the faculty members as a mark of honour to them. A day long programme was organised with presentations by students on science topics and painting/drawing competition on the theme EUPHORIA, meaning happiness at all times. All teachers expressed views about fulfilling their dreams of achievements The programme was inaugurated with a dedicated song to the "Guru" followed by thoughts and views on the celebration of Teacher's Day and its features. A three minute video was made using the pictures of past and present and was dedicated to the teaching members.

20.10. Annual Sports meet – 2018

Sports day was organized at the campus to bring everyone under one roof. All the members of PPISR including the director Dr. Aanand B. Halgeri participated in the event. The event was well planned and organized for the first time at the Bidalur campus. Director expressed his happiness and mentioned that such events are necessary for the students and scientist involved in research and this kind of events unite the members of any organization. Many sports, such as Cricket, Tug-of-war (men and women), volleyball, shuttle, Carom, Slow motorcycle race, Table Tennis, along with athletic games of 100Mts sprint, marathon of 2.5kms and one minute games such as skipping, filling the bottle with water and so forth were conducted.

20.11. Board of trustees meeting of Admar Mutt Education Foundation (AMEF)

The meeting was held at Sadashivnagar campus on October 27, 2018 in the presence of Chairman, H H Sri Vishwapriya Theertha Swamiji and Vice- chairman

H H Sri Eeshapriya Theertha Swamiji along with trustee members and invited members. Dr. Anand B. Halgeri made a presentation on overall progress of the institution, which was highly applauded by the trustee members and the chairman. In this meeting, Annual Report of the institution for the year 2017-18 was released by the Chairman and the first issue of the Newsletter for the year 2018 was released by the Vice-Chairman. Also, the AMEC annual general body meeting was held at Sadashivnagar on October 21, 2018.

20.12 Other Events

- **Felicitation of the Ph.D student**: Dr. Manjunathan P. was felicitated by H H Sri Vishwapriya Theertha Swamiji and H H Sri Eeshapriya Theertha Swamiji for receiving PhD award from MAHE, Manipal during the year 2018. He was presented with a "Certificate of Appreciation" for his achievements.
- **A Tribute to Sri Atal Behari Vajpayee:** A Tribute was paid to Sri **Atal Behari Vajpayee**, the former Prime Minister of India and the person who was associated on laying the foundation stone for Poornaprajna Institute of Scientific Research in 1998, at his sad demise on August 16, 2018.
- **One Day Organizational Development Workshop :**Dr. Suresh Rao from UK along with some of his colleagues from Manipal Management Institute have jointly organized One Day Organizational Development Workshop on 15th Jan 2019 at our research campus in Bidalur. The main objective of this Workshop was to to emphasize the inculcation of key personal, professional and team leadership skills through capability in coaching, mentoring and perspective-taking styles which was then followed by Panel Discussion by Facilitators and Questions and Answers.
- **Support for Flood Victims**: The natural disaster of flood in the Karnataka state made huge damage to many places including Coorg (Kodagu) district. A support for the victims of flood affected area was organised from PPISR in association with Poornaprajna Education centre, Sadashivanagar. The food items, clothes, sanitation items, medicines, tonned milk, vessels etc were collected and despatched through SRS transport. Ms. Vaishnavi, Research Scholar took the initiative in organising the flood relief help.
- **Independence day celebrations:** The 71st Independence Day was celebrated at Bidalur Campus on August 15, 2018. The director of the institute Dr. Anand B Halgeri hoisted the flag and addressed the gathering. Later on saplings were planted in the campus to mark the celebration of Independence Day and to enrich further the greener gardens of the campus.
- **Republic Day Celebrations**: The 69th Republic Day Celebrations were organized at our Bidalur Campus on January 26, 2019. Shri. P. Sreenivasa Rao, Financial Advisor, PPISR, Bengaluru was invited as the guest on the occation. After unfurling flag, Shri. Rao, addressed the gathering of students, staff and faculties and spoke about the institute and its mission to the gathering.

21. VISITORS' VIEWS

- **Prof. UMESH V WAGHMARE,** TSU, JNCASR, Bengaluru
  It was a very enjoyable visit to this beautiful campus where interesting research in Biology and Materials is going on with a focus on goals to connect with real applications for the betterment of society. My discussions with faculty were very informative and many good questions during my talk made it a very vibrant experience. I appreciate a great contribution, efforts and vision of Dr. Halgeri in this pristine institute of learning envisioned by Swamiji.

- **Dr. C V RODE, Senior Scientist (G**), Chemical Process Development Division, DSIR-NCL Pune.
  It was an excellent opportunity to be at PPISR and had fruitful interaction with the Director and Dr. Ganapati Shanbhag and colleagues and students. I am very much impressed by the work being carried out here on both fundamentals and application to the industry which is evidenced from excellent PhDs, publication and funding from the industry projects. The institute has state-of-the-art facilities resourceful faculty and dedicated research students. In a very short span of time, the result oriented work is visible. I wish all the best to the faculty and the students who, I am confident will reach to higher heights in near future

- **Prof. BALA IYER,** Simons Visiting Professor, ICTS-TIFR, Bengaluru.
  Thank you for the invitation to deliver a talk on "gravitational waves" and interact with colleagues here. The work done in the theory group by Dr. Sujit Sarkar and Dr. Srikanth is of high quality consistently. I wish them and their students and PPISR all the best in the coming years and grow to great academic heights.

- **Prof. G SATYANARAYANA,** Senior Vice President and Head, Shilpa Medicare Limited, Bengaluru.
  Good interaction visit. I see young boys and girls doing research in applied areas. Interesting place to perform research. I really enjoyed interacting with the researchers and faculties. All the best.

- **Prof. S M SHIVAPRASAD MATH**, Director, Karnataka State Higher Education Academy, Dharwad and JNCASR.
  I am grateful to the great Swamiji who have promoted Scientific Research to attain complete consciousness. The unit has done very well in a short time and I can clearly see this institute soon becoming an important centre. This is only because of the commitment and motivation as a part of Prof. C N R Rao's vision.

- **Dr. GAUTAM SONI,** Raman Research Institute, Bengaluru. Excellent campus with very enthusiastic students. Very privileged to be invited here. Hope to come again.

- **Prof. RAVISHANKAR**, FEMSI, FASc, Professor, Materials Research Centre, IISc, Bengaluru
  I am extremely happy to visit PPISR. I see great excitement and enthusiasm in the faculty and students. They have significantly improved their facilities from when I visited last and have been producing high quality research. I wish them all success and hope to see them reach greater and greater heights.

- **Prof. RAGHAVENDRA.S,** Department of Studies and research in Physics, SDM college, Ujire.
  I feel very privileged to have been invited here. The lush green campus, the calm ambience, research oriented people and comfortable stay. I wish the very best of luck to the entire team of PPISR.

- **RAVI PANGAL,** Philanthropist, San Roman, California, U S A. PPISR is an assemblage of intellectuals with passion, who are working on bringing Shri Vibudhesha Teertha Swamiji's vision and deeper insight to Reality, they are a group of researchers who think about what nobody else has thought and thrive to give back to the community with their research. I am very fortunate to have visited PPISR and got to know Dr. Halgeri, Dr. Udupi Ramagopal and Dr. Ananda. Thanks to Dr. Srihari for making this happen. I would be glad to help PPISR in it's mission to give back to the community to best of my ability.
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- **Prof. S. YASHONATH SUBRAMANIAN,** SSCU, IISc, Bengaluru.
  As we approach the campus of PPISR, we see the beauty and greenery of the place. Once inside, one can see the harmonious mixture of science with philosophy. The campus is manned by excellent scientists who also work in different areas and have come out with high quality results. The institute is focused on its research and education. Dr. Halgeri and its faculty have created and brought up a place which needs to be nurtured to make it into a world class institution.

A tribute was paid to the former Prime Minister of India Sri Atal Bihari Vajpayee who laid the foundation stone for PPISR in 1998 for his sad demise on August 16, 2018.

Dr. Manjunathan P. of PPISR was presented the memento by H H Sri Vishwapriya Theertha Swamiji, Chairman PPISR and H H Sri Eeshapriya Theertha Swamiji on 21st October, 2018 upon completion of PhD programme with good publications in internationally reputed journals

A meeting with Prof. V Nagaraja, President, JNCASR Bengaluru was held at PPISR Sadashivanagar campus on October 10, 2018

Sri Vibudhesha Teertha Swamiji memorial second Endowment lecture by Prof. G. U. Kulkarni, Director, CeNS, Bengaluru was delivered on February 26, 2019 at PPISR

The newsletter for the first half of the year 2018 was released during the AMEF Board of Trustees meeting on October 27, 2018

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