



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
2020-21



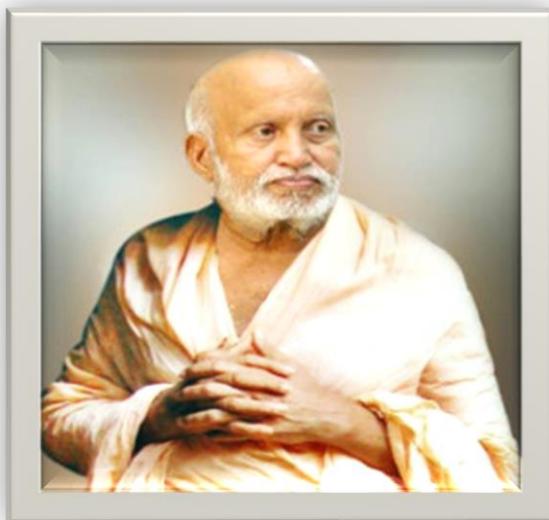
Poornaprajna Institute of Scientific Research Bengaluru, India

Annual Report 2020-2021



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of Higher Education (MAHE), Manipal

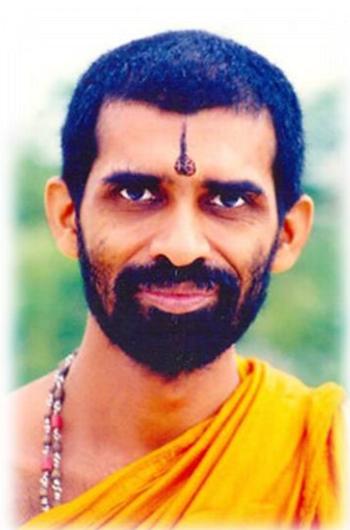
Founder's Message



Knowledge is Power! Providing facilities to conduct research in basic sciences has become very necessary. Our brilliant youth go outside the country to do research and settle there. Until we check this trend, India cannot make real progress in any field. Hence, an attempt is made to establish the Poornaprajna Institute of Scientific Research (PPISR) under the guidance of many eminent scientists of this country. The more the investment by the nation in science and technology, the stronger the country will evolve. All well-wishers of this country are approached hereby for all possible assistance to this project, so that India may better serve the world. I pray for divine guidance. May the Lord grant the necessary strength to develop this Institute for the benefit of the nation and the world.

**H H Sri Vibudhesha Theertha Swamiji,
Founder, PPISR**

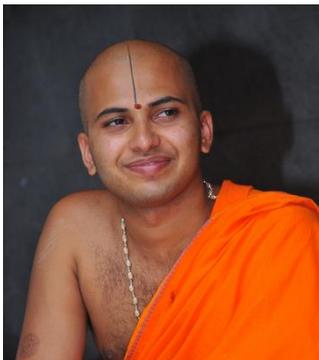
Chairman's Message



Founded by my beloved Guruji, an illustrious predecessor, H H Sri Vibudhesha Theertha Swamiji, the Poornaprajna Institute of Scientific Research (PPISR), is often cherished as the crest jewel among the Poornaprajna family of Institutions. PPISR is steadily yet firmly marching towards his dream of becoming a world-class research institute in the areas of Physical, Material, and Biological Sciences. The research work is carried out here with immense curiosity and spirit of service to the Motherland, just like the Rishis of yore into the spiritual sciences. The worldwide pandemic has not weakened the vigor of research activities and progress at PPISR but only altered how it is pursued with an emphasis on online interaction. The number of students who obtained their PhD at PPISR has now increased to Seventeen. Several new research projects have been initiated, with the possibility of the Theoretical Sciences group venturing into experiments to develop cutting-edge technology. I do not doubt that the stewardship of PPISR rests in the hands of capable and dedicated Scientists and staff. Their hard work will one day fulfill H H Sri Vibudhesha Theertha Swamiji's vision of India playing a pivotal role in scientific contribution to the scientific world globally. May Lord Sri Krishna bless and guide all the members of PPISR.

H H Sri Vishwapriya Theertha Swamiji
Chairman, AMEF

Vice-Chairman's Message



Having an academic background both in traditional studies as well as in technology, I am delighted to share duties with my beloved Guruji H. H. Vishwapriya Theertha Swamiji in witnessing and overseeing the considerable educational and academic strides being made by the Poornaprajna Institute of Scientific Research (PPISR), founded by the patriot saint H. H. Sri Vibudhesha Theertha Swamiji. Starting first with a modest size and having only the Theoretical Sciences department, we have now grown to include two currently well-established departments for Materials Science, and Biological Sciences, where frontier research on industrial-grade catalysts and protein structure analysis are undertaken, among many others. It is especially noteworthy that, even while the core of our research is curiosity-driven, part of the research we undertake is devoted to societally useful issues, such as medicinal applications, green chemistry, solar energy use, and quantum. I am happy to share that M/s. Karnataka Bank Limited has provided financial support for the installation of Solar Power Plant under the Bank's CSR green initiative scheme which has quite immensely helped the organization. I appreciate that now PPISR is making efforts to leverage their joint expertise in these diverse fields towards studies where machine learning and artificial intelligence (AI) can be applied in areas such as catalysis design, the discovery of immunity-boosting molecular medical studies, novel solar energy materials and quantum technologies. Given the quality of publications and that of our research scholars, the management, for their part, has deemed it fit to support research at PPISR by making available funds for additional built-up area, faculty expansion, and student scholarships. May the blessings of Lord Shri Krishna provide constant guidance to the PPISR family members both scientifically and spiritually

H H Sri Eeshapriya Theertha Swamiji

Vice Chairman – AMEF

Contents

1. Message from Hon. Secretary, AMEC & AMEF	11
2. Foreword from the Director	13
3. Board of Trustees	15
4. Research Advisory Committee	15
5. Doctoral Advisory Committee	16
6. Organization	17
7. About the institute	18
8. Division Structure	19
9. Mission	20
10. List of sponsored projects	21-22
10.1 Government sponsored	21
10.2 Industry sponsored	22
11. National and International Collaborations	23
12. Materials Science Division	24
12.1 Mission research highlights	24
12.2 Faculty Profile	27
13. Biological Sciences Division	55
13.1 Mission and research progress.....	55
13.2 Faculty profile.....	56
14. Theoretical Sciences Division	67
14.1 Mission and research progress.....	67
14.2 Faculty profile.....	68
15. PPISR Publications	75
16. New Research Students	79
17. Highlights of Research Activities	79
18. Conferences/workshop	81
19. Invited Lectures at PPISR	83
20. In-house Seminars	84
21. Events and meetings	85
22. Poornaprajna Analytical Centre (PAC)	87

1. Message from Hon. Secretary, AMEC & AMEF



Uniquely among the heads of various spiritual organizations of this country, His Holiness Sri Vibudhesha Theertha Swamiji, the then chief Pontiff of Udupi Sri Admar Mutt, Udupi, not only conceived but also created the thriving scientific research institute that PPISR has today become. His interest and curiosity about scientific matters were

such that he would enthusiastically interact with scientists, sometimes even placing himself in the position of a student attending science classes and lectures. His deep vision was not only for India's excellence in scientific research but for the unification of science and spirituality in the spirit of the ancient Rishis of this Country. While the thirty-three Poornaprajna Institutions or schools all founded by him all over the Country, each excels in its own right. Yet, for him, Poornaprajna Institute of Scientific Research established in Bidalur, Bengaluru during 1998, held a position of pride, a "*choodamani*" (a crest jewel). PPISR may thus rightly be considered tangible as symbolizing Saint's love for science. He was not only an idealist but a man with a practical bent of mind, who carefully planned the operational aspects of running such an institute as a premier research institute producing top quality Ph.D. students.

Since H.H. Sri Vibudhesha Theertha Swamiji attained the Lotus Feet of Lord Sri Krishna, the mantle of providing sacred guidance of PPISR has been graciously taken up by H.H. Sri Vishwapriya Theertha Swamiji, the present Pontiff of Sri Admar Mutt, Udupi, the President of AMEC and Chairman of AMEF. Since the setting up of Bharat Ratna Prof C. N. R. Rao Laboratory for Materials Science, the Materials Science division (since renamed as Materials Science and Catalysis Division). There can be little doubt that H. H. Sri Vibudhesha Teertha Swamiji is watching these developments from Above with joy and pride. PPISR has been pursuing a healthy mix of both fundamental ("blue sky") research as well as applied and applicable research. Among many achievements by PPISR over the past year, perhaps it is apt to especially mention that now 17 doctoral students have obtained their Ph.D. degrees of which three students in the current academic year have obtained their PhD degrees. They

have moved on for a postdoc in reputed institutes in India or abroad and that PPISR has now crossed the milestone of 320 publications in peer-reviewed journals of international repute. The students have won several best presentation awards during this period. In PPISR's journey in pursuit of the sacred, scientific vision set forth by H. H. Sri Vibudhesha Theertha Swamiji and guided by H. H. Sri Vishwapriya Theertha Swamiji and H.H. Sri Eeshapriya Teertha Swamiji, all activities of PPISR are being funded mainly by AMEF. At the same time, a larger part of student scholarships is obtained from academic and industrial projects. It is our fond hope that our achievements would inspire more members from the Corporate World and the General Public to support our activity for service to the world's scientific knowledge through Indian science.

Dr. K. Srihari
Professor (Rtd), UAS, Bengaluru
Hon. Secretary, AMEC and AMEF

2. Foreword from the Director



I have great pleasure in presenting the tenth Annual Report on the account of research and academic activities of Poornaprajna Institute of Scientific Research (PPISR) for the year 2020-21. We are steadily making progress in highly competitive scientific research and is coming into limelight on the national and international stage by maintaining the uniqueness in the research field. The Institute has chosen contemporary frontier areas of research in the fields of Materials Science and Catalysis, Biological Science and Theoretical Sciences. PPISR is successfully forging ahead a fruitful academia-industry partnership by innovating, designing, and developing novel multifunctional materials that have wide-ranging applications in catalysis, nanotechnology, etc. Several new research projects have been initiated with sponsorship from industries like Sulzer-GTC Technology Inc, USA, Hindustan Petroleum Corporation Ltd. (HPCL), Deepak Novochem Technologies Ltd, Pune and Sravathi Advanced Process technologies Bengaluru and Government agencies like VGST, DST, DRDO, etc. Currently, 26 doctoral students are actively involved in research activities on many sponsored projects both from Government agencies as well as from industries. PPISR has been pursuing nearly 38 research projects in different areas which are both fundamental as well as applied sciences. These projects have shown significant progress in terms of publications and patents.

Ms. Archana K. M., who was pursuing under the guidance of Dr. Nalini G Sundaram of Materials Science & Catalysis Department and Mr. Sathyapal, who carried out research work under the guidance of Dr. Sanjeev P Maradur has successfully submitted their PhD thesis and have awarded their Ph.D. degrees from Manipal Academy of Higher Education, (MAHE), Manipal during this period. Three doctoral students namely Mr. Shrikant Utagi, pursuing research under the guidance of Dr. R. Srikanth, Mr. S K Kempanna under the guidance of Dr. Sanjeev P Maradur and Mr. Nagendra Kulal under the guidance of Dr. Ganapati V Shanbhag have submitted their Pre PhD thesis.

One of our faculty members, Dr. Sanjeev P. Maradur, has been awarded the 'Award for Research Publication in Metallurgical & Materials Engineering Category from the Vision Group on Science and Technology, Govt of Karnataka for 2019-20 and one of our doctoral students, Ms. Shrilakshmi S, has been awarded the prestigious CSIR Senior Research Fellowship. Ms. Marilyn E. D'Mello was selected as the Winner of Dr. KVR Rao Scientific Society- Young Scientist Award-2020, a highly reputed nationally known award. This award is given to the young research scholars who are pursuing research in chemistry by Dr. KVR Rao Scientific Society Hyderabad every

year. It carries a citation and cash award. Ms. Chethana A and Mr. Kempanna have got their Best oral Presentation awards at the International Conferences held at Tamil Nadu and Kerala respectively. Mr Shankar Kundapura received an Award for Science story communication organized by DST AWSAR.

In 2020-21 alone, the Institute has published 40 research papers in all areas of sciences and overall, PPISR has crossed 320 publications in peer-reviewed high impact factor international journals. Dr. Shanbhag was invited as a speaker at 6th Indo-French symposium which is scheduled during July 5-7, 2021 in Strasbourg, France under the auspices of the CNRS, France and CSIR, India as well as at the Fifth Edition of Catalysis and Chemical Engineering during February 22-24, 2021 in San Francisco, CA, USA. Recently students of PPISR initiated 'PPISR Activity Forum' which serves as a platform to nurture and showcase the hidden talents of all the members of PPISR in various fields. Various creative programs are being organized every month which includes paintings, sketches, write-ups, poems etc. Several workshops like Research Orientation Workshop for undergraduate students of Poornaprajna College Udupi, Second DFT workshop and One day programme on Introduction to Python were organized during this period.

On the whole, the entire year 2020-21 was much more productive and successful with the unstinted support and blessings from H. H. Sri Vishwapriya Theertha Swamiji, H. H. Sri Eeshapriya Theertha Swamiji and also enthusiastic support from the management of Admar Mutt Education Foundation and Trustee members, and also with the support of all faculty members, students, and staff of PPISR.

Dr.A B Halgeri
Director

3. MEMBERS OF BOARD OF TRUSTEES/ MANAGEMENT

H. H. Sri Vishwapriya Theertha Swamiji Sri Admar Mutt, Udupi	Chairman
H. H. Sri Eeshapriya Theertha Swamiji Sri Admar Mutt, Udupi	Vice-chairman
Dr. K. Srihari , Professor (Rtd), UAS, Bengaluru	Hon. Secretary
Sri. M. Ashok Kumar , Chartered Accountant	Hon. Treasurer
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
Prof. V. Nagaraja , President, JNCASR, Bengaluru	Member
Dr. Anand B. Halgeri , PPISR	Director
Sri P. Sreenivasa Rao , PPISR	Financial 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. S Natarajan, SSCU, IISc, Bengaluru
4. Prof. G. U. Kulkarni, Director CeNS and Professor, JNCASR, Bengaluru
5. Prof. A J Rao, Retired Professor, DST Raja Ramanna Fellow, IISc, Bengaluru
6. Prof. T.N. Guru Row, Professor, SSCU, IISc, Bengaluru
7. Prof. Chandrabhas Narayana, Director, RGCB, Thiruvananthapuram
8. Prof. S. Ramakumar, Professor, Bioinformatics Centre, IISc, Bengaluru
9. Prof Uday Kumar Ranga, Professor, MBGU, JNCASR, Bengaluru
10. Prof B Gopal, Professor, MBU, IISc, Bengaluru
11. Prof Jayanth Murthy, Professor, IIA, Bengaluru
12. Prof. A. B. Halgeri (Member Secretary), Director, PPISR

5. DOCTORAL ADVISORY COMMITTEE

1. Prof. C. Sivaram	Indian Institute of Astrophysics, Bengaluru
2. Prof. S. Ramakumar	Physics Dept., IISc, Bengaluru
3. Prof. S Natarajan	SSCU, IISc, Bengaluru
4. Prof. B. R. Jagirdar	IPC Dept, IISc, Bengaluru
5. Prof. Anjali A Karande	Dept of Biochemistry, IISc, Bengaluru
6. Prof. Dipankar Nandi	Dept of Biochemistry, IISc, Bengaluru
7. Prof. Rajeev Ranjan	Materials Engineering, IISc, Bengaluru
8. Prof. PrabeerBarpanda	Materials Research Centre, IISc, Bengaluru
9. Prof. Chandrabas N.	Director, RGCB, Thiruvananthapuram
10.Dr. Tapas Kumar Maji	CPMU, JNCASR, Bengaluru
11.Dr.Govindaraju T.	New Chemistry Unit, JNCASR, Bengaluru
12.Dr.Meher K. Prakash	Biophysics group, JNCASR, Bengaluru
13.Prof. Ramachandra	Chairman and Director, CFRCE, Bengaluru
14.Prof. H. G. Nagendra	MVIT Eng. College, Bengaluru.
15.Dr.R.Ravishankar	Deputy General Manager, HPCL, Bengaluru.
16.Dr. G S. Rao	Sr. Scientist, SABIC Technology Centre,Bengaluru
17.Prof. N. Nagaraju	St. Joseph College, Bengaluru
18.Dr. Ramakrishna Matte	CeNS, Bengaluru
19.Dr. D. A. Nagegowda	CSIR-CIMAP, Bengaluru
20.Prof Rajeev Joshi	Central University of Karnataka, Kalburgi
21.Dr. Shanti K.N.	PES University, Bengaluru
22.Prof. S. K. Srivatsa	Atria Institute of Technology, Bengaluru
23.Dr. G Mohan Rao	Indian Institute of Science, Bengaluru
24.Prof Sundaresan A	JNCASR, Bengaluru
25.Dr Putla Sudarsanam	National Chemical Laboratory (NCL)Pune
26.Dr. Naveen V. Kulkarni	Amrita Vishwa Vidyapeetham Kerala,

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 K.

Dr. Ganapati V. Shanbhag

Dr. Sanjeev P. Maradur

Dr. D. H. K. Murthy

Honorary Professor:

Dr. Rajappan Vetrivel

Administration:

Senior Administrative Officer Mr. Kishore L. Gaikwad

Accounts Officer Mr. Nagarajan R.

Sr. Secretary to Director Mrs. Latha Srinivasan

Secretary 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 Scientific Research (PPISR) is situated near Bengaluru International Airport on a sprawling campus spread over 27 acres. It was conceptualized and founded by the pontiff of Admar Mutt Udipi H. H. Sri Vibudhesha Theertha Swamiji. His vision was 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 Institute was laid in 1998 by the then Prime Minister of India Sri Atal Bihari Vajpayee. The Institute is recognized by the 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. There are three departments; Theoretical Sciences, Materials Science & Catalysis and Biological Sciences, where advanced cutting-edge research activities are being conducted.

The present both Chairman, H. H. Sri Vishwapriya Theertha Swamiji and Vice Chairman, H H Sri Eeshapriya Theertha Swamiji are enthusiastically carrying forward to make Poornaprajna Institute of Scientific Research a Centre of Excellence to realize the dreams of their Guruji H. H. Sri Vibudhesha Theertha Swamiji. Both have a keen interest in the research activities of PPISR. The infrastructure is being constantly upgraded to meet the advanced research facility and scientists & student activities. During the last decade, H. H. Sri Vishwapriya Theertha Swamiji had built new facilities like a new Biological Sciences laboratory, a new hostel building, and a world-class research laboratory for Materials Science donated by Bharat Ratna Prof. C. N. R. Rao at the Bidalur campus.

In the Institute at this period, eight-core faculties, many distinguished adjunct and honorary professors, and more than 25 research students are working. So far, seventeen students from PPISR have obtained their Ph.D. degrees from MAHE, Manipal. Presently, 18 doctoral students and several project assistants are actively involved in research projects sponsored, both from Government agencies and Industries. To date, the Institute has published more than 320 papers in International peer-reviewed journals. PPISR has filed three international patents in collaboration with HPCL Bengaluru and out of which two US patents have been granted. The average impact factor of PPISR publications is >3.0 which is on par with many elite institutes of the country.

PPISR is promoted and managed by Admar Mutt Education Foundation (AMEF). It is a part of a large family of sister institutions, including around thirty-three Poornaprajna Schools, Poornaprajna Preuniversity colleges, Poornaprajna colleges for degree and post graduations, and the Poornaprajna Institute of Faculty improvement, all governed by the Udipi 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 H. H. Sri Eeshapriya Theertha Swamiji. The excellent support from the management of Admar Mutt Education Foundation, and the cooperation of all faculty members, students, and staff of PPISR is greatly appreciated. They have immensely contributed to realise the vision of our founder Chairman H. H. Sri Vibudhesha Theertha Swamiji.

8. DIVISION STRUCTURE

Faculty	Research Scholars/ Project Students
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MATERIALS SCIENCE AND CATALYSIS

Dr. A. B. Halgeri (Catalysis)
Professor and Director

-

Dr. G. V. Shanbhag
(Heterogeneous Catalysis)
HOD & Associate Professor

Mr. Nagendra Kulal, Mrs. Vaishnavi B. J.,
Mr. Manjunath D., Mr. Sujith S.,
Ms. Archana K. M., Ms. Chethana A.,
Ms. Marilyn E Dmello,
Ms. Chaitra Mallannavar,
Ms. Srinidhi Patil

Dr. Sanjeev P. Maradur
(Heterogeneous Catalysis)
Associate Professor

Mr. Satyapal Churipard, Mr. Kempanna
Kanakikodi, Ms, Bhavana Kulkarni
Mr. Puneeth Kumar

Dr. D. H. K. Murthy,
Assistant Professor

Ms. Sujana

BIOLOGICAL SCIENCES

Dr. U. A. Ramagopal
(Structural Biology)
Academic Dean & Associate
Professor

Mrs. Swetha L, Mr. Shankar Kundapura,
Mr. Akshaya Bhat, Ms. Salima Parveen

Dr. K. Ananda (Microbiology)
Associate Professor

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 conduct research in the selected frontier areas of basic and applied sciences.

* To encourage and support sponsored research programs 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 the 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 institute's faculty.

* 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

Government-sponsored projects

1. “Quantum non-Markovianity: characterization, measure and resources”,
Sponsored by Science & Engineering Research Board (SERB), DST, Govt. of India under MATRICS Scheme
Principal Investigator Dr. Srikanth R.
Duration:2020-2023.
2. “Topological States of Superconducting Nanowires and interacting light-matter systems at nano scales”
Sponsored by DST-SERB, Govt. of India
Principal Investigator. Dr.Sujit Sarkar
Duration: 2018-2021
3. “Experimental realization of a quantum random number generator and development of strategies for quantum hacking”
Sponsored under Interdisciplinary Cyber-Physical Systems (ICPS) programme of DST, Govt of India Collaborative project with IIIT, Noida
Co-Principal Investigator: Dr. R. Srikanth
Duration: 2019-2021
4. “Chemical fixation of CO₂ by converting into value-added chemicals using metal-modified ordered nanoporous silicate catalysts”
Sponsored VGST, Govt. of Karnataka under Centre of Excellence in Science, Engineering and Medicine (CESEM) grant
Principal Investigator: Dr. Ganapati Shanbhag
Duration: 2015-2021
5. “Structural and evolutionary investigations on antibiotic-resistant conferring rRNA methyl transferases for designing novel strategies of drug development”
Sponsored by DST, Govt. of India
Principal Investigator: Dr. Udipi Ramagopal
Duration: 2017-2020
6. “ α -Amylase and α -glucosidase inhibitors from endophytic fungi for treating Type 2 diabetes”
Sponsored by Vision Group for Science and Technology, Govt. of Karnataka (CESEE) Principal Investigator: Dr. Ananda K.
Duration: 2017-2022
7. “Computational speed-up in generalized probability theories”
Sponsored by DST-SERB, Govt. of India
Principal Investigator: Dr. R. Srikanth
Duration: 2017-2020

Industry-sponsored projects

1. Catalyst and process development for hydrocarbon synthesis via halogen mediation

Sponsored by: Sulzer-GTC Technology Inc, USA Duration: February 2021-January 2022

Principal Investigator: Dr. Ganapati V Shanbhag

Co-PI: Dr. D. H. K. Murthy

2. Catalyst and process development for CO₂ hydrogenation reaction

Sponsored by Hindustan Petroleum Corporation Ltd., Govt. of India, Duration: 2 years, 2020-2022

Principal Investigator: Dr. Ganapati V Shanbhag

Co-PIs: Dr. R. Vetrivel, Dr. Sanjeev. P. Maradur

3. Computational discovery of materials and active ingredients through machine learning

Sponsored by Shrivathi AI Technology, Bengaluru Duration Jan 2021 to Jan 2022)

Principal Investigator: Dr. D. H. K. Murthy

Co-PI: Dr. Ganapati Shanbhag

4. Catalyst and process development for aromatics alkylation to make higher aromatics

Sponsored by Deepak Novochem Technologies Ltd., Pune) from November 2020-October 2021

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

5. Development of Catalyst and Process for Specific CO₂ Transformation

Sponsored by: Hindustan Petroleum Corporation Ltd. (HPCL)

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Vetrivel and Dr. Sanjeev P. Maradur

Duration: 2020 – 2022

6. Structure-Based Rational Design of Pd1 Mutants to create Lead Molecules for Cancer Immunotherapy

Sponsored by: Bristol Myers Squibb, USA

Principal Investigator: Dr. Udupi A Ramagopal

Duration: 2019 – 2020

11. NATIONAL AND INTERNATIONAL COLLABORATIONS

PPISR has MOU with many institutes for collaborative research like Argonne national laboratory, Chicago, IIT-Madras, Central University, Gulbarga, 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”)

NATIONAL COLLABORATORS:

- Dr. C. S. Gopinath, HOD, Catalysis Division, CSIR-NCL, Pune
- Dr. G. Valavarasu, DGM, HP Green R & D Centre, Bengaluru
- Prof. Shubhangi Umbarkar, Sr. Scientist, CSIR-NCL, Pune.
- Prof. Rajendra Srivastava, Associate Professor, IIT-Ropar, Punjab
- Prof. A. Sakthivel, Central University of Kerala, Kasargod.
- Prof. Dinesh Rangappa, Professor & Chairman, VTU, Chikkaballapura
- Dr. Ankur Bordoloi, Sr. Scientist, CSIR-IIP, Dehradun
- Dr Jyoti Roy Choudhary, Department of Chemistry, BMSIT, Bengaluru.
- Prof. Nagaraja. M from IIT Ropar
- Dr. Mahesh Padaki from Jain University, Bengaluru
- Dr. Satadeep Bhattacharjee from IKST, Bengaluru
- Prof. Ramakumar S., Indian Institute of Science, Bengaluru, India
- Prof. Udaykumar Ranga, JNCASR, Bengaluru, India.
- Prof. Hemalatha Balaram, JNCASR, Bengaluru, India.
- Dr. Dibyendu Samanta, Indian Institute of Technology, Kharagpur, India
- Department of Biochemistry, St. Aloysius College, Mangalore
- Department of Chemistry, Manipal Institute of Technology, MAHE, Manipal.
- Prof. M. Kumar, S. N. Bose Centre, Kolkatta
- Prof. Prosenjit Singhdeo, S. N. Bose Centre, Kolkatta

INTERNATIONAL COLLABORATORS:

1. Prof. Ajayan Vinu, University of Newcastle, Australia
2. Dr. Ding Zhong Yi, Technology Manager, PWT Inc, USA
3. Prof. Matjaž Spreitzer from Jožef Stefan Institute (JSI), Ljubljana, Slovenia.
4. Prof. Kazunari Domen from Shinshu University, Japan
5. Prof. C. D. Hu from The National Taiwan University.
6. Prof. Masaki Tesuzaka, Tokyo, Japan
7. Prof. Igor Goryni, Karlsruhe, Germany.
8. Dr. Vinayak Jagadish & Prof. Francesco Petruccione of University of Durban

12. MATERIALS SCIENCE AND CATALYSIS DIVISION



Established in May 2010 by the present Director, Prof. A. B. Halgeri with the help of the Executive Committee of AMEF, the department now consists of core faculty members hailing from diverse backgrounds as industrial chemistry, catalysis, polymers, and materials science. A new materials synthesis laboratory, with several sophisticated equipments has been established in the division. Bright students passionate about research were interviewed and inducted into Doctoral Programme in the Department. The research laboratories are now equipped with state-of-the-art instruments to give every advantage to the students and faculty pursuing research here. 9 students have obtained PhD from PPISR during 2015-2020 and at present, there are several students pursuing research and diligently working towards their Ph.D. degrees. More than 120 publications have been published in reputed national/ international journals in the last 10 years with an average impact factor of >4.0. About 26 students have received the best paper presentation awards in prestigious national/ international conferences. The faculty of the division has completed 23 Govt & industry-sponsored projects by 2020. Several conferences and workshops have been organized by the division.

12.1 The mission of the Division

- To innovate, design and develop novel multi-functional materials that have wide applications in various fields like heterogeneous catalysis, photocatalysis, nanotechnology, gas sensing, absorbents, photoluminescence, etc, and thus pave way for fruitful academic-industry partnership.
- The division is committed to train many doctoral students through a research program that promotes excellence and original thinking.
- The division also plans to interact with many national and international academic research institutions through collaborations, educational training, and other outreach activities

Specific areas of research:

- Heterogeneous catalysis
- Shape selective acid-base catalysis
- Novel micro/mesoporous materials for green chemical processes
- Biomass conversion to value-added products
- Catalytic CO₂ utilization by converting into useful chemicals

- Mesoporous polymers for catalysis and other applications
- Metal-organic frameworks for catalysis and gas sensing
- Functional inorganic nanomaterials as applied to photoluminescence
- Hybrid nanomaterials
- Photocatalysis
- Gas sensing
- H₂ generation
- Solar cells
- 2D materials for optoelectronics
- Computational studies (DFT) for 'structure-property correlations.

Academic and sponsored research highlights:

Dr. Ganapati Shanbhag and his group conduct research in the frontier area of catalysis for the design of novel catalysts for green chemical processes such as the catalytic conversion of CO₂ into value-added chemicals, conversion of biomass by-products like glycerol and furfural to value-added chemicals, pore engineering of microporous materials for shape-selective catalysis and gas adsorption. It also works on novel materials design for photocatalysis and gas sensors. Till 2021, the group has published 34 research articles in internationally reputed journals, three book chapters, and co-inventors in 4 patents. Three students, Mr. Nagendra Kulal, Mrs. Vaishnavi B. J. and Ms. Marilyn DMello joined as Senior research fellows of CSIR, Govt. of India, New Delhi in November 2020. Ms. Marilyn E. DMello was selected as Winner of Dr. KVR Rao Scientific Society- Young Scientist Award in Chemistry for 2020 and one best Oral Presentation Award in an international conference was received by Ms. Chethana A. Two publications in high-impact journals [Chemical Engineering Journal (IF: 13.2) and ACS Applied Nanomaterials (IF 5.1)] were published on CO₂ carbonylation to synthesize glycerol carbonate and substituted urea as a part of the project sponsored by VGST, Govt. of Karnataka. Two articles on the synthesis of alkyl levulinates from biomass derivative furfuryl alcohol were published in reputed journals. A research article in a prestigious Scientific Reports (Nature publishers) journal has also been published. A book chapter on *Heterogeneous Catalysis for Chemical Fixation of CO₂ via Carbonylation Reactions* was published by Springer, Singapore and authored by Dr. Shanbhag and his students Nagendra and Vaishnavi. Overall, 9 publications and 1 book chapter have come out of this group in international journals this year and 4 sponsored projects have been executed. During this year, Dr. Shanbhag gave several invited talks in conferences and workshops in virtual mode and was also invited as a PhD thesis examiner. A two-day workshop on Density Functional Theory (DFT) for computational catalysis was conducted by PPISR in a virtual mode as a part of a collaborative project. The training on DFT was given to the researchers by Dr. R. Vetrivel, Hon. Professor and an expert in this field.

During 2020-2021, 4 sponsored projects were executed by Dr. Shanbhag's Group. A new industry project sponsored by Sulzer-GTC Technology Inc, the USA titled "Catalyst and process development for hydrocarbon synthesis via halogen mediation" was initiated by Dr. Ganapati Shanbhag as PI and Dr. D. H. K. Murthy as Co-PI. The second industry project sponsored by Deepak Novochem Technologies Ltd (DNTL), Pune titled "Catalyst and process development for aromatics alkylation to make higher aromatics" was initiated by Dr. Ganapati Shanbhag as PI for the period of 1 year during 2020-2021. The DNTL has sponsored this project after the successful completion of the previous one-year project

in 2018-2019. The third sponsored project on “Catalyst and process development for CO₂ hydrogenation to produce methanol” sponsored by Hindustan Petroleum Corporation Ltd. (HPCL), Govt. of India is underway. A Govt. project sponsored by VGST under CESEM grant on “Chemical fixation of CO₂ by converting into value-added chemicals using metal modified mesoporous silicate catalyst” is also under progress. In the midst of COVID-19 pandemic setbacks and hurdles, overall, the group could achieve significantly in sponsored and academic research programmes due to the hard work of all the researchers involved.

Dr. Sanjeev Maradur’s group is working on mesoporous materials and metal-organic framework (MOF) for catalytic applications. Mr. Sathyapal Churipard R, SRF, the first student from the group, has been awarded PhD on the title “Synthesis and Characterization of Mesoporous Polymers and their Application in Adsorption and Catalysis” by the Manipal Academy of Higher Education on February 16, 2021.

The group published a work on Upgrading of lignocellulosic biomass-derived furfural: an efficient approach for the synthesis of bio-fuel intermediates over γ -alumina supported sodium aluminate catalyst. The major findings have been published in Molecular Catalysis Journal, Elsevier Publishing. Also, the group is working on metal-organic frameworks (MOF) catalysis. The MIL-101(Cr) metal-organic framework was successfully utilized for olefin-aldehyde condensation for the sustainable synthesis of nopol. Nopol finds various applications in fragrances and household products and is also used in agrochemicals as a pesticide and as an aroma in soaps, detergents, and polishes. The manuscript has been communicated to an international journal of high repute. In another work, the Pd/UiO-66 MOF catalyst has been successfully utilized for the selective hydrogenation of phenylacetylene (PA) to styrene (ST) is a pivotal step to eliminate the alkyne impurities and to increase the purity of the monomers in polymer industries. The project is ongoing and soon the results will be communicated for publication. The scope of the Pd/UiO-66 MOF has been successfully extended for the One-pot hydrogenation-esterification (OHE) of furfural to furfuryl acetate is a model reaction for upgrading of bio-oil.

The industry-sponsored project from Sravathi Advanced Process Technologies, Bengaluru on selective hydrogenation of aromatics with Dr Maradur as PI and Dr. Shanbhag as Co-PI has been successfully completed on Jan 2021. A new research proposal has been submitted to Hindustan Petroleum Green R&D center for possible funding to work on mesoporous alumina and it is under consideration.

Dr. D. H. K. Murthy’s group works on innovating novel energy materials towards scalable and cost-effective green hydrogen generation. The design of material and their desired properties (structural/surface/electronic) are rationally decided based on the insights from a range of computational/spectroscopy analyses. The Group is actively working with Researchers from India and abroad with an emphasis on advancing the efficiency of green hydrogen generation using photocatalyst modules that directly captures abundantly available sunlight, unlike the expensive electrolyzer.

12.2 Faculty Profile



Dr. A. B. Halgeri

Professor and Director

Email: abhalgeri@gmail.com,

director@poornaprajna.org

Homepage: <https://ppisr.res.in/faculty/b-halgeri/>

EDUCATIONAL QUALIFICATIONS:

Master's Degree in Chemistry from Karnataka University, Dharwad

Ph.D. in Physical Chemistry (Heterogeneous Catalysis) from Bengaluru University

Postdoctoral researcher under the UNESCO fellowship on Zeolite Catalysis at Department of Tokyo Institute of Technology, Japan

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

INDUSTRIAL PROJECTS COMPLETED: 07

CURRENT INDUSTRIAL PROJECTS (2020-2021): 04

ONGOING GOVERNMENT AGENCY SPONSORED PROJECTS:

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

MAJOR ACHIEVEMENTS AT PPISR

1. During his tenure as the Director, 17 research scholars have obtained their Ph.D. degrees at PPISR
2. Completed several industry-sponsored projects under his leadership

3. Under his leadership as a Chairman, several Workshops including the prestigious 23rd National Symposium on Catalysis (CATSYMP-23) were successfully conducted.

PUBLICATIONS AND PATENTS

He has published 150 research papers in national and international peer-reviewed journals and has also obtained 38 Indian and International patents.

PREVIOUS R & D ACCOMPLISHMENTS IN INDUSTRY

- Served as Vice President and Head of R&D Division of the Public Sector Indian Petrochemicals Corporation Ltd. Baroda, Gujarat after joining the Research Centre of the Indian Petrochemicals Corporation Ltd (IPCL), Baroda – Gujarat, in 1976.
- Worked as head of research and Development Centre of Reliance Industries Ltd and led a team of 150 Scientists and Engineers on the catalysts research in the Petrochemical units and Refineries.

Ph.D. STUDENTS GUIDED:

Three doctorates under his guidance are:

1. Mrs. Swetha Sandesh (Guide)
2. Mr. Vijayakumar Marakatti (Co-Guide)
3. Mr. Janardhan H L (Co-Guide)

AWARDS AND HONOURS

- 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, Kolkata
- 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] Lifetime achievement award by CSI-Bengaluru Chapter for his contribution towards Catalysis research in India during CATSYMP-23 in January 2018.
- 9] Lifetime achievement award by Material Society India for his contribution in Materials Research during International Conference on Advances in Materials Research (ICAMR-2019) in July 2019



Dr. RAJAPPAN VETRIVEL

Honorary Professor

Materials Science and Catalysis Division

Email: Rajappan.vetrivel@poornaprajna.org

Brief CV:

2019 - --- Chief Scientist – Sravathi AI Technology Pvt. Ltd., Bengaluru

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

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

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:

- Computational Material Science
- “Structure-Property-Performance” correlations in catalyst materials
- Electronic properties of catalyst surfaces
- Modeling and simulation for the 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:

1. Visiting Associate Professor at Tohoku University, Sendai, Japan from 1993 to 1994 and conducted research under Indo-Japan collaboration program
2. Visited University of Cambridge & University College London, UK to perform research studies in Indo-UK collaborative research program
3. Visited ‘Ecole Nationale Supérieure de Chimie’, Montpellier, France in 1988 & 1989 for an Indo-French project
4. Received the Best Young scientist award – Gold medal (1998) of Catalysis Society of India
5. Life Member of the Catalysis Society of India, Elected executive committee member, and Assistant Editor of Bulletin of the Catalysis Society of India.
6. Life Member of the Polymer Society of India
7. Elected Fellow of the Maharashtra Academy of Sciences

8. Supervised 3 research students of NCL, Pune who were awarded a Ph.D. degree by the University of Poona, Pune
9. Research publication actions in peer-reviewed journals
10. I have filed 7 global patents and 4 patent applications
11. I obtained management recognition awards in the form of company shares for leading R&D projects that led to business benefits
12. Currently Co-investigator for two industry-sponsored (by HPCL and Sravathi AI Technology Pvt. Ltd.) projects

PUBLICATIONS AND PATENTS (Latest)

I have published 125 research papers in national and international peer-reviewed journals and have also obtained Indian and International patents. Some of the selected publications from 1990 are:

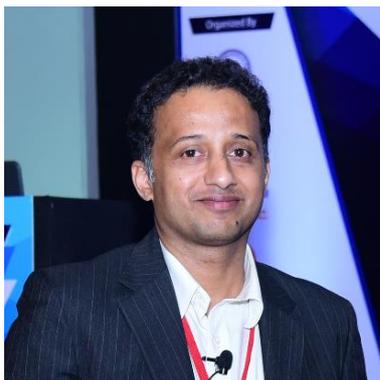
1. R. Vetrivel And Coworkers, Guidelines for Mastering the Properties of Molecular Sieves, (Eds. D. Barthomeuf Et Al), Plenum Press, New York, 1990, P.263. [Nato Asi Series B: Physics, Vol. 221].
2. R. Vetrivel And Coworkers In: Polymer Science - Contemporary Themes, (Ed. S. Sivaram), Tata Mc Graw-Hill Publishing Co Ltd., New Delhi, 1991, P.630. (Proc. Polymers'91 Symp., Pune, India.)
3. R. Vetrivel, Zeolites, 12, 424 (1992)
4. R. Vetrivel And Coworkers J. Phys. Chem. 96, 3096 (1992)
5. R. Vetrivel And Coworkers, Macromolecules, 25, 2215 (1992)
6. R. Vetrivel, Appl. Catal., 92(2), N16 (1992)
7. R. Vetrivel And Coworkers, Appl. Surface Sci., 82/83, 516 (1994)
8. R. Vetrivel And Coworkers, J. Am. Chem. Soc., 120, 4752 (1998)
9. R. Vetrivel And Coworkers, J. Am. Chem. Soc., 120, 11426 (1998)
10. R. Vetrivel And Coworkers, J. Catal., 174, 88 (1998)
11. R. Vetrivel And Coworkers, Langmuir, 18, 932 (2002)
12. R. Vetrivel And Coworkers, Combinatorial Chemistry and High Throughput Screening, 6, 1 (2003)
13. R. Vetrivel And Coworkers, J. Phys. Chem., B108, 11541 (2004)
14. R. Vetrivel, And Coworkers, Proc. 10th International Conference on Advanced Materials (Iumrs-Icam 2007) Held in Bengaluru, India, Oct. 2007
15. R. Vetrivel, 'Gtl Experience' Proc. 4th R&D Conclave (Organized by Petrotech Society) Held at Goa, India, Jan. 2010
16. R. Vetrivel, Invited Talk at JNCASR Winter School On "Materials and Processes for Applications in Energy and Environment", Bengaluru, Jan. 2015
17. R. Vetrivel And Co-workers, 'How Supercomputers Help to Overcome the Technical Challenge of Keeping Satellites Working Smoothly Hundreds of Kilometers Above Earth?', Shell Business Innovations; 2016.
<https://www.shell.com/inside-energy/smooth-moves-in-space.html>
18. R. Vetrivel And Coworkers, 'Computational Catalysis'

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

N. Kulal, R. Vetrivel, N.S.G. Krishna and G.V. Shanbhag, ACS, Applied Nano Materials, 4, 4388 (2021)

N. Kulal, R. Vetrivel, C.S. Gopinath, R.K. Ravindran, V.N. Rao, M. Shetty, R. Shrikanth D. Rangappa and G.V. Shanbhag, Chem. Engg. J., 419, 129439 (2021)

Faculty Profile



Dr. Ganapati V. Shanbhag

Associate Professor and HOD
Materials Science and Catalysis Division
E-mail: shanbhag@poornaprajna.org

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, India
- ❖ 1999: M.Sc. Organic Chemistry, Karnatak University, Dharwad, India

RESEARCH INTERESTS:

➤ Research on novel catalytic materials

There has been an increasing interest in recent years in developing novel heterogeneous catalysts for the selective synthesis of fine and specialty chemicals. In such an attempt, our group studied extensively several materials and was able to discover two materials as solid acid and base catalysts for the first time. Both studies have been published in a reputed RSC Advances journal. Metal hydroxychlorides are well known as minerals found in various parts of the world. One such example is tin(II)hydroxychloride, a mineral known by the name abhurite. The crystallographic and mineralogical properties of tin(II)hydroxychloride are well understood but its application has been overlooked so far. Its insolubility in water and organic solvents stimulated our curiosity to study its properties and application as a heterogeneous catalyst for Prins reaction.

In another study, zinc hydroxystannate ($\text{ZnSn}(\text{OH})_6$) has been reported for the first time as a solid bifunctional catalyst and has been applied for the synthesis of glycerol

carbonate from glycerol and urea. It has a perovskite-type crystal structure with metal atoms octahedrally coordinated with corner-sharing hydroxyl groups to form $\text{Sn}(\text{OH})_6$ and $\text{Zn}(\text{OH})_6$ octahedra. We found that it has strong basicity along with Lewis acidic Zn which makes it a bifunctional heterogeneous catalyst.

➤ **Designing catalysts for biofuel synthesis**

Increasing demand for petroleum fuels and depleting availability of crude oil has made to look for alternative sources of energy. The major challenge for the scientific community is to develop a technology compatible with the existing source in terms of quality at an affordable price. Biodiesel is one such source that attracted many researchers since it can be easily synthesized by transesterification of vegetable oil with alcohol in presence of an acid or base catalyst. To overcome these issues of homogeneous catalysts, heterogeneous catalysts are being developed to make biodiesel synthesis, an eco-friendly process.

Glycerol is obtained as a by-product during transesterification of vegetable oil which accounts for one-tenth of every gallon of biodiesel produced. It is well known that glycerol can be converted into chemicals by catalytic processes namely, acetalization, oxidation, hydrogenation, esterification, etherification, transesterification, dehydration, oligomerization and pyrolysis. Hence, there is a great commercial interest to design green and chemoselective catalysts for these processes. Our group has reported KF/alumina, metal hydroxystannate, and zeolite beta catalysts for transesterification, carbonylation and acetalization reactions respectively which were published in reputed international journals *viz.* Catalysis Letters, RSC Advances and Journal of Molecular Catalysis A.

➤ **Pore engineering of microporous materials for shape-selective organic transformations**

Vapor phase alkylation and disproportionation of aromatics are important reactions practiced in petrochemical industries. For these reactions, thermodynamic equilibrium mixtures of all the regioisomers are obtained with nonselective catalyst. Selectivity towards para-isomer can only be increased by the application of shape-selective catalyst. The para-isomer being commercially important than the other two for many organic reactions, post-synthesis modification is desirable to improve the product selectivity. Zeolites are known as shape-selective catalysts due to the presence of micropores with pore diameter close to the molecular diameter of the products. However, pore modification is essential for substantially improving the

shape selectivity towards a particular product. Post synthesis modification has been carried out by silanation, selective coking and metal/non-metal oxide impregnation. Phosphate modification was studied extensively by our group to explore the generation of new active sites, correlation of shape selectivity with phosphate modification and several model reactions such as toluene alkylation, ethyl benzene ethylation and disproportionation and competitive reaction of meta-xylene and ethyl benzene. Three papers are published in Applied Catalysis A journal and Chemical Engineering Science.

➤ **Chemical fixation of CO₂ by converting into valuable chemicals.**

CO₂ activation and valorization into value-added products is an emerging area of research considering the increasing environmental concerns caused by the emission of CO₂ into atmosphere by various modes resulting in the greenhouse effect and health hazards. Designing catalysts for CO₂ fixation to produce important products like cyclic carbonate, substituted urea, cyclic urea, glycerol carbonate is challenging as the catalyst should activate CO₂ and enhance the activity & selectivity towards the essential product. Tuning the nature and number of active sites on the catalyst surface is vital for these carbonylation reactions as CO₂ and the substrate are activated by basic and acidic sites respectively. After receiving a project sponsored by VGST, GOK through CESEM grant, the design of solid acid-base bifunctional catalysts for CO₂ transformation into value-added chemicals has been conducted since last few years. Several research works have been published by this group in internationally reputed journals like Chemical Engineering Journal, ACS Applied Nano Materials, Journal of CO₂ Utilization, Applied Catalysis A, and a book chapter with Springer Nature publishers.

RECOGNITIONS/ACHIEVEMENTS/AWARDS/MEMBERSHIP:

- Received Award for Research Publications (ARP) for the year 2016-17 for best publications by VGST, Govt of Karnataka which contains cash award + Citation.
- Chemical Today magazine published an interview in June 2016 issue.
- Received plaques by GTC Technology Inc in 2012, 2014, and 2015 for completing projects as PI and developing 1st and 2nd generation catalysts for the toluene methylation process.
- Co-inventor of two US patents (granted) filed by HPCL in the collaborative project.
- 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.

- An invited member of the Technical Committee and Session Chair for the National Conference on “Frontiers of Catalysis Science & Technology and its applications” held at St. Joseph's College, Bengaluru on January 10-11, 2020.
- A member of the technical committee and a member of Panel Discussion for the “International Conference on Advances in Materials Research”, organized by Ramaiah University of Applied Sciences, Bengaluru on July 25-27, 2019.
- Delivered several invited talks at prestigious national/ international conferences such as 1) 3rd International conference on emerging advanced nanomaterials 2018 (ICEAN-2018)” organized by University of Newcastle, in Newcastle, Australia; 2) International Conference on World biodiesel Congress & Expo at San Antonio, USA, 2016; 3) 5th Indo-French symposium at CSIR-National Chemical Laboratory (NCL), Pune 2019; 4) International conference on "Carbon capture & its Utilization" at CSIR-NCL, Pune conducted in association with Royal Society of Chemistry, 2018; 5) Asia-Pacific Congress on Catalysis (APCAT – 7) organized by ICT in Mumbai, 2017; 6) 23rd National Symposium on Catalysis (CATSYMP-23) organized by Catalysis Society of India in Bengaluru, 2018; 7) National Workshop on Catalysis organized by Catalysis Society of India held at CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad, 2016
- Received International Travel Grant from SERB, DST, Govt. of India to travel to Australia to attend ICEAN conference in 2018.
- Ph.D. Thesis Examiner for reputed CSIR institute and prestigious universities.
- Committee Member of the Syllabus revision committee for Chemistry for Siddaganga Institute of Technology (SIT), Tumkur 2013-2018.
- Reviewer for international journals like Chemical Communications, RSC Advances, Catalysis Science and Technology, Applied Catalysis A, Catalysis Communications and Journal of Chemical Sciences, ChemCatChem., New Journal of Chemistry, ACS Sustainable Chemistry, and Engineering, etc since the last 10 years.
- Subject Resource person for FDP, Refresher, TEQIP and National Training Course programmes for degree and engineering colleges.
- Life member of International Zeolite Association (IZA) and Catalysis Society of India (CSI) and member of American Chemical Society.

STUDENTS (2020-2021):

Ph.D. students		Project Fellows	
1	Mr. Nagendra Kulal	6	Mr. Sujith S.
2	Mrs. Vaishnavi B. J.	7	Ms. Chaitra Mallannavar
3	Ms. Marilyn DMello	8	Ms. Shrinidhi Patil
4	Ms. Chethana A.	9	Mr. Harsha Murudappa
5	Ms. Madurya Gowda	10	Mr. Vithobha Hugar
		11	Mr. Rajashekhar Vaibhav

GROUP ALUMNI:**A) PhDs**

1. **Dr. Vijaykumar Marakatti:** Present Position: Marie Skłodowska-Curie Postdoctoral Fellow, Universite catholique de louvain (UCLouvain), Belgium
2. **Dr. Janardhan H L:** Present Position: Team Leader, Materials Research, Dhio Research and Engineering Pvt. Ltd, Bengaluru.
3. **Dr. Manjunathan P.** Present Position: Post-Doctoral Fellow, Korea Research Institute of Chemical Technology (KRICT), South Korea.
4. **Dr (Mrs). Swetha Sandesh** Present Position: CEO, Niranthara Scientific Solutions Pvt Ltd, Bengaluru.

B) M. Tech Thesis Guided:

- 1) **Mr. Satish Burla** 2011-2012. Currently, he is Scientist in SABIC Research Centre, Bengaluru
- 2) **Mr. Prashant Kumar K.** 2012-2013. Currently, he is Scientist in SABIC Research Centre, Bengaluru
- 3) **Mr. Girish Kamath** 2015-2016. Currently, he is pursuing his PhD at Univ. of Saskatchewan, Canada

C) Post-Doctoral Fellows:

- 1) **Dr. Ramesh S.** 2012-2013: He worked in a project sponsored by Shell Technology Centre, Bengaluru and GTC, USA for the period of 1 year.
- 2) **Dr. Prakash Chandra** 2015-2016: He worked in the project sponsored by PW Technology Inc, USA for the period of 1 year.
- 3) **Dr. Subba Reddy Marri** 2016-2017: He conducted research in industry project sponsored by HP Green R & D Centre Bengaluru and worked during 2016-2017.

NATIONAL AND INTERNATIONAL COLLABORATORS:

1. Prof. Ajayan Vinu, University of Newcastle, Australia
2. Dr. Ding ZhongYi, Sulzer-GTC Technology Inc, USA
3. Dr. C. S. Gopinath, HOD, Catalysis Division, CSIR-NCL, Pune
4. Dr. G. Valavarasu, DGM, HP Green R & D Centre, Bengaluru
5. Dr. Raman Ravishankar, DGM, HP Green R & D Centre, Bengaluru
6. Prof. Shubhangi Umbarkar, Principal Scientist, CSIR-NCL, Pune.
7. Prof. Rajendra Srivastava, Associate Professor, IIT-Ropar, Punjab
8. Prof. A. Sakthivel, Central University of Kerala, Kasargod.
9. Prof. Dinesh Rangappa, Professor & Chairman, VTU, Chikkaballapura
10. Dr. Ankur Bordoloi, Sr. Scientist, CSIR-IIP, Dehradun

RESEARCH 2020-2021:**CURRENT SPONSORED PROJECTS:****1) Catalyst and process development for hydrocarbon synthesis via halogen mediation**

Sponsored by: Sulzer-GTC Technology Inc, USA Duration: 1 year February 2021-January 2022

Principal Investigator: Dr. Ganapati V Shanbhag

Co-PI: Dr. D. H. K. Murthy

Research fellows: Ms. Shrinidhi, Patil, Mr. Harsha M., Mr. Vithobha Hugar

A new project sponsored by Sulzer-GTC Technology Inc, USA has been initiated by procurement of chemicals and labwares. Initially, a series reactor was set up and required solid catalyst developed by PPISR in the previous project was freshly synthesized and tested for this reaction. A few process parameters were changed to see the effect on the catalyst performance. Another work on estimation of halogen in distillate was parallelly conducted in a new customized distillation set-up. The results are sent to the sponsors on a daily basis and review meetings are conducted on weekly basis.

Status: Ongoing

2) Catalyst and process development for CO₂ hydrogenation reaction

Sponsored by Hindustan Petroleum Corporation Ltd., Govt. of India, Duration: 2 years, 2020-2022

Principal Investigator: Dr. Ganapati V Shanbhag

Co-PIs: Dr. R. Vetrivel, Dr. S. P. Maradur

Research fellows: Mr. Sujith S., Ms. Chaitra Mallannvar, Ms. Shrinidhi Patil

Several catalysts for CO₂ hydrogenation have been synthesized and characterized at PPISR. They were then sent to HP Green R & D Centre for catalyst testing experiments. The initial catalysis activity studies have been received from HPCL and results are encouraging. Based on these results, the catalyst recipes were further fine-tuned to achieve better performance. During this period, DFT calculations for this reaction have also been carried out. The method, model, basis sets, and related parameters are standardized for the reactant and product molecules. The calculations were carried out for reactants and product molecules. The studies on adsorption of CO₂ in different orientations over metal oxide catalyst systems are carried out using their known crystal structures, crystal planes with various possible terminations. The adsorption energy of CO₂ is predicted for the model catalyst. The Quarterly and six-month review meetings with HPCL committee have been conducted during the last 1 year.

Status: On going.

3) Catalyst and process development for aromatics alkylation to make higher aromatics

(Sponsored by Deepak Novochem Technologies Ltd., Pune) from November 2020-October 2021)

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 2020 by recruiting the project fellows and purchasing the 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 screenings were conducted. A good mass balance was obtained for the reactions and all the analytical procedures were established. The reactions were conducted in a single and series reactor and initial catalytic reaction results have been shared with DNTL. The process parameters were optimized both in single and two reactors in series for different aromatic substrates. A high conversion of ~80% conversion with > 60% selectivity for the desired product was obtained. Further catalyst testing with changing process parameters is under progress. Status: Ongoing

4) Exploring characteristics of Sn-Ni oxide as solid acid-base catalyst for carbonylation of amines with CO₂ and theoretical study for predicting the best suited active sites

Sponsored project CESEM, VGST, Govt. of Karnataka

Research fellow: Mr. Nagendra Kulal

Principal Investigator: Dr. Ganapati V Shanbhag

The reaction between n-alkylamine and CO₂ has gained interest due to the demand for the dialkylurea for various applications. We have successfully used the tool 'Mathematica' for the first time to analyze the experimental data with an idea to derive an equation that predicts the product yield for any given input set of dependent parameters. The usage of this tool in heterogeneous catalysis provides a novel methodology for future research to design better-performing catalysts. Among several Sn containing mixed oxides, Sn-Ni oxide (Sn-Ni-O) was found to be the better performing catalyst. There are two main reasons for improved catalytic performance; one, mixing of SnO₂ into NiO decreases the number of holes (h⁺) localized on lattice oxygen (O²⁻+ h⁺→ O^{•-}) and two, smaller SnO₂ particles are dispersed on the bigger particle NiO which alters the acidic and basic active sites in the catalyst. The high performance of Sn_{1.1}-Ni-O-600 catalyst could be attributed to the presence of appropriate number and strength of acidic and basic sites. The reactions of various amines with CO₂ show that the catalyst works well for aliphatic amines, diamine and amino alcohol, whereas trace conversions were obtained for aromatic and secondary amines. Under optimized reaction condition, Sn_{1.1}-Ni-O-600 gave 77.3 % of n-butylamine conversion and 75.7% of yield for 1,3-dialkylurea.

Status: Manuscript is accepted in Chemical Engineering journal

5) Zn-Doped CeO₂ Nanorods for Glycerol Carbonylation with CO₂ Sponsored project CESEM, VGST, Govt. of Karnataka

Research Guide: Dr. Ganapati V Shanbhag

Research fellow: Mr. Nagendra Kulal

Nickel, copper and zinc doped CeO₂ nanorods were synthesized by hydrothermal method and their physicochemical properties were correlated with catalytic activity for carbonylation of glycerol with CO₂ to yield GlyCO₃. CeO₂ nanorod gave higher GlyCO₃ yield than cube and mixed CeO₂ because it contains a greater number of oxygen vacancy sites leading to the formation of catalytic active sites. The activity of the catalyst increased in the order; Zn/CeO₂ > Ni/CeO₂ > Cu/CeO₂ > CeO₂ nanorod, which followed the trend of capacity of CO₂ adsorption. As the concentration of Zn increased in Zn/CeO₂ catalyst, there was an increase in both acidic and CO₂ chemisorption sites and increase in surface oxygen vacancy of Ce³⁺ concentration. The reducibility of Ce in 10.5%Zn/CeO₂ and 15.3%Zn/CeO₂ catalysts at similar temperatures indicating 10.5% of Zn as the optimum amount of doping into CeO₂. Hence, the results suggested that 10.5%Zn/CeO₂ catalyst was the best for this reaction which gave 90.4% of glycerol conversion and 89.5% of yield for GlyCO₃ under optimized reaction condition. Overall, Zn/CeO₂ was highly active, selective and reusable catalyst for carbonylation of glycerol with CO₂.

Status: This manuscript was published in *ACS Applied Nano Materials* journal

6) Interactions of cobalt/ceria promoting oxygen vacancy for boosting dimethyl carbonate synthesis from CO₂ and methanol

Sponsored project CESEM, VGST, Govt. of Karnataka

Research Guide: Dr. Ganapati V Shanbhag

Research fellow: Mr. Nagendra Kulal

The oxygen vacancy on the catalyst had a strong impact on the activation of CO₂ by filling the oxygen vacancy with one oxygen atom of the CO₂ molecule. The Co@CeO₂ catalyst exhibits multiple reduction behavior as Co²⁺ and Co³⁺ metal species differ in the strength of their interaction with CeO₂. This causes the reduction of surface and bulk Ce⁴⁺ to Ce³⁺ in solid solution Co-O-Ce. This work presents how the reduction behavior of Co@CeO₂ catalyst influence CO₂ activation by changing the Co concentration for dimethyl carbonate synthesis. Catalysts were characterized by various techniques and catalytic activity was correlated with oxygen vacancy. The reaction under optimized conditions with CO₂ and methanol resulted in > 80% dimethyl carbonate yield using Co@CeO₂ catalyst. DFT calculations for predicting the best CO₂ adsorption sites and reaction mechanism are completed.

Status: Manuscript under preparation

7) Utilization of renewable resources: Investigation on role of active sites in zeolite catalyst for transformation of furfuryl alcohol into alkyl levulinate

Research fellow: Ms. Vaishnavi B.J.

Research Guide: Dr. Ganapati V Shanbhag

Alkyl levulinates are compounds derived from furfuryl alcohol, which act as a versatile building blocks for the synthesis of various chemicals. They are widely used in the food industry, as green solvents and plasticizing agents.

The transformation was studied using ZSM-5 catalyst by investigating its active sites. The manuscript was revised as suggested by the reviewers by additionally studying the B//L ratio using pyridine FTIR for all the post modified ZSM-5 catalysts. We could correlate the catalytic activity of all these modified ZSM-5 prepared by desilication, dealumination, metal ion exchange and phosphate modification with their B/L ratio. The manuscript was thoroughly modified to meet the journal standards by addressing most of the comments suggested by the reviewers.

Status: Published in Molecular Catalysis Journal

8) Designing eco-friendly solid acid catalyst for esterification of furfuryl alcohol to produce furfuryl acetate

Principal Investigator: Dr. Ganapati V Shanbhag

Research fellow: Ms. Vaishnavi B J

Esterification of furfuryl alcohol yielding furfuryl acetate is one of the transformations of our interest where the desired product is commercially used in fragrance and flavouring industries. The reaction was carried at a controlled temperature of 70°C and various solid acid catalysts such as Zeolite-Y, H-Beta, Ferrierite, Amberlyst15, Silicoaluminophosphate-SAPO11, SAPO-34, Sulfated Zirconia, Al-SBA-15 were screened for this transformation. The catalytic performance with respect to TON is in the following order Sulfated Zirconia > Al-SBA-15 > SAPO-11 > Ferrierite > HZSM-5 > H-BETA > SAPO-34 > Amberlyst-15 > Y-Zeolite. From these results, sulfated zirconia was chosen for further studies as it has very high TON over all the conventional catalysts. Due to the inherent character of sulfated zirconia containing leachable sulfate species, the various concentration of sulfate exchanged sulfated zirconia were synthesized and the materials were subsequently washed to get rid off all the leachable sulfate ions at 80°C for 6hours. Hence after removing the physisorbed sulfate ions, the catalysts were screened to get the optimum molar sulfate ion concentration at the reaction temperature of 100°C. Sulfated zirconia with 2.5M sulfation has shown the best catalytic performance with 79% furfuryl alcohol conversion and 75% furfuryl acetate selectivity.

Status: Under progress

9) Rational design of MOF based catalyst for hydrolysis of furfuryl alcohol to produce levulinic acid

Research fellow: Vaishnavi B. J.

Principal Investigator: Dr. Ganapati V Shanbhag

Aiming at the development of novel solid acid catalysts for efficient hydrolysis of furfuryl alcohol to levulinic acid, metal-organic frameworks were planned as a catalysts for this transformation. Therefore, for preliminary screening,

the catalytic activity of UiO-66, BUT-Cr, BUT-Cr-SO₃H, MOF-808, MOF-SO₃H were compared with the reported H-ZSM-5 in a sealed tube at 120°C. Catalyst loading was 3wt% and the furfuryl alcohol to water to solvent (diglyme) mole ratio was 1:15:60. Though sulfonated MOF-808 showed better catalytic performance than other MOFs, it could not compete with the reported HZSM-5 catalyst. This might be due to the mild sulfonation (0.25M) on MOF-808 done, which resulted in yielding lesser amount of Brönsted acidity in the material. The catalytic performance can be enhanced by increasing the concentration of sulfonic group in MOF-808 as the reaction demands strong Brönsted acidity. Also the sulfonation done to BUT-Cr was using H₂SO₄, whereas as the report suggests the sulfonation using the aid of fuming sulfuric acid.

Status: Under progress

10) Designing efficient supported metal catalysts for hydrogenolysis of furfuryl alcohol to 1,2-Pentanediol and 1,5-Pentanediol

Research Guide: Dr. Ganapati V. Shanbhag

Research fellow: Ms. Vaishnavi B.J.

1,2-Pentanediol (1,2-PeD) is used widely as an intermediate of low-toxic microbicides and polyesters feedstock. α,ω -Diols, are used for the production of elastic fiber, polyesters and polyurethane. These can be potentially replaced by 1,5-Pentanediols (1,5-PeD). Initially Mⁿ⁺/Al₂O₃ catalysts were prepared and screened in a low-pressure stainless-steel reactor that showed a very good selectivity towards 1,2PeD which is due to the presence of Pt which is hydrogenating active species in the catalyst. When the reaction temperature was 130 and 200°C, undesired humins were formed with very less or no selectivity towards either of the desired isomers (1,2PeD and 1,5 PeD). Initial catalyst screening is under progress.

Status: In progress

11) Designing catalyst for the synthesis of difurfuryl carbonate via carbonate interchange reaction

Research Guide: Dr. Ganapati V. Shanbhag

Research fellow: Ms. Madurya Gowda

Difurfuryl carbonate has several useful applications in liquid fuel, lubricant and engineering plastic. Difurfuryl carbonate is synthesized by carbonate interchange of dimethyl carbonate using furfuryl alcohol. Initially the reaction was studied by employing reported homogeneous catalysts (potassium carbonate and cesium carbonate) at 70°C for 2h by using different reactor setup like Seal tube and Low-pressure reactor. The reactions carried out in low pressure reactor yielded with high conversion and selectivity compared to seal tube, which implies the reaction should be carried out at pressurized conditions. Synthesis of new catalytic material based on the required active sites and catalytic activity study is being carried out.

Status: In progress

12) 2D Redox active conductive MOFs for the development of chemiresistive gas sensors

Principal Investigator: Dr. Suresh B Kalidindi

Co-investigator: Dr. Ganapati Shanbhag

Research fellow: Ms. Marilyn E. DMello

In recent studies, to boost electrical conductivity and long-range magnetic order in 2D MOFs, an excellent work has been done by K.S. Pederson et.al and group. They synthesized structurally simple layered coordination solid, $\text{CrCl}_2(\text{pyz})_2$ using transition chromium ion in conjugation with ditopic redox active ligand-pyrazine. The claimed $\text{Cr}^{\text{III}}\text{Cl}_2(\text{pyz})_2$ is generated by transition metal-ion reduction of pyrazine via formation of pyrazine anion radical. In our study, we present a feasibility study of a different approach on using redox active $\text{CrCl}_2(\text{pyz})_2$ for an effective dispersion of palladium nanoparticles and studied for chemiresistive hydrogen gas sensing. Aromatic amines are known to be redox-active when coordinated to moderately reducing transition- metal ion centers. The developed material is required to allow fast transport/diffusion of hydrogen to have enough sensing response, time and reproducibility with high selectivity compared to pristine $\text{CrCl}_2(\text{pyz})_2$. Further we explored $\text{Pd}@\text{CrCl}_2(\text{pyz})_2$ for chemiresistive hydrogen sensing and have established a proof-of concept that can be considered as an ideal solution to solve inherent issues associated with MOF-based chemiresistive sensors. Based on the results obtained in this study, one can expect that the use of ligand redox activity for metal@MOF hybrid systems-based sensors is a powerful approach to address the poor selectivity and reproducibility issues in palladium-based sensors.

Status: The manuscript is under preparation. DFT studies to propose the chemiresistive hydrogen sensing mechanism is under progress.

13) High Dispersion of Pd (II) over Chromium based Metal-Organic Framework for Rapid Detection of Hydrogen

Principal Investigator: Dr. Suresh Babu Kalidindi

Co-investigator: Dr. Ganapati V. Shanbhag

Research fellow: Marilyn DMello

Hydrogen gas is one of the cleanest and the most promising clean-energy carriers for future applications and presently used in many industrial processes. Nevertheless, the use of H_2 gas is associated with several safety issues and its detection has its own challenges. H_2 sensing has stirred much interest with nanostructures of metals like palladium majorly due to the strong affinity to H_2 . However, this hinders a long-time usage of Pd-based sensors for H_2 and often resulting in high sensing recovery times. In recent studies, two- dimensional electrically conductive MOFs have been receiving increasing attention for their application as versatile sensors. Here in this work, in a new approach we anchored Pd (II) over $\text{CrCl}_2(\text{pyrazine})_2$ MOF which acted as an effective chemiresistor for rapid selective sensing of hydrogen gas at low temperatures (60°C) with response/recovery times of 5-7 sec. Integration of Pd(II)(rather than Pd(0) nanoparticles) maximized

signal transduction which played vital role in overall performance of the sensor. The high dispersion of Pd²⁺ not only maximized the metal- MOF interactions but also allowed minute quantities (1.25 wt%) of noble metal loadings leading to a development of cost effective device. Importantly, the sensor is found to be stable up to six months when stored under ambient conditions. Further, this work encourages future studies in the area of single metal atom-MOF chemiresistors that will ensure the development of rapid low temperature H₂ sensors.

Current Status: Manuscript under preparation

14) Exfoliation of Cr-based Metal-Organic Framework for Ultra-high Dispersion of Palladium to Detect Hydrogen. (Collaboration work with Dr. H S S Ramakrishna Matte @ CENS, Jalahalli)

Research fellow: Ms. Marilyn DMello

Research Guide: Dr. Suresh Babu K.

Research Co-Guide: Dr. Ganapati V. Shanbhag

Layered MOF- CrCl₂(pyz)₂ are formed by stacking the 2D layers along the vertical direction via weak interactive van der Waals forces, allowing them to be easily exfoliated into 2D nanosheets by the top-down methods, just like the top-down exfoliation of graphene and transition metal dichalcogenides. Single or few-layer MOF nanosheets have been prepared via sonication exfoliation using acetonitrile solvent after carefully choosing solvents (among methanol, iso-propanol and NMP organic solvents). Further the exfoliated Pd@CrPy was characterized by using transmission electron microscopy and high resolution XPS to provide insights into the structure, (dispersion of Pd over CrPy matrix and oxidation state of Pd in exfoliated CrPy MOF sheets). Further, gas sensing studies were carried out by drop casting a few layers of Pd@CrPy (exfoliated using acetonitrile) onto inter- digitated electrodes.

Current Status: In progress

15) Multifunctional Covalently linked Graphene-MOF hybrid: An Effective Chemiresistive Gas Sensor

(Collaboration work with Dr. K. Jayaramulu, IIT Jammu, Jammu & Kashmir, Prof. R. Zboril, Palacky University, Czech Republic and Prof. Roland Fischer, University of Munich, Germany)

Research fellow: Ms. Marilyn DMello

Research Guide: Dr. Suresh Babu K.

Research Co-Guide: Dr. Ganapati V. Shanbhag

CO₂ is a greenhouse gas and its sensing over a wide range of concentrations is of utmost importance in the control and/ or monitoring of emissions. In recent times, the inclusion of active sites for adsorption/desorption on nanostructured carbon-based materials, two dimensional materials and metal-organic frameworks-based materials where CO₂ gas can cause changes of electrical parameters (e.g resistance) can further change the future of designing effective CO₂ gas sensors. Here, in this work the covalent assembly of graphene acid (GA) with amine functionalized UiO-66-NH₂.

In this material, UiO-66-NH₂ is covalently bonded with GA via amide bonds, creating the hybrid GA@UiO-66-NH₂. The material displays hierarchical porous architecture facilitates easy gas diffusion to provide faster access to the amine/amide active sites. The easy gas diffusion pathway is due to the MOF and GA layers that construct the mesoporous diffusion channels. The amide bridge at GA@UiO-66-NH₂ (GA-MOF interface) connecting the graphene basal plane and -NH₂ functionality on the pristine UiO-66-NH₂ are the affinity sites towards CO₂.

Current Status: This manuscript under communication

16) Chemiresistive Gas sensing and Photocatalytic Dye Degradation studies using Conducting polymer@MOF Composite

(It is a collaboration work with Dr. J. Bosco, SASTRA University, Tamil Nadu and the Photocatalytic Dye Degradation studies is a collaboration work Prof. N. Rao Peela, IIT Guwahati).

Principal Investigator: Dr. Suresh Babu Kalidindi

Co-investigator: Dr. Ganapati V. Shanbhag

Research fellow: Marilyn DMello

Hybridization of MOFs with flexible materials like polymers is an emerging trend in many MOF research field. The attractive properties of MOFs including porosity, high surface area, pore surface functionalization, host guest interaction have always fascinated many researchers. In this work, initially UiO-66-NH₂@PANI, was successfully prepared by polymerizing the conductive polyaniline (PANI) polymer around the metal-organic framework UiO-66-NH₂. Due to good water, chemical stability, and the abundance of amine groups possessing a band gap of 2.7 eV, UiO-66-NH₂ was selected as a representative MOF support. PANI can effectively enhance the conductivity/charge migration of the composite materials by speeding up the electrons/ion's diffusion in the matrix. UiO-66-NH₂ not only serves as backbone for PANI, but also provides high surface area and more adsorption sites. Currently, characterization of UiO-66-NH₂@PANI by TEM, Raman and XPS to get information on the structure is under progress. UV-DRS of UiO-66-NH₂@PANI and calculation of the band gap is going on. Photocatalytic dye degradation studies will include: effect of catalyst to substrate, effect of visible light on the dye degradation, time studies, and catalyst recyclability.

Current Status: Under progress

17) Designing of Ca substituted LaFeO₃ perovskite oxide for the selective detection of low concentration SO₂ gas.

Research fellow: Ms. Chethana A.

Research Guide: Dr. Nalini Sundaram

Research Co-Guide: Dr. Ganapati V. Shanbhag

The present work is based on the synthesis of Ca substituted LaFeO₃ for the selective detection of SO₂ gas. Herein, we have made a comparative study of gas-sensing performance of La_{1-x}Ca_xFeO₃ (0.4 ≤ x ≤ 0.8) nanoparticles both in pellet and thin film. Based on this work we had submitted a manuscript titled "*Selective SO₂*

Detection at Low Concentration by Ca Substituted LaFeO₃ Chemiresistive Gas Sensor: A Comparative Study of LaFeO₃ Pellet vs Thin Film” to “Sensors and Actuators: B Chemical” journal. As per reviewer’s suggestions, we have done additional sensing studies for the La_{1-x}Ca_xFeO₃ (0.4≤x≤0.8) material. We have explored the effect of operating voltage and operating temperature on gas sensitivity of La_{0.6}Ca_{0.4}FeO₃ pellets as well as thin films. Further, to study the stability of La_{0.6}Ca_{0.4}FeO₃ sample, the used pellet was characterized by the P-XRD technique after repetitive gas sensing measurements. There was no change in the particle size or stability issues with respect to these samples. The XRD peaks of used pellet were same as before the gas sensing measurement with no change in the peak width confirming that the particle size was preserved even after gas sensing measurements. With these additional data, this work has been successfully accepted and published in “Sensors and Actuators: B Chemical” journal.

18) Designing of hybrid (Ta₂O₅-SnO₂)-Polyaniline material to improve the sensitivity of gas detection

Principal Investigator: Dr. Nalini G. Sundaram

Co-investigator: Dr. Ganapati V. Shanbhag

Research fellow: Ms. Chethana A.

In the present work, we have synthesized an inorganic-organic hybrid semiconducting material for the gas sensing study of CO gas. The hybrid (Ta₂O₅-SnO₂) composite with Polyaniline (PANI) was synthesized by polymerization complex method, where in as prepared (Ta₂O₅ (5wt %) -SnO₂) nano composite was incorporated in the PANI matrix. The synthesized materials were characterized by P-XRD and FTIR techniques. Further, The pellet of hybrid material was subjected to gas sensing studies for the detection of CO gas. From the optimization of results, we have arrived at best composition as 1: 0.50 weight ratio of (Ta₂O₅-SnO₂): PANI when compared with other compositions (1:0.25, 1: 0.75). The measurements were carried out from room temperature and we observed a good response of 5.2% for 10 ppm CO gas at room temperature with well-defined response and recovery curves. Although, the (Ta₂O₅-SnO₂) composite does not detect CO gas at room temperature, the hybrid material with PANI helped in decreasing the operating temperature. In addition, the hybrid material showed increased conductivity which could be due to the conducting properties of Polyaniline. The material was able to detect the CO gas up to 125 °C with low response and recovery time. This is the best results we have obtained and it is comparable with the literature reports available for CO sensing.

Status of the work: Manuscript under preparation

EVENTS AND ACHIEVEMENTS:**A) New sponsored projects**

1) An industry project sponsored by Deepak Novochem Technologies Ltd (DNLT), Pune titled “Catalyst and process development for aromatics alkylation to make higher aromatics” was initiated by Dr. Ganapati Shanbhag as PI for the period of 1 year during 2020-2021. The DNLT has sponsored this project after the successful completion of the previous one-year project in 2018-2019.

2) An industry project sponsored by Sulzer-GTC Technology Inc, USA titled “Catalyst and process development for hydrocarbon synthesis via halogen mediation” was initiated by Dr. Ganapati Shanbhag as PI and Dr. D. H. K. Murthy as Co-PI in February 2021 for the period of 1 year. The Sulzer-GTC has sponsored this project after the successful completion of their previous 8 sponsored projects from GTC during 2010-2019 by Dr. Shanbhag’s group.

B) Number of Publications

Total publications: 54

Total No of Patents granted: 04

Publications for the year 2020-21: 09

C) Book Chapters

Total Book Chapters: 03

Book Chapters for the year 2020-21: 01

D) Papers Presented In Conferences/ workshops

Total Best presentation awards: 20

Total Best presentation awards for the year 2020-21: 01

Other Presentations in Conferences

Total presentations: 50

Presentations for the year 202-21: 06

Awards/recognitions of the students in the lab: 01

Ms. Marilyn E. DMello was selected as Winner of Dr. KVR Rao Scientific Society-Young Scientist Award in Chemistry for 2020.

F) Invited talks in conferences/workshops:

Total invited talks: 20

For the year 2020-21: 05

G) Other scientific activities in 2020-21

1. Reviewed the manuscripts in international reputed journals like Applied Catalysis B. Environmental, Applied Catalysis A. General, Sustainable Energy & Fuels, Journal of Industrial & Engineering Chemistry, ChemCatChem, ACS Sustainable Chemistry and Engineering, Asia-Pacific Journal of Chemical Engineering, International Journal of Polymer Science. The manuscripts have been promptly reviewed and comments have been submitted to the journals during these 3 months.
2. Delivered a talk in One day conference during Founder's Day on the topic "PPISR-A Decade's Review" on July 2, 2020, as a tribute to our beloved Funder HH Sri Vibudhesha Theertha Swamiji.
3. Dr. Ganapati Shanbhag attended the virtual 4th National Symposium on the "Shaping the Energy Future: Challenges & Opportunities" organized by CSIR-Indian Institute of Petroleum, Dehradun on June 5, 2020.
4. Ms. Chethana A. attended an International Webinar on "X-ray spectroscopy as a tool in understanding biological catalysis" by Prof. Dr. Serena DeBeer, Director department of inorganic spectroscopy Max Plank institute for Chemical energy conversion, organized by the Department of Chemistry, St. Joseph's College (Autonomous), Bengaluru on July 29th 2020.
5. Ms. Chethana A. attended online workshop on Rietveld refinement method during September 22-24th, 2020, organized by UGC-DAE Consortium for Scientific Research Mumbai Centre in association with Indore Centre.

Faculty Profile



Dr. Sanjeev P. Maradur

Associate Professor

Materials Science & Catalysis Division

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RESEARCH INTERESTS:

- 1. Nanoporous Materials:** Nanoporous materials have gained scientific and technological importance because of the presence of their pore structures of tuneable dimensions at manometer 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 main 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 the 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.
- 2. 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 an industrial scale. Supports play a significant role in such systems. The microenvironment around the catalyst active site will be the deciding factors in achieving high conversions with high selectivity. Heterogenization of homogeneous catalysts onto supports such as zeolites, nonporous materials like silica and polymers would be of much interest in the design and development of processes for fine chemical production.
- 3. Synthesis and Catalytic Applications Metal-Organic Framework (MOFs):** The metal-organic frameworks (MOF's) are advanced materials with exceptional textural properties. Catalysis by MOFs mainly depends on the active sites, both metal centres and organic linkers. Organic bridging linkers are used as scaffolds to which distinct catalytic complexes, biomolecules, and homogeneous catalysts can be immobilized or encapsulated. These materials are

known for their textural properties such as high surface area, intrinsic porosity, a high percent of transition metal content, and accessibility of guest molecules into the pores. The beneficial properties of the metal-organic frameworks made them excellent materials for catalytic applications. In the last two decades, MOFs have presented a significantly amplified role in heterogeneous catalysis as they have been considered as eco-friendly alternatives for catalysis. The ongoing research work in our group aims at the synthesis of MOFs with good thermal stability and high surface area. In addition, MOF-derived carbon-based materials are used in the proposed organic transformations.

Training of Students:

PHD AWARDED	: 01
Guiding as PI/Co-PI	: 02
MSc Project completed	: 03
B. TECH/M. TECH. PROJECT COMPLETED:	07

RECOGNITIONS/ACHIEVEMENTS:

1. Received “**Award for Best Publication**” in Metallurgical and Materials Science Category, from Vision Group on Science & Technology (VGST, Govt. of Karnataka 2019-2020).
2. Received **Seed Money for Young Scientist Research Program Award** from Vision Group on Science and Technology, Govt of Karnataka in 2014.
3. 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.
4. 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.
5. Life member of International Zeolite Association (IZA).
6. Life member of Catalysis Society of India (CSI).

STUDENTS

PhD Award:

1. Mr. Sathyapal Churipard R has been awarded PhD on the title “Synthesis and Characterization of Mesoporous Polymers and their Application in Adsorption and Catalysis” by Manipal Academy of Higher Education on February 16, 2021 under the guidance of Dr. Sanjeev P. Maradur. Associate Professor, Materials Science & Catalysis Division, PPISR.

PhD Students

1. Mr. Kempanna S. K.
2. Ms. Bhavana B. Kulkarni

Project Fellow

1. Mr. Puneeth Kumar MS.

RESEARCH:

INDUSTRY SPONSORED PROJECT: “Selective reduction of aromatics: Catalyst screening and process optimization” Aug 2020 to Jan 2021

Sponsored by: - Sravathi Advanced Process Technologies, Bengaluru

Principal Investigator: Dr. Sanjeev P. Maradur, Co-PI- Dr. G. V. Shanbhag

Research Student: Mr. Puneeth kumar M. S & Bhavana Kulkarni

The catalyst screening and process optimization work for the selective reduction of the aromatics had been undertaken and various commercial catalysts have been screened. The final technical report has been submitted with recommendations of how to take it further for process scaleup.

ACADEMIC PROJECTS

1. **Polyoxotungstate $[\text{PO}_4\{\text{WO}(\text{O}_2)_2\}_4]^{3-}$ Immobilized on Mesoporous Polymeric support for Selective Liquid-Phase Oxidation of alcohols using H_2O_2 ”**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Mr. Sathyapal R. C. & Mr. Kempanna S. Kanakikodi

Oxidation reactions are one among the most significant reactions in organic synthesis. However, they are amongst the most hazardous and problematic processes which often entail high E-factor and environmental risks. In the present study, we synthesized a mesoporous polymer supported peroxotungstate anion, $[\text{PO}_4\{\text{WO}(\text{O}_2)_2\}_4]^{3-}$ (PW4), and evaluated as a potential catalyst for green oxidation of alcohols using H_2O_2 . The concentration of quaternary functional groups in the material was varied to investigate the effect of hydrophilic environment on the substrate wettability and catalyst activity. The findings has been published in the international journal of high repute.

2. **Carboxymethylation of alcohols with dimethyl carbonate over solid acid catalysts under mild conditions**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Mr. Kempanna S. Kanakikodi & Mr. Sathyapal R. C.

Acid catalyzed carboxymethylation of alcohols is an emerging organic transformation that has grabbed the attention of the scientific community in recent years. In the present study, sulfonated mesoporous polymer (MP- SO_3H) is presented as a highly active solid acid catalyst to convert a wide range of alcohols into alkyl methyl carbonates. The catalyst is recyclable, resistant towards leaching and can be used in successive runs without losing the original activity. To the best of our knowledge, MP- SO_3H is the first solid acid catalyst to exemplify the highest activity for the synthesis of different alkyl methyl carbonates using DMC. The major findings of the research have been published in an international journal of high repute.

3. **Exploring the Acidity of Functionalized Mesoporous Polymer Catalyst (P-SO₃H) for Glycerol tert-butyl ethers Synthesis**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Mr. Kempanna S. Kanakikodi & Sathyapal R. C.

Etherification of glycerol with alcohols/olefins is of great importance in the chemical processing industry for the valorization of biomass feedstocks. In this

project, the functionalized mesoporous polymer (divinylbenzene-co-sodium p-stryrene sulfonic acid/ P-SO₃H) catalysts were synthesized solvothermally and characterized by different techniques to understand the physico-chemical properties. Etherification of glycerol with tert-butyl alcohol/isobutylene was studied in the high pressure stirred autoclave using P-SO₃H catalyst. The material exemplified the complete glycerol conversion with a very high yield of the desired product. The results achieved herein presented P-SO₃H as an efficient catalyst that can be used for the large-scale synthesis of potential additives for diesel. This work has been published in an international journal of high repute.

4. **Towards the upgrading of lignocellulosic biomass: An efficient approach for the synthesis of bio-fuel intermediates over γ -Alumina Supported Sodium Aluminate**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Mr. Kempanna S. Kanakikodi & Rama Bai

Synthesis of value-added chemicals from simple molecules originating from biomass is of great interest today. Herein, we presented a simple and green approach for the synthesis of γ -Al₂O₃ supported sodium aluminate (SA) catalysts for the aldol condensation of furfural with acetone. The catalyst 25SA/ γ -Al₂O₃ surpassed the activity of state-of-the-art materials reported for this transformation. This remarkable activity of the material is ascribed to its intrinsic properties such as the distribution of active sites over the high surface area, amount of basic sites, and inherent mesoporosity. The catalytic activity of 25SA/ γ -Al₂O₃ is superior among the screened materials. On top of it, recycling experiments have proven that the material is stable and resistant to the leaching of active sites. This work has been published in an international journal of high repute.

5. **Selective hydrogenation of Phenyl Acetylene to Styrene on Pd-supported Metal-Organic Frameworks**

Principal Investigator: Dr. Sanjeev P. Maradur and Dr. Suresh

Research Student: Mr. Kempanna S. Kanakikodi & Bakuru Vasudevarao

The selective removal of the acetylenic hydrocarbons from the olefins is a challenging task but crucial to achieve high purity monomers. Currently, this problem is solved by the hydrogenation of acetylene derivatives in presence of Pd and Ag based materials. Despite of high activity and selectivity, they are rapidly deactivated/poisoned by oligomers of the acetylene formed during the course of reaction. Therefore, it is still a challenging problem to find new approaches to the synthesis of highly efficient and selective hydrogenation catalysts. Pd/Hf-MOF demonstrated the good catalytic activity with high selectivity to the styrene. The reaction parameters are optimized to get the better conversion selectivity. The experimental part of this work is completed and preparation of manuscript is in progress.

6. **Carboxymethylation of bio-alcohols with dimethyl carbonate: effect of morphology on the catalytic activity of CeO₂**

Principal Investigator: Dr. Sanjeev P. Maradur & Co-PI- G.V. Shanbhag

Students: Kempanna S. Kanakikodi & Nagendra Kulal

An effective and highly selective protocol has been realized for the synthesis of asymmetric organic carbonates using dimethyl carbonate (DMC) as a reactant and solvent. Herein, the performance of CeO₂ nanostructures with different morphology was explored in the carbonate interchange reaction (CIR) of alcohols to synthesize asymmetric organic carbonates. The CeO₂ nano-catalyst with rod morphology having the highest oxygen vacancy enabled remarkable enhancement in the conversion, to the best of our knowledge this is superior to most of the reported heterogeneous catalytic materials. The CeO₂ was recovered by simple centrifugation and used in more than four recycles with consistent catalytic activity. Manuscript preparation is in progress and soon it will be communicated to a suitable journal for publication.

7. **Catalytic performance of MIL-101(Cr) metal-organic framework in nopol production by Prins condensation**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Bhavana B. K. & Kempanna S. K.

The conversion of pinenes into value-added chemicals is an interesting area of research. Nopol, a condensation product of β -pinene and paraformaldehyde, is an important starting material for the synthesis of fragrances and household products and also used in agrochemicals as a pesticide and as an aroma in soaps, detergents, and polishes. Herein, MIL-101(Cr) MOF catalyst was synthesized and used in Prins condensation of β -pinene and paraformaldehyde. The MIL-101(Cr) MOF demonstrated a high conversion of β -pinene (97%) with 99% selectivity to nopol under mild reaction conditions in contrast to reported catalysts. This superior catalytic activity of the material is ascribed to its high surface area and Lewis acid sites offered by unsaturated metal ions. Recyclability and heterogeneity tests have proven that the material is stable and resistant towards the leaching of active sites. The major findings of the project have been communicated to an international journal of high repute.

8. **Catalytic performance of MIL-101(Cr) metal-organic framework in nopol production by Prins condensation**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Bhavana B. K. & Kempanna S. K.

The conversion of pinenes into value-added chemicals is an interesting area of research. Nopol, a condensation product of β -pinene and paraformaldehyde, is an important starting material for the synthesis of fragrances and household products and also used in agrochemicals as a pesticide and as an aroma in soaps, detergents, and polishes. Herein, MIL-101(Cr) MOF catalyst was synthesized and used in Prins condensation of β -pinene and paraformaldehyde. The MIL-101(Cr) MOF catalyst was characterized by different techniques such as Powder X-ray diffraction analysis, BET analysis, TGA analysis, and FTIR. Different materials have been screened for nopol production and MIL-101(Cr) MOF demonstrated high conversion of β -pinene (97%) with 99% selectivity to nopol under mild reaction conditions contrast to reported catalysts. This superior catalytic activity

of the material is ascribed its high surface area and Lewis acid sites offered by unsaturated metal ions. The different reaction parameters such as, catalyst concentration, mole ratio between reactants, effect of temperature, effect of time, effect of solvents were optimized. Recyclability and heterogeneity tests have proven that the material is stable and resistant towards the leaching of active sites.

9. **One-pot hydrogenation-esterification of furfural with acetic acid over Pd@UiO-66 (Hf) metal-organic framework**

Principal Investigator: Dr. Sanjeev P. Maradur

Research Student: Bhavana B. K. & Kempanna S. K.

One-pot hydrogenation-esterification (OHE) of furfural to furfuryl acetate is a model reaction for upgrading of bio-oil which is typically catalyzed by composite or physically mixed bifunctional catalysts. The reaction scheme involves hydrogenation of furfural to furfuryl alcohol over redox metal sites and subsequent esterification with acetic acid over-acidic sites. Herein, Pd@UiO-66(Hf) MOF catalyst was synthesized and used in one-pot conversion of furfural to furfuryl acetate. The project is ongoing, and the manuscript will be communicated soon.

RESEARCH HIGHLIGHTS:

A) Published papers:

Total publications:**25**

Publications for the year 2020-21: **05**

B) Book Chapters

Publications for the year 2020-21: **01**

C) Papers Presented in Conferences/ workshops: 03

Total Best presentation awards for the year 2020-21: **01**

D) Other Scientific Activities

1. Technical Review meeting to discuss the proposal on "Development of a cost-effective process for the synthesis of mesoporous alumina" was held on 2nd December 2020. Dr. Maradur & Dr. Shanbhag from PPISR, Dr. K Raja, Dr. N V Choudray, Dr. Arun Basrur and Dr. P Satyanarayana Murthy from HPCL Green R&D were present during the meeting.
2. Dr. Sanjeev P. Maradur submitted a proposal on "Development of a cost-effective process for the synthesis of mesoporous alumina" to HPCL Green R&D Center Bengaluru for a Possible Project Funding 23rd December 2020.
3. Dr. G Jayaramanan and Prof. Rajanandam, Scientists from Kumar Organics Pvt Ltd (KOPL) had visited PPISR 19th March 2021 to discuss a possible sponsorship to work on catalyst and process development on the synthesis of 3,5-xyleneol. Dr. Sanjeev Maradur has submitted a preliminary proposal to KOPL and waiting for their approval.
4. Sravathi Advanced Process technologies Bengaluru sponsored project on Selective ring hydrogenation of aromatics was successfully completed. A final technical report has been submitted on 15th March 2021.



Dr. D. H. K. Murthy

Assistant Professor
Materials Science & Catalysis Division
E-mail: murthy@ppisr.res.in

Brief CV:

2020-Present: Assistant Professor, PPISR, Bengaluru, India
2019-2020: Research Fellow, Nanyang Technological University (NTU), Singapore.
2015-2019: AIST Special Researcher, National Institute of Advanced Industrial Science and Technology, (AIST) and Tokyo University in Japan.
2014-2015: Research Associate, CPMU, JNCASR, Bengaluru, India.
May 2009-Sep 2013: Ph.D. Candidate at Dept. of Chemical Engineering, Delft University of Technology (TU Delft), The Netherlands.

Research interests

Our research group innovates novel photocatalysts that exploit abundantly available solar energy to produce useful chemicals/fuels (NH₃, H₂, hydrocarbons, etc). Our strategy revolves around the artificial photosynthesis principle which can potentially transform various molecules to value-added chemicals and/or fuels via photocatalytic reaction. Few examples include sunlight-drive water splitting to generate green hydrogen, CO₂ reduction, nitrogen fixation to form ammonia, photocatalytic reforming of abundantly available biomass waste to form fuels/chemicals.

We emphasize revealing the correlation between the material properties (electronic, structural, surface and photophysical) and the photocatalytic performance/efficiency. Such rational insight will aid in the understanding of the factors limiting the efficiency of given materials while offering unique insight on how to further tune the materials properties. In this direction, we employ a range of computational and spectroscopy tools.

PhD Student

Ms. Sujana C

National & International collaborators

- Professor Kazunari Domen, Shinshu and Tokyo University, Japan
- Professor Akihiro Furube, Tokushima University, Japan
- Dr. M. S. Santosh, CSIR-Central Institute of Mining and Fuel Research (CIMFR)
- Professor Jayant K Singh, IIT Kanpur
- Professor Arnab Dutta, IIT Bombay
- Professor Jayaram Kolleboyina, IIT Jammu
- Dr. Satadeep Bhattacharjee, India-Korea science and technology (IKST) centre
- Professor Tom Savenije, Delft University of Technology, The Netherlands
- Professor Satyaprasad Senanayak, NISER, Bhuvaneshwar

Events and achievements

An industry project sponsored by Sravathi AI Technology, Bengaluru on the computational discovery of materials and active ingredients through machine learning (Jan 2021 to Jan 2022) was initiated Dr. D. H. K. Murthy as PI and Dr. Ganapati Shanbhag as co-PI.

An industry project sponsored by Sulzer-GTC Technology Inc, USA titled “Catalyst and process development for hydrocarbon synthesis via halogen mediation” was initiated by Dr. Ganapati Shanbhag as PI and Dr. D. H. K. Murthy as Co-PI in February 2021 for 1 year.

Delivered an invited talk as a resource person on “Let's go green: Hydrogen production and application to industries & energy sectors” conducted by Department of Chemistry, Sai Vidya Institute of Technology, Bengaluru on 23rd July 2021.

Participated as a Resource person during the Half-Yearly Research Review Meeting (RRM) Department of Chemistry, M.S. Ramaiah Institute of Technology (RIT) Bengaluru. Evaluated the performance of >20 Ph.D. students and suggested ideas/guidance to take their research forward on 10th July 2021.

Delivered an invited talk on “The status and prospects of green hydrogen to the energy sector” Department of Chemistry, M.S. Ramaiah Institute of Technology (RIT) Bengaluru on 10th July 2021.

Delivered a popular science talk to PUC and B.Sc. students of National College Bengaluru on the topic of Renewable Energy on 1st September 2021.

Publications

For the year 2020-21: **04**

Summer internship students

Ms. Jyosna Dsouza and Mr. Simon Galbao, M.Sc. students from St. Aloysius college, Mangalore spent two months investigating the synthesis and application of novel semiconductors (July - September 2021) for a range of photocatalytic reactions.

13. BIOLOGICAL SCIENCES DIVISION

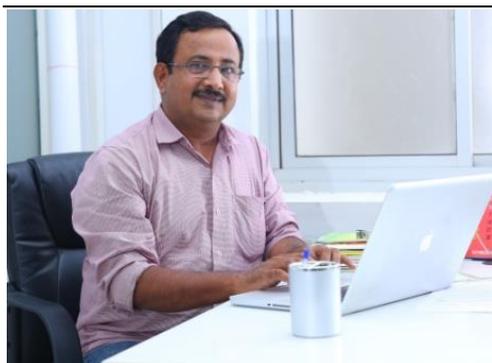
13.1 Mission and research progress

The Biological Sciences division was established in 2010 by the present director Prof. A. B. Halgeri together with support from executive committee members of AMEF. Currently, there are two groups, one headed by Dr. Udupi A. Ramagopal, a structural biologist, and the other by Dr. Ananda, K. a microbiologist. These groups work in the areas, such as cancer immunotherapy, purine and pyrimidine pathways of pathogenic microorganisms, the discovery of natural inhibitors for viral proteases, natural inhibitors for diabetic control, chemical modification of proteins for therapeutic purposes. Etc. The division possesses facilities for 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 assays are also available. The research activities in the department are supported by PPISR and as well as grants from government funding agencies such as the 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). We also work with pharmaceutical companies and conduct research to provide valuable input in the areas of our expertise. We also collaborate with national international researchers such as those from IISc and JNCASR, Bengaluru, IIT-Kharagpur, India, Albert Einstein College of Medicine, USA, MAHE Manipal, Mangalore University, NITK Suratkal and so on. Till today around 5 students have completed their Ph.D. from the Biological Sciences division registered under Manipal Academy of Higher Education (MAHE), Manipal. We have also contributed more than 25 protein structures to the worldwide Protein Data Bank (wwwPDB) and more than 35 fungal sequences and published more than 30 articles in reputed international Journals.

Major Areas of Research

1. Structural studies of viral proteases and discovery of natural inhibitors of viral proteases.
2. Structure-guided modification of T-cell costimulatory molecules to generate lead biologics to treat autoimmune disorders and cancer.
3. Structural and functional studies of antibiotic resistance-conferring methyltransferases and 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 Profile



Dr. Udupi A. Ramagopal

Associate Professor & Dean-Academics

Email: udupi.ramagopal@poornaprajna.org

Lab Website: <https://ppisr.res.in/udupi-ramagopal/>

H-Index= 29, I₁₀ index= 41, Publications =54, Citation/article ~ <60>

<https://scholar.google.co.in/citations?user=d7t9weUAAAAJ&hl=en>

Brief CV

- Associate Professor (2014 to 2020) and Dean Academics (2018-Current), PPISR, Bengaluru, India.
- Assistant Professor 2011 – 2014, (Ramalingaswami Fellow – DBT, 2011-2016), PPISR, Bengaluru, India.
- Visiting Faculty, 2011 – Present: Albert Einstein College of Medicine, New York, USA. <https://einsteinmed.edu/faculty/9276/udupi-ramagopal/>
- 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.
- PhD: Indian Institute of Science, India – 2001

Mentoring:

PhD Awarded: **1**

MS thesis: **4**

Post-doctoral trainees: **4**

Interns and trainees: **12**

Current PhD students (PI/Co-PI): **3**

Current Research Projects:

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

Modulation of T-cell co-stimulatory/inhibitory pathways has been proven to be one of the main immunotherapeutic approaches in the treatment of cancer. CD28/CTLA-4: B7-1/B7-2 family of molecules being one of the key proteins in the T-cell co-stimulatory/inhibitory pathway, they are the most explored targets for immune checkpoint inhibitors. This project aims at the structure-guided rational modification of human B7-2 and B7-1 proteins, to create economically viable and more efficacious

immune-modulator than the existing antibody-based drugs. Other than designing lead molecules for immunotherapy this project works on fundamental aspects such as oligomerization and their association into clusters, understanding of which plays a critical role in signalling. Towards this goal, we have done an extensive structural analysis of molecules involved in T-cell signalling and their preferred association into 1D and 2D cluster. Together with structural analysis, bioinformatics, biochemical and biophysical studies have revealed, how the clustering of cell-surface molecules, in some cases, hide the ligand-binding surface and avoid spurious signalling and produce robust and reproducible signals. While the research is of both fundamental and of medicinal importance in nature, such an endeavour requires facilities and collaborations to produce these molecules and to test *in vitro* and *in vivo* efficacy. We are looking for funding opportunities to pursue research in the area of exemplary importance.

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

Treatment of cancer has been given a new lease of life by immune checkpoint inhibitors since the early 2010s. Most of these immune checkpoint inhibitors are monoclonal antibodies and were found to be effective. Further, the majority of approved checkpoint-blockade antibodies are the blockers of this PD1:PD-L1/PD-L2 pathway and are found to be effective. This project aims at the structure-guided rational modification of PD-1, to create lead molecules that are expected to be more efficacious immune-modulators with fewer side-effects than the existing antibody-based drugs. To design these mutants, as a first step, we have done a critical analysis of structures of immune receptor complexes. It was observed that although IgV domains of antibodies and immune receptors share a very high structural similarity, the binding of IgV domain of immune receptor reveals specific differences in the mode of binding to their cognate partner in comparison to the interaction observed between the IgV domains of light and heavy chains of the antibody. This work has been published in the prestigious journal *Scientific Reports* (Nature group). Based on this analysis, we have created several mutants of PD-1 to mimic the function of anti-PD-L1 (PD-L1 is a cognate receptor of PD-1) antibodies. Biophysical experiments confirm that several of these PD-1 mutants are showing an expected higher binding affinity to PD-L1. The efficacy of these PD-1 mutants in the context of the cell should be tested and their ability to block PD-L1 should be ascertained yet.

Structural studies of viral proteases and structure-based identification of natural protease inhibitor

The aim of this project is to identify natural inhibitors of viral proteases using structure guided approach supported by biophysical and biochemical techniques. A recently developed method in the lab, wherein the inhibitor of interest can be selectively picked from the crude plant extract which will be used for the initial identification of the molecule of interest. Here, we have selected three proteases from virulent viruses, (1) Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), (2) Dengue virus (DENV) and (3) Kyasanur Forest disease virus (KFDV). The molecule

will be identified using mass-spectroscopy, X-ray diffraction and structure determination of the protease in complex with the natural inhibitor. The identified molecules will be purified in large quantity for other biophysical experiments and competitive assay.

Awards and Recognitions/Achievements

- Ramalingswami fellow, DBT, India (2011 - 2016).
- Best thesis “Kumari L. A. Meera Award and a Gold Medal”, 2001, IISc, India.
- Visiting Fellow (2001 – 2003, NIH, USA).
- Visiting Faculty (Albert Einstein College of Medicine, 2011 – current).
- 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/>), CCP4 workshops, crystallography workshops at RRCAT.
- Proposal reviewer: Macromolecular Crystallography, APS, Argonne National Laboratory.
- Served in the "User Executive Committee 2002-2003" of National Synchrotron Light Source, Brookhaven National Laboratory, USA.
- Jeffery Award (poster award - IUCr 2002, co-author).
- Contributed > 250 protein structures to Worldwide Protein Data Bank (wwPDB).
- The referee for various International Journals such as *Acta-D*, *Protein Science*, *BioChem Journal*, *Nature Scientific Reports*, *ACS Omega* and so on.
- Reviewer of a doctoral thesis from national research institutes like National Institute of Immunology (New Delhi), NISER (Bhubaneswar, India) and JNCASR (Bengaluru).
- Doctoral Advisory committee member for a few students registered under Manipal University and served as an external examiner/thesis reviewer for NIMHANS, JNCASR, NII, and NISER
- Scientific Advisor “Genelon Life Science Ltd.”, Yelahanka, Bengaluru
- Collaborated/collaborating with pharmaceutical industries working towards novel biologics for auto-immunity and cancer.
- Co-authored publications with Prof. James Allison, Nobel Laureate in Physiology and Medicine 2018.

Current PhD students

Ms. Swetha Lankipalli (Registered for PhD under MAHE, Manipal, Thesis submitted)

Mr. Shankar Kundapura (Registered for PhD under MAHE, Manipal)

Ms. Shrilakshmi (Co-PI, graduate student, registered under MAHE, Manipal)

Ms. Salima Parveen (Registered for PhD under MAHE, Manipal)

Project Fellows/trainees (2020)

- 1 Ms. Preeti Nayak
- 2 Ms. Manasa Upadhyaya

Alumni and Post-Doctoral Fellows

1. Dr. Raghurama Hegde 2012-2018-currently working at Elletra, Trieste, Italy)
2. Dr. Debayan Day :DBT-Research Associate and currently working at USA
3. Dr. Pavithra G. C.: currently working at NCBS, Bengaluru, India)
4. Dr. Srinivasulau :Currently working as Dr. K. S. Kothari postdoctoral Fellow, IISc

Grants:

1. Structure based rational design of PD-1 mutants to create lead molecules for cancer immunotherapy, Bristol Mayers Squibb, USA (ongoing/extension applied)
2. X-ray data collection and travel grant to synchrotron sources at (1) SOLEIL, France, ESRF, France (2 proposal approved), XRD2, Trieste, Italy (2 proposal approved) and X29 USA.
3. Bhat Biotech, India, Discovery of natural inhibitors of key proteins (2021-ongoing)
4. Ramalingaswami Fellowship titled “Co-stimulatory molecules: Biology and therapeutic intervention”, Department of Biotechnology (DBT), New Delhi, India (completed).
5. 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 (completed).
6. Structural and evolutionary investigations on antibiotic resistance-conferring rRNA methyltransferases for designing novel strategies of drug development, Department of Science and Technology, India.

NATIONAL AND INTERNATIONAL COLLABORATORS

- Prof. Steven C. Almo, Albert Einstein College of Medicine, New York, USA.
- Prof. Udaykumar Ranga, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.
- Dr. Dibyendu Samanta, Indian Institute of Technology, Kharagpur, India.
- Dr. Gaythri Mukharjee, Indian Institute of Technology, Kharagpur, India
- Dr. Deepak Kumaran Nair, Indian Institute of Science, Bengaluru, India.
- Prof. Hemalatha Balaram, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India.
- Prof. Ramakumar S., Indian Institute of Science, Bengaluru, India

RESEARCH INTEREST:

- (1) Modification of immune checkpoint blockade receptors for cancer immunotherapy.
- (2) Structural and functional characterization of enzymes from pathogenic bacteria.
- (3) *De novo* structure determination of proteins and methodology development in protein crystallization.
- (4) Discovery of natural inhibitor(s) for a medicinally important enzyme.

PUBLICATIONS:

Total publications: **55**

Publications for the year 2020-21: **05**

OTHER ACTIVITIES/ACHIEVEMENTS:

- Submitted research proposal for funding titled “Modification of PD1 to create lead molecules for check-point-blockade immunotherapy” together with co-PI, Dr. Gayathri Mukharjee, IIT-Kharagpur to Department of Biotechnology, India.
-
- Received Approval for the allotment of time at the beamline XRD2 at Elettra synchrotron Facility, Trieste, Italy and IISc/DST for the proposal titled “Novel role of Mtb surface protein LpqH and its mutants in host-pathogen interaction”
-
- Submitted an extension request with a completion report for the project “Structure-based rational design of PD-1 mutants to create lead molecules for cancer immunotherapy” to Bristol Myers Squibb, USA.
-
- Dr. Ramagopal and colleagues have used the new “remote single-crystal X-ray diffraction facility at the beamline XRD2, Trieste, Italy on 15th February 2015 for the first time and collected data on several crystals.
-
- Conducted the pre-PhD examination and Viva Voce as an external examiner for two PhD students from NIHMANS, Bengaluru
- Executed an MTA with the University of Oulu, Finland for CyDisCo plasmids, to express disulfide bridge containing protein in soluble form.
- Research collaboration made with Prof. Kanagaraja Sekar, IISc Bengaluru on MD simulation of IGF.
-
- Dr. Ramagopal submitted a manuscript titled: “How does ectodomains of membrane associated proteins stand upright and exert robust signal?” to BioRxiv <https://biorxiv.org/cgi/content/short/2020.07.29.226837v1>

Faculty Profile



Dr. Ananda K

Associate Professor

Biological Sciences Division

E-mail: ananda.at.poornaprajna.org;

ananda.at.ppISR.res.in

RESEARCH INTERESTS:

1. Natural Enzyme Inhibitors from plants and endophytic fungi for controlling type 2 diabetes

Metabolic disorders leading to one of the major problems like type 2 diabetes in recent years becoming a tough challenge all over the world. Amongst the plenty of oral drugs for type 2 diabetes, the partial inhibition of starch digesting enzymes such as alpha-amylase and intestinal alpha-glucosidase enzymes being focused to control the postprandial hyperglycaemia. These enzymes exclusively catalyse the hydrolysis of α -1,2, α -1,4 and α -1,6-glycosidic linkages in oligosaccharides and thereby release absorbable monosaccharides. Many of the plant extracts have been used in the treatment of diabetes because of their safety, low cost, more effective and availability. Hundreds of compounds have been purified from plants and being used to control glycaemic index. Extensive usage of medicinal plants might be endangered for few of the valuable rare plants. As an alternative for the medicinal plants, we are targeting endophytic fungi which are living inside these plants for the isolation of anti-diabetic compounds. Endophytes are known for the production of secondary metabolites similar to that of their host plants. In this regard we are isolating secondary metabolites from endophytic fungi and purifying inhibitors of digestive enzymes by *in-vitro*, *in-silico* and *ex-vivo* analysis. Further, we want to explore on the interactions of natural digestive enzyme inhibitors with genetically cloned, expressed and purified human enzymes.

2. Rational modification of Insulin to improve its half-life and other therapeutic properties

Treatment of type -1 diabetes can be done using the only drug Insulin. There are multiple analogues of insulins are available in the market, most of them are either produced by a genetic mutation or chemical modification. Our group at PPISR is also initiated similar activities where insulin is chemically modified by bioconjugation and selectively mutated to get genetic analogues of insulin using unique methods. Though there are many insulin analogues, the half life of these are not more than 24 hrs and few leads to other complications after long treatment. There is high demand for novel insulin analogues or for its modified forms which should have low production cost, lesser side effects and longer half life than any of the existing insulin in the market. We have achieved few interesting miles stones by generating new analogues and some are expected to throw some lights in diabetes treatment in near future.

3. Fungal laccase for the industrial and pharmaceutical waste detoxification

Laccases are multicopper oxidases found in plants and microorganisms. Fungal laccases are well studied as these are known to degrade different phenolic compounds present as contaminants in soil and water. Synthetic dyes including triphenyl methane class of dyes (Malachite green, crystal violet, aniline blue, acid violet, basic green and more) are extensively used in industrial processes like textile dyeing, biological stains, leather industries, paper colorants and many more. These dyes contribute momentous hazard as they are potent carcinogen to animals and confer toxicity to the growth of plants and micro-organisms as well. White-rot fungi are profuse producers of laccase which efficiently decolorize triphenyl methane dyes and we have found some interesting results from our recent studies. We would like to apply these laccases to produce some useful compounds like vanillin, curcumin

Training of Students:

PHD AWARDED	: 03
Guiding as PI/Co-PI	: 03
MSc Project completed	: 03
BSC/BE PROJECT COMPLETED	: 09
BSc Inspire students	: 03
PhD students in collaboration	: 03

RECOGNITIONS/ACHIEVEMENTS:

- Recognised as Visiting Professor of Dept. of Biochemistry, Mangalore University, Mangalore since 2020.
- PhD Co-coordinator at PPISR for Manipal University, 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 Award:

1. Ms. Kavitha K N awarded PhD on the title "Studies on Effect of Radiation on Laccase Producing Endophytic Fungi and Applications of Fungal Laccase" under Manipal Academy of Higher Education on July 20, 2020 under the guidance of Dr. Ananda K. Associate Professor, Biological Sciences, PPISR.

PhD students

1. Mr. Kirana M P
2. Ms. Shrilakshmi S
3. Ms. Shreya Kanth (Co-PI)

Project Fellows

1. Ms. Anusha , B.E, N.M.A.M. Institute of Technology, Nitte, Karkala,Udupi
2. Ms. Arye Sudershan, MSc. AMRITA VISHWA VIDYAPEETHAM, Kerala

RESEARCH:**SPONSORED PROJECTS (ongoing):**

1. “ α -amylase and α -glucosidase inhibitors from endophytic fungi for treating Type 2 diabetes” funded by VGST-Karnataka for 3 years.

ACADEMIC PROJECTS:**1. Inhibition of alpha-glucosidase enzyme and antioxidant activity of the metabolites purified from an endophytic fungus of *Simarouba glauca* DC. PI:**

Dr. Ananda K, Research Scholar: Mr. Kiran M P.

In the present study, an endophytic fungus showing AGI activity was isolated from the bark of *Simarouba glauca* DC., a well-known medicinal plant used traditionally against several ailments. The endophytic fungus was identified, cultured in lab scale for extracting its secondary metabolites and a highly active purified fraction was selected based on the AGI activity. Further, purified fraction was analysed by GC-MS technique and identified the possible AGI compounds with the help of database. The identified compounds were docked against the yeast and human AG enzymes and reported the best compound which has highest binding affinity.

2. A study on synthesis and evaluation of insulin-albumin conjugates with prolonged glycaemic control.

PI: Ananda K, Research Scholar: Shrilakshmi S

Insulin is the only drug available for the treatment of type -1 diabetes and advanced stages of type-2 diabetes. There are multiple analogues have been prepared and evaluated for their better properties based on the requirements. Some of these analogues are in the clinical studies and few are got FDA approval for treating diabetes in human. In this scenario, there are efforts are being made in chemical modification of insulin which includes bioconjugation. In this project we have planned to bioconjugate albumin with the insulin using different types of linkers. The plan was to keep multiple insulin molecules on the surface of albumin by conjugating through covalent linkage. Purpose of the idea is to keep the insulin in the physiological circulation for longer time than the normal insulin, the latter usually lasts for few minutes in the circulation otherwise. Further, in this proposal we are using both proteins are of internal origin and their bioconjugate products should not have any problem with the immune system. The albumin-insulin_n ((n=2-8) had good half life better than the native insulin and needs further authentications in animal models. The manuscript is prepared and need to be published.

3. Insight into the molecular docking analysis of natural compounds from Simaroubaceae family against alpha-amylase and alpha-glucosidase enzymes for the effective management of type 2 diabetes.

PI: Dr.Ananda K, Research Scholar: Mr.Kiran M P

There are more than 200 compounds have been isolated from the Simaroubaceae family and tested them for different diseases including to control diabetes. In this project we have analysed more than 200 compounds from the Simaroubaceae family for their alpha amylase and alpha glucosidase activity using the in-silico docking analysis. There are more than 5 compounds have shown very good drug like properties which have shown highest binding energy while with some of the seven tested enzymes. One of the alpha-glucosidase inhibitor identified by our earlier study also listed one among the best seven compounds and it has very good binding energy at least for 3 tested enzymes. The binding energy is better than the acarbose which is used as an standard drug control. The manuscript related to this is communicated to the journal for the publication.

4. Phylogenetic, sequence and structural analysis of Insulin superfamily proteins reveal an indelible link between evolution and structure-function relationship.

PI: Ananda K. Co-PI: Udupi A Ramagopal , Research Scholar: Shrilakshmi S

One of the objectives of this study was to learn, if any tolerable mutations could be borrowed from other ISP members to produce insulin mutants with improved therapeutic value. In fact, insulin Lispro marketed as *Humalog*, is a rapid acting insulin analogue produced by the swapping of the residues -B28Pro-B29Lys- to -B28Lys-B29Pro-. This swapping of -B28Pro-B29Lys- has been observed in IGF-1 naturally. Our analysis indicates that these swapped C-terminal residues of B chain is highly conserved across IGF-1 sequences, suggesting that borrowing mutation from close family members of insulin is an effective way to modify insulin. Considering ISPs have evolved from a single ancestral gene, it is possible that the evolutionary conservation and variations of residues among ISPs, could provide critical clues for rational modification of insulin with therapeutic value.

5. A study on the alpha-glucosidase inhibition and antioxidant activity of *Ensete superbum* (Roxb.) Cheesman seed: a GC-MS based profiling of the metabolites and molecular docking study against alpha-glucosidase.

PI: Dr.Ananda K, Research Scholar: Mr.Kiran M P

In the present golden era of biochemistry, metabolic engineering and understanding the natural product biosynthesis, the discovery of compounds from untapped natural sources can be one of the alternatives to the synthetic route of drug discovery. Within this circumstance, the present study aims to uncover the alpha-glucosidase inhibition (AGI) and antioxidant activities of *Ensete superbum* (Roxb.) Cheesman seed extract. The AGI activity of the crude extract and silica gel column purified fraction was excellent when compared to the standard acarbose . Also, the DPPH and ABTS

free radical scavenging ability of the purified fraction was comparable to the standard antioxidant; ascorbic acid. Among the five compounds identified from the purified fraction using the GC-MS technique, two compounds had very good binding energy against the C-terminal maltase glucoamylase (Ct-MGAM) and yeast alpha-glucosidase (YAG) enzyme. However, ADME/Toxicity evaluation of these five compounds revealed that the compounds would require further structural scrutiny and *in-vivo* studies before recommending them as an alternative to the present alpha-glucosidase inhibitors (AGI's) to treat T2D. The manuscript will be communicated.

6. Alpha-glucosidase inhibition and antioxidant activity of different extracts of *Simarouba glauca* DC.: HPLC based detection of gallic acid and quercetin in high active leaf extract.

PI: Dr.Ananda K, Research Scholar: Mr.Kiran M P

The *Simarouba glauca* plant is one of the well-known medicinal plants used for the ailment of various diseases such as cancer, diabetes, fever, etc. The extracts from leaves, fruits, seeds were prepared and tested for their anti-diabetic properties and anti-oxidant properties. Different solvents were used for the extraction of polar to non-polar compounds from the dry and raw materials. These extracts were analysed for the alpha glucosidase inhibitors and active extracts were further purified using column chromatography. The crude compounds are characterised using different biochemical assays and data is ready for publication.

7. Alpha-glucosidase inhibition activity and LC-MS/MS based metabolite profiling of *Daldinia* sp.: an endophytic fungus of *Ensete superbum* (Roxb.) Cheesman.

PI: Dr.Ananda K, Research Scholar: Mr.Kiran M P

Ensete superbum is a medicinally important plant has been extensively studied for their use in traditional medicine. Except the traditional usages, there have been no detailed studies on the biological properties of their endophytic fungi. Thus, the present study aims to disclose the endophytic fungi of *E. superbum* and their bioactivities. Among the endophytic fungi of *E. superbum*, one of the isolates was identified as *Daldinia* sp. which was studied in detail for its AGI and antioxidant activities. Also, the extract of *Daldinia* sp. was purified using silica gel chromatography and HPLC technique, and the plausible compounds which are responsible for its bioactivities were identified using LC-MS/MS analysis.

RESEARCH HIGHLIGHTS:

Published papers:

Total publications: 48

Publications for the year 2020-21: 04

Resource person/papers presented in conferences:

Total presentations: 26

For the year 2020-21: 01

Other Scientific Activities

1. Delivered eight lectures as visiting Professor to MSc students of Biochemistry at Mangalore University, Mangalore on “Diabetes and cancer biology” in the year 2020-21.
2. Ms. Shrilakshmi S cleared the CSIR-SRF interview and has been awarded the fellowship in February 2021.
3. Mr. Kirana MP was shortlisted for the CSIR-SRF fellowship under the Life Science group. And attended the interview on November 26, 2020.
4. Dr. Ananda K, has submitted a research proposal on endophytic fungi for bioactive compounds to “Vitaliz Biosciences Pvt. Ltd” a biopharmaceutical company for research collaboration and had three rounds of discussions and finalized proposal needs to be submitted
5. Research proposal titled “Production of recombinant human maltase-glucoamylase (MGAM) and discovery of inhibitors from medicinal plant *Simarouba glauca* and its endophytic fungi” was submitted to SERB India for the fund by Dr. Ananda K as Principal Investigator and Dr. U A Ramagopal as Co-PI in March 2021.
6. Dr. Ananda is a Co-guide for PhD Registration of Ms. Shreya Kanth, Dept. of Chemistry MIT, Manipal on the title “Synthesis and characterization of antimicrobial polymers and their coating studies” at MAHE, Manipal. PI’s (Dr. Yashoda M P) host institute (MIT, Manipal).
7. Ms. Shrilakshmi S and Mr. Kirana MP presented their Six months Ph.D. progress report on August 19th, 2020 to DAC members, and the report was sent to MAHE, Manipal.

RESEARCH COLLABORATION:

1. St. Aloysius College, Mangalore
2. Genelon Institute of Life sciences, Yelahanka, Bengaluru.
3. Department of Chemistry, Manipal Institute of Technology, MAHE, Manipal
4. Mangalore University, Mangalore

14. THEORETICAL SCIENCES DIVISION

Mission and research progress Theoretical science seeks to unravel the scientific and mathematical structure underpinning Nature and Her physical laws, and how these relate to the macro-world in a testable way. The broad research areas of the Division include quantum many-body and mesoscopic physics, nanoscience, quantum information theory, quantum foundations, and Solar physics. Currently, there are five PhD students in the group, Mr. Rahul S, Mr. Ranjith Kumar R and Mr. Y R Kartik with Dr. S. Sarkar and Mr Shrikant U and Mr Vinod N Rao with Dr R. Srikanth. Two students have already obtained their PhD with Dr. R. Srikanth, and a postdoc had worked under Dr S. Sarkar. The students were all hired under DST/SERB or DRDO projects. All of our former students have moved on either to postdoctoral work in eminent research groups or taken up faculty positions in a university.

The Doctoral Advisory Committee (DAC) members overseeing the current set of students are Prof. C. Sivaram (Emeritus, IIA, Bengaluru), Prof. B. S. Ramachandra (Director, CFRCE, Bengaluru), Prof. Rajeev Joshi (Dept. of Physics, Central University of Karnataka, Dharwad) and Dr S. K. Srivatsa (DEPA, Bengaluru), whose areas of expertise span theoretical astrophysics, black hole cosmology, soft condensed matter, and crystallographic studies.

14.1 Mission & Goals

- Probing the nature of the quantum state and correlations by operational means including cryptography and measurement disturbance, rather than a specific ontological framework.
- Exploring the interplay of topology and interactions in light-matter systems, and its specific manifestations such as Zak-Berry phase
- Exploring theoretical problems pertaining to practical quantum information processing, in particular in the context of quantum open systems and quantum cryptography.
- Temporal and spatial analysis of Solar supergranulation.

Glimpses of Current Research

- Quantum field theoretical study of interacting disordered systems
- General conditions for producing eternal quantum non-Markovianity of quantum channels.
- Counterfactual quantum cryptography
- Solitons and spin transport in an antiferromagnetic spin chain
- (Non-)Markovianity and channel singularities obtained by mixing Pauli qubit channels
- An interplay of topology and quantized geometric phase for two different symmetry-class Hamiltonians
- Fractal dimension of Solar supergranulation

14.2 Faculty Profile



Dr. Sujit Sarkar

Associate Professor

E-mail:sujit.tifr@gmail.com

BRIEF CV:

- Associate Professor, PPISR: Jan 2018 (cont..)
- Assistant Professor, PPISR: 2007 -- 2017
- Faculty Fellow, PPISR: 2005 -- 2007
- IISc Physics Department (1997-1998)
- Bar-Ilan University, Physics Department (1999-2000)
- Max-Planck Institute, Germany as a Guest Scientist (2000-2002)
- The Weizmann Institute of Science (2002-2005).
- Associateship position at S. N. Bose National Centre for Basic Sciences (since 2016 and continue)
- 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.

The physics of one-dimensional quantum many-body is interesting in its own right. One dimensional quantum many-body system has strong quantum fluctuations that do not allow spontaneously broken continuous symmetries. As a result of this, the pairing instabilities do not lead to any ordered density wave. This many-body has a critical phase with power-law decay of various correlation functions, universally known as a Luttinger liquid. In one-dimensional quantum, many-body systems whether it is the weakly correlated or strongly proper treatment of the quantum fluctuations leads in both cases to a Luttinger liquid characterized by phonon-like collective density fluctuation modes. In this process, there is a one-to-one correspondence between excitations of a one-dimensional free Fermi gas and free bosons. This can be used to attack the strongly interacting fermion problem by turning it into a weakly interacting boson problem via the method of bosonization followed by the quantum field theoretical renormalization group study. In the present study, we use the bosonization process to recast the model Hamiltonian in continuum field theory followed by the renormalization group method.

(2). Cavity Quantum Electrodynamics.

Recently there are few successful experimentations, where researchers have engineered the strong interaction between the photons and atoms in high-quality micro-cavities. This has created a platform to use the light-matter system as quantum simulators for many-body physics. Many interesting results are coming out to understand the complicated quantum many-body system. With this quantum simulator, quantum criticality in conventional condensed matter systems can be studied by manipulating the interaction between photons and atoms.

(3). Emergence of parity time-symmetric quantum critical phenomena

The emergence of different interesting and insightful phenomena at different length scale is the heart of the quantum many-body system. We show that the physics of parity-time (PT) symmetry is one new addition to them. We show explicitly that the emergence of different topological excitation at different length scale for the PT-symmetry system through the analysis of renormalization group (RG) flow lines.

(4). Emergent Quantum Phases for the Interacting Topological State of Matter.

Our study is based on the quantum field theoretical renormalization group (RG) calculations. The behaviour of the RG flow lines gives the emergence of different quantum phases for the non-interacting and interacting topological state of matter. We show the emergent of two different quantum phases, one is the Luttinger liquid phase and the other is the topological phase for the non-interacting topological state of quantum matter along with an exact solution. We show explicitly the emergence of another three different kind of quantum phases over the topological superconducting phase as a function of interaction and chemical potential. The most interesting emergent phase is the flat phase. We also show explicitly that higher values of strong correlation destroy the topological state of quantum matter. We also present the results of the scaling equation. We present explicitly the analysis of fixed point.

(5). Quantum Field Theoretical Study of Interacting Disorder System.

According to the presence or the absence of certain symmetries, we provide a detailed classification for the behavior of some physical quantities, like the density of states, the spin, and the quasiparticle charge conductivities. Following the original Finkel'stein approach, we finally extend the effective functional method to include residual quasiparticle interactions, at all orders in the scattering amplitudes. We consider both the superconducting and the normal phase, with and without chiral symmetry, which occurs in the so-called two-sublattice models.

RECOGNITIONS/ACHIEVEMENTS:

Seminars, Lectures, Workshops, and Conferences:

In this Covid-Period, I have not attained any offline conference/workshop /meeting. But I have attained several online seminar/mini-workshop across the world upon request. Especially my whole group has been benefited from the virtual PHHQ seminar participant.

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 nanoscales

Principal Investigator: Sujit Sarkar

Project Student: Mr. Rahul Sharma, Mr. Ranjith Kumar R, Mr. Kartik Y R

Progress: We have already been done six research work on this project. DST has already been sent the second installment of the fund.

Research Highlights:

(1). The hardest and beautiful problem of quantum many-particle physics is the quantum field theoretical study of interacting disorder system. My main area of research interest in this field to explore the effect of interaction on the calculation of scaling function for 10-fold different symmetry classes for the topological state of quantum matter.

(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 for the system lost periodic boundary condition.

List of Publications:

Publications for the year 2020-21: 09

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).
- (5). Prof. Prosenjit Singhdeo (S. N. Bose Centre)

Faculty Profile



Dr. R. Srikanth

Associate Professor

Theoretical Sciences Division

E-mail:srik@poornaprajna.org

RESEARCH INTERESTS:

1. Quantum information theory: Memory effects in quantum channels; mixing of (non-)Markovian channels, counterfactual quantum cryptography; entanglement dynamics in two-qubit systems; noiseless quantum attacks on cryptography, quantum hacking and privacy amplification.

2. Foundations of quantum mechanics: Operational characterization of quantum state reduction and nonlocality; study and classification of entanglement of quantum identical particles.

3. Solar physics: Latitude and rotation dependence of Solar supergranular fractal dimension; magnetic activity level across the Solar cycle and supergranular structure.

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

Training of Students:

PHD AWARDED	: 03
Guiding as PI/CoPI	: 05
MSc Project completed	: 02
BSC/BE PROJECT COMPLETED	: 07
PhD students in collaboration	: 02

RECOGNITIONS/ACHIEVEMENTS:

- Various invited talks and lectures. Most recently:
 - Presented at “National Conference on Contemporary Mathematics and Applications (NCCMA 2021)” a talk titled “Device-independent cryptography in operational quantum mechanics and generalized probability theories” dated 23rd October 2021.
 - Presented at Quantum Information and Computation: From Foundations to Applications -2021 (QFA-2021) from 18-23 October 2021a talk titled ‘Counterfactual security for quantum cryptography’
 - Presented at the National Quantum Symposium at IIIT Hyderabad a talk titled “Quantum non-Markovianity & Mixing quantum channels” 26th July and 3rd August 2021

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

STUDENTS

Current PhD students

1. Mr U. Shrikant: PhD awarded on Oct 12, 2021 on the topic of "ASPECTS OF NON-MARKOVIANITY IN OPEN QUANTUM SYSTEM DYNAMICS AND QUANTUM COMMUNICATION"
2. Mr 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)

PROJECT STUDENTS:

1. Mr Keertan Shetty (MAHE)
2. Mr Rohan Joshi (DTU, Delhi)
3. Mr Akhil Gupta (DTU, Delhi)

RESEARCH

Sponsored ACADEMIC PROJECTS:

1. Quantum non-Markovianity: characterization, measure, and resources

Principal Investigator: Dr. R. Srikanth

Funding Agency: MATRICS, DST/SERB, India

2. DST-QuEST project "Designing of Devices and Protocols for Quantum Hacking, Random Number Generation, and Secure Communication"

Investigators: Prof Anirban Pathak (PI), Dr. R. Srikanth (coPI)

Students: Mr Vinod N Rao and Ms Charu Gupta

Funding agency: DST-SERB

CURRENT PROJECTS:

1. Hierarchy of quantum corrections under non markovian dynamics :(along with postdoc Dr Paulson and prof. Subhashish Banerjee of IIT-Jodhpur) we investigate the dynamics of quantum correlation (QC) under the effects of reservoir memory, as a resource for quantum information and computation tasks. Quantum correlations of two-qubit systems are used for implementing quantum teleportation successfully, and for investigating how teleportation fidelity, violation of bell-cash inequality, quantum steering, and entanglement are connected with each other under the influence of noisy environments. Both markovian and non-markovian channels are considered, and it is shown that the decay and revival of correlations follow the hierarchy of quantum correlations in the state space. Noise tolerance of quantum correlations is checked for different types of unital and non-unital quantum channels, with and without memory. The quantum speed limit time is investigated from the perspective of memory of quantum noise, and the corresponding dynamics are used to analyze the evolution of quantum correlations. We establish the connection between information backflow, quantum speed limit time and dynamics of quantum correlations for non-markovian quantum channels.

2.Counterfactual quantum indistinguishability: (With student Mr Vinod N Rao) Indistinguishability and counterfactuality are two counterintuitive facets of quantum mechanics. The latter refers to the possibility of detecting a particle without an interaction, whilst the former refers to the indistinguishability of identical particles. Here we describe a unification of these two facets, whereby the blocking actions on an indistinguishable particle lead to a detection of another indistinguishable particle.

3.An eternally non-Markovian non-unital quantum channel is impossible:

(With student Mr Shrikant Utagi and Prof Subhashish Banerjee of IIT-Jodhpur) We show that a non-unital channel cannot be eternally non-Markovian (ENM), which we demonstrate with the generalized amplitude damping (GAD) channel. This contrasts to the case of unital channels, where an ENM Pauli channel is known. Under the circumstance, at best one can construct a quasi-ENM GAD channel, characterized by a time $t^* > t_0$ (where t_0 is the initial time) such that one of the two canonical decay rates remains negative for time $t \geq t^*$. We introduce an example of a quasi-GAD channel wherein the non-Markovianity occurs in the non-unital part.

4.Mixing qudit semigroups: (With Dr Vinayak Jagadish and Prof Francesco Petruccione of Univ. of Durban, South Africa) We study general conditions under which mixing non-invertible qudit channels produces semigroups. Further, we quantify the measure of channels obtained by mixing the three Pauli channels of a given non-invertible form, which are Markovian and non-Markovian.

5.Hide and seek with quantum resources: New and modified protocols for quantum steganography:

(with Prof Anirban Pathak (JIIT, Delhi), Dr Kishore Thapliyal (Palacky University, Czech Republic) and Students: Akhil Gupta and Rohan Joshi (DTU, Delhi) Steganography is the science of hiding and communicating a secret message by embedding it in an innocent-looking text such that the eavesdropper is unaware of its existence. Previously, attempts were made to establish steganography using quantum key distribution (QKD). Recently, it has been shown that such protocols are vulnerable to a certain steganalysis attack that can detect the presence of the hidden message and suppress the entire communication. In this work, we elaborate on the vulnerabilities of the original protocol which make it insecure against this detection attack. Further, we propose a novel steganography protocol using discrete modulation continuous variable QKD that eliminates the threat of this detection-based attack. Deriving from the properties of our protocol, we also propose modifications in the original protocol to dispose of its vulnerabilities and make it unsusceptible to steganalysis.

6.The operational reality of quantum nonlocality: whence no-signaling?

-- Does the remote measurement-disturbance of the quantum state of a system B by measurement on system A entangled with B , constitute a real disturbance -- i.e., an objective alteration-- of B in an operational sense? Employing information-theoretic criteria motivated by operational considerations alone, we argue that the disturbance of B is real in a class of steerable correlations. The main consequence of this observation is that it draws attention to the question of why QM is non-signaling. In foundational studies aimed at axiomatizing QM or characterizing it in the space of more general theories, no-signaling is generally taken to be an axiom inspired by relativistic signal locality. We point out why this does not seem appropriate in light of our result, in the process of revisiting the Einstein-Podolsky-Rosen paradox. Finally, we discuss a natural reason why one may expect QM or indeed any convex operational theory to be non-signaling: namely, to ensure the consistency between the properties of reduced systems and those of single systems.

Other research / academic highlights:

Dr U. Shrikant has been awarded his doctorate on Oct 12, 2021, and has since joined the group of Prof C M Chandrashekhara (IISc / IMSc) as a postdoc.

1. Our former student Dr Srikrishna Amkar was invited to join as a scientist with UK / Canadian quantum technology firm "Orca".
2. Our former student Dr S Aravinda has joined as Assistant Professor with the Physics Department of IIT Tirupati.
3. International collaboration with Dr Vinayak Jagadish and Prof Francesco Petruccione of University of Durban, South Africa)

List of Publications:

Publications for the year 2020-21: **10**

15. PPISR PUBLICATIONS (2020-21)

1. Kulal N., Vetrivel R., Ganesha Krishna N. S., Shanbhag G. V., Zn-Doped CeO₂ Nanorods for Glycerol Carbonylation with CO₂, (2021) *ACS Applied Nano Materials*, 4 (5), 4388-4397 DOI: [10.1021/acsanm.0c03166](https://doi.org/10.1021/acsanm.0c03166)
2. Kulal N., Vetrivel R., Gopinath C. S., Ravindran R. K., Rao V. N, Shetty M., Shrikanth R., Rangappa D., Shanbhag G. V., Green route for carbonylation of amines by CO₂ using Sn-Ni-O bifunctional catalyst and theoretical study for finding best suited active sites (2021) *Chemical Engineering Journal*, 419, 129439 DOI: [10.1016/j.cej.2021.129439](https://doi.org/10.1016/j.cej.2021.129439)
3. Vaishnavi, B. J., Sujith, S., Kulal, N., Manjunathan, P., Shanbhag, G. V., Utilization of renewable resources: Investigation on role of active sites in zeolite catalyst for the transformation of furfuryl alcohol into alkyl levulinate (2021) *Molecular Catalysis*, 502, 111361 DOI: [10.1016/j.mcat.2020.111361](https://doi.org/10.1016/j.mcat.2020.111361)
4. Manjunathan, P., Shanbhag, D.Y., Vinu, A., Shanbhag, G.V., Recognizing soft templates as stimulators in multivariate modulation of tin phosphate and its application in catalysis for alkyl levulinate synthesis (2021) *Catalysis Science & Technology*, 11, 272-282 DOI: [10.1039/D0CY01637C](https://doi.org/10.1039/D0CY01637C)
5. Chethana Aranthady, Teena Jangid, Kapil Gupta, Abhishek Kumar Mishra, S.D.Kaushik, V. Siruguri, G. MohanRao, Ganapati V. Shanbhag, Nalini G.Sundaram. Selective SO₂ detection at low concentration by Ca substituted LaFeO₃ chemiresistive gas sensor: A comparative study of LaFeO₃ pellet vs thin film. *Sensors and Actuators B: Chemical*. (2021) 329, 129211. DOI: [10.1016/j.snb.2020.129211](https://doi.org/10.1016/j.snb.2020.129211)
6. Sahu, P., Tincy, A., Sreenavya, A., Shanbhag, G. V., Sakthivel, A. Molybdenum Carbonyl Grafted on Amine-Functionalized MCM-22 as Potential Catalyst for Iso-Eugenol Oxidation (2021) *Catalysis Letters* 151 (5), 1336-1349. DOI: [10.1007/s10562-020-03388-5](https://doi.org/10.1007/s10562-020-03388-5)
7. Devi, K.R.S., Prasanna, V., D'sa, F., Shetty, K.R., Miranda, J. R., Pinheiro, D., Shanbhag, G.V., Response surface optimization and process design for glycidol synthesis using potassium modified rice husk silica (2021) *Materials Today: Proceedings* 41, 506-512 DOI: [10.1016/j.matpr.2020.05.234](https://doi.org/10.1016/j.matpr.2020.05.234)
8. Kempanna S. Kanakikodi, Sathyapal R. Churipard, Rama Bai and Sanjeev P. Maradur ,“Upgrading of lignocellulosic biomass-derived furfural: An efficient approach for the synthesis of bio-fuel intermediates over γ-alumina supported sodium aluminate” *Molecular Catalysis* 510 (2021) 111716
9. Chandrappa, S.; Murthy, D. H. K. et al. (as corresponding author), Utilizing 2D materials to enhance H₂ generation efficiency via photocatalytic reforming industrial & solid waste. *Environmental Research*, 2021, Volume 200, page 111239

10. Jagadeesh Babu, V.; Rao, N.V.; Murthy, D. H. K. et al., Significantly enhanced cocatalyst free H₂ evolution from defect engineered brown TiO₂, *Ceramics International*, 2021, Volume 47, page 14821-14828
11. Swetha Lankipalli and Udupi A. Ramagopal *. 2021, Structural perspective on design of decoy immune modulators, 2021, *Pharmacological Research*, 170, 105735.
12. Swetha Lankipalli, Mahadeva Swamy H. S., Deepak Selvam, Dibyendu Samanta, Deepak Nair and Udupi A. Ramagopal *. Cryptic association of B7-2 molecules and its implication for clustering. 2021, *Protein Science*, 2021, <https://doi.org/10.1002/pro.4151>, Impact factor 6.73.
13. Weifeng Liu, Ting-Fang Chou, Sarah C. Garrett-Thomson, Gooyoung Seo, Elena Fedorov, Udupi A. Ramagopal, Jeffrey B. Bonanno, Kiyokazu Kakugawa, Hilde Cheroutre, Mitchell Kronenberg, Steven C. Almo. HVEM structures and mutants reveal distinct functions of binding to LIGHT and BTLA/CD16, 2021, *Journal of Experimental Medicine*, 218 (12): e20211112.
14. Kavitha Keshava Navada and Ananda Kulal (2021). Kinetic characterization of purified laccase from *Trametes hirsuta*: a study on laccase catalyzed biotransformation of 1, 4-dioxane. *Biotechnology Letters* 43, 613-626.
15. Ranjith R. Kumar, Y. R. Kartik, S. Rahul, Sujit Sarkar. Multi-critical topological transition at quantum criticality. *Scientific Reports* 11, 1004 (2021)
16. Sujit Sarkar, A study of quantum Berezinskii–Kosterlitz–Thouless transition for parity time symmetric quantum criticality. *Scientific Report* 11, 5510 (2021) ;<https://doi.org/10.1038/s41598-021-84485-2>
17. Y. R. Kartik, Ranjith R. Kumar, S. Rahul, Nilanjan Roy, Sujit Sarkar. Topological quantum phase transitions and criticality in a longer-range Kitaev chain. *Phys. Rev. B* 104, 075113 (2021).
18. S. Rahul, Ranjith R. Kumar, and Y. R. Kartik and Sujit Sarkar. Majorana Zero Modes and Bulk-Boundary Correspondence at Quantum Criticality. *Journal of the Physical Society of Japan* 90, 094706 (2021).
19. Y. R. Kartik, Ranjith R. Kumar, and Sujit Sarkar, Quantum simulation of quantum BerezinskiiKosterlitz-Thouless transition for interacting light-matter system: A few exact solutions. *Journal of the Physical Society of Japan* 90, 114001 (2021).
20. Shrikant Utagi, Subhashish Banerjee, R. Srikanth, On the non-Markovianity of quantum semi-Markov processes *Quantum Inf. Process.* (2021; to appear) arXiv:2004.11208

21. Vinod N. Rao and R. Srikanth, Noiseless attack and counterfactual security of quantum key distribution., *Phys. Rev. A.*,104, 022424 (2021)
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Book Chapter

1. Shanbhag G.V., Kulal N., Vaishnavi B.J. Heterogeneous Catalysis for Chemical Fixation of CO₂ via Carbonylation Reactions. In: Goel M., Satyanarayana T., Sudhakar M., Agrawal D.P. (eds) (2021) Climate Change and Green Chemistry of CO₂ Sequestration. *Green Energy and Technology*. Springer, Singapore. DOI: 10.1007/978-981-16-0029-6_10 (Book Chapter)
2. Satyapal. R. Churipard, K. S. Kanakikodi, Sanjeev P. Maradur. "Metal Nanoparticles Supported Mesoporous Polymers: Realizing the Synergetic Effect to Achieve Superior Catalytic Performance", *Book Chapter Accepted for Publication in ACS Symposium Series: Advanced heterogeneous Catalysts Volume 1: Applications at the Nano-Scale* Chapter 16 (2020) 483-511,

16. New Recruitments

Students

1. **Ms. Madurya Gowda** has been enrolled for PhD Programme in Dr. Shanbhag group at PPISR in September 2020. She obtained her MSc (Organic Chemistry) from Dept. of Chemistry, Mysore University in 2019.
2. **Mr. Harsha Murudappa** completed his MSc with Analytical Chemistry specialization from St Joseph's College (Autonomous), Bengaluru in 2020 and joined as Research fellow under the guidance of Dr. Ganapati Shanbhag in a project sponsored by DNTL, Pune
3. **Mr. Rajashekhar Vaibhav** secured his MSc in Physics from Central University of Karnataka in 2020 and joined PPISR as Research Fellow under the guidance of Dr. Ganapati Shanbhag in a project sponsored by HPCL.
4. **Mr. Vithobha Hugar** obtained MSc from Indian Academy Degree College, Bengaluru in 2020 and joined as Research Fellow in Dr. Shanbhag's group to work in DNTL sponsored project in October 2020.
5. **Ms. Sujana**: Completed MSc from St. Joseph College, Bengaluru and joined as Research Fellow under the guidance of Dr.D.H.K. Murthy in 2020.

17. HIGHLIGHTS OF RESEARCH ACTIVITIES & ACHIEVEMENTS

PhD defence Viva and award

Ms. Archana K. M.: Ph.D. defence Viva of Ms. Archana K. M was held virtually on November 28, 2020 via Google Meet. The title of her thesis is "Design of alkali rare earth double tungstates for photoluminescence, electrochemical and theranostic applications". Dr. Vausdeva Siruguri, Director, UGC-DAE CSR, BARC, Mumbai center was the external examiner appointed by MAHE, Manipal. PhD Guide, Dr. Nalini Sundaram was the internal examiner. She received her PhD award from MAHE, Manipal.

2. Mr. Sathyapal R. Churipard: Ph.D. defence Viva of Mr. Sathyapal R. Churipard was held on February 16, 2021. He pursued research under the guidance of Dr. Sanjeev P Maradur, defended his thesis with the title "Synthesis and Characterization of mesoporous polymers and their application adsorption and catalysis". He received his PhD award from MAHE, Manipal.

Other Awards/recognitions

Dr. Sanjeev P. Maradur has been awarded the 'Award for Research Publication in Metallurgical & Materials Engineering Category from the Vision Group on Science and Technology, Govt of Karnataka for 2019-20

Ms. Marilyn E. D'Mello was selected as Winner of Dr. KVR Rao Scientific Society-Young scientist award in chemistry for 2020. It is highly reputed nationally known award given by Dr. KVR Rao Scientific Society, Hyderabad. It carries a citation and cash award.

Ms. Shrilakshmi S have been awarded the prestigious CSIR Senior Research Fellowship in February 2021

Mr. Shankar Kundapura received an award for science story communication organized by DST AWSAR for the story titled "Reprogramming the Immune System to Fight Cancer

Ms. Chethana A. received Best ORAL Presentation Award for the paper entitled "Selective SO₂ detection at low concentration by Ca substituted LaFeO₃ thin film sensor" in the 5th International Conference on Recent Advances in Material Chemistry (ICRAMC-2021) organized by Department of Chemistry, SRM University, Tamil Nadu, India during February 18- 20, 2021.

Mr. Kempanna S. Kanakikodi has got the best oral presentation" award at *International Conference on Advances in Material Science and Chemistry*" (ICAMSC) hosted by Department of Chemistry, Amrita School of Arts and Sciences, Amrita Vishwa Vidyapeetham, Amritapuri Campus, Kerala August 2020.

Mr. Kempanna S. Kanakikodi: presented his PhD colloquium, who was pursuing his PhD programme under the guidance of Dr. Sanjeev Maradur submitted his Pre-PhD thesis titled "Designing Functionalized Mesoporous Materials for Catalytic Conversion of Biomass Platform Chemicals to Value Added Products" on Feb 08 2021

Mr. Nagendra Kulal, pursuing research programme under the guidance of Dr Ganapati Shanbhag submitted his Pre-PhD thesis titled "Chemical fixation of CO₂ by converting into value added chemicals using heterogeneous catalysis" on March 18, 2021.

Mr. Shrikant Utagi, doctoral student, who is pursuing research under the guidance of Dr. Srikanth R., presented his thesis colloquium on "Aspects of non-Markovianity in open quantum system dynamics and quantum communication" was held on December 16, 2020.

Dr Udupi A Ramgopal's proposal to collect data of the crystals of LpqH protein was accepted by Elettra, synchrotron, Trieste, Italy and they have transported few LpqH: E-cadherin crystals to Trieste, Italy and collected several sets of data from their crystals remotely.

Dr. Ganapati Shanbhag was invited by Chemistry, Department, MVJ College of Engineering, Bengaluru to become a member of the Advisory Board and Member of the Research council of Department of Chemistry in March 2021.

Orientation Program: Seven new PhD students of Materials Science and Catalysis Division of PPISR are selected to participate in Orientation Programme in Catalysis organized virtually by NCCR, IIT-Madras, Chennai during January-May, 2021.

18. CONFERENCES/SEMINARS/WORKSHOPS

1. Dr. Ganapati V Shanbhag was invited as Speaker at Fifth Edition of Catalysis and Chemical Engineering during February 22-24, 2021, in San Francisco, CA, USA.
2. Dr. Maradur Delivered an invited talk in the webinar organized by Department of Chemistry, Presidency University on 7th September 2020.
3. Dr. D.H.K. Murthy gave an invited webinar talk on 19th August 2020 to students and faculties of Physics department at Reva university, Bengaluru. The title of the talk was "Realizing largescale and cost-effective solar H₂ production through photocatalytic water splitting"
4. Mr. Nagendra Kulal made ORAL presentation on "Utilization of CO₂ by converting into substituted urea using Sn-Ni oxide catalyst: Structure-activity correlation and mechanistic studies" in virtual UK Catalysis Conference 2021 during 6th – 8th January 2021 organized by The School of Chemistry and Chemical Engineering, Queen's University Belfast.
5. Ms. Vaishnavi B. J. made an ORAL presentation on the work titled "Valorization of bio-derived furfuryl alcohol to make furfuryl acetate over solid acid catalysts: Effect of acidity and porosity on activity" in virtual UK Catalysis Conference 2021 during 6th – 8th January 2021 organized by The School of Chemistry and Chemical Engineering, Queen's University Belfast.
6. Mr. Sujith S. presented a POSTER on "Transformation of bio-derived furfuryl alcohol to produce alkyl levulinate over zeolite catalyst" at the virtual UK Catalysis Conference 2021 during 6th – 8th January 2021 organized by The School of Chemistry and Chemical Engineering, Queen's University Belfast.
7. Ms. Chethana A. presented a POSTER entitled "Highly Efficient Chemiresistive CO Sensor Based On Nano Structured Ta₂O₅-SnO₂ Composite Material" in the International Conference on Nanoscience and Nanotechnology (ICONN 2021)

organized by Department of Physics and Nanotechnology, SRM IST, India during February 01 – 03, 2021.

8. Mr. Kempanna delivered an Oral Presentation titled “Carboxymethylation of Bio-alcohols with Dimethyl Carbonate: Effect of Morphology on the Catalytic Activity of CeO₂” in 7th UK Catalysis Conference (UKCC, 6-8th January 2021).
9. Mr. Nagendra Kulal and Ms. Vaishnavi B.J. delivered talks on Materials Characterization and Heterogeneous Catalysis respectively at the “Workshop on Orientation: Research & Development” for BSc undergraduates online organized by Poornaprajna College, Udupi from December 30, 2020 to January 1, 2021.
10. Dr. Ananda K. attended a three-day International virtual conference on ‘Plant specialized metabolism and metabolic engineering (PSMME-2020)’ organized by CSIR-CIMAP, India on 14-16 October, 2020
11. Ms. Marilyn DMello and Nagendra Kulal presented their research work for Dr. K. V Rao Scientific Society Award through online mode on June 13, 2020.
12. Mr. Kempanna delivered an Oral Presentation titled “Towards the upgrading of lignocellulosic biomass: An efficient approach for the synthesis of bio-fuel intermediates over γ -Alumina Supported Sodium Aluminate” at International Conference on Future Aspects of Sustainable Technologies (FAST 2.0) organised by Department of Chemistry, Central Institute of Technology (CIT), Kokrajhar, Assam, on 20-21st October-2020.
13. Mr. Kempanna delivered an Oral Presentation titled “Functionalised mesopolymers for the carboxymethylation of bio-alcohols: an efficient approach for the synthesis of alkyl methyl carbonates” at International Online Conference on Macromolecules (ICM) organized by School of Energy Materials (SEM), Mahatma Gandhi University, Kottayam, Kerala, on 13-15th November-2020.
14. Mr. Shankar was invited to give a presentation at the PES Institute of Technology, Bengaluru on the topic titled “*Rational modification of immune checkpoint receptors of PD-1 inhibitory pathway for cancer immunotherapy*” on 12th November 2020 via Microsoft Teams.
15. Mr. Kempanna’s abstract titled “Carboxymethylation of Bio-alcohols with Dimethyl Carbonate: Effect of Morphology on the Catalytic Activity of CeO₂” got accepted in 7th UK Catalysis Conference
16. Ms. Swetha L presented a talk on “structure based drug discovery” in the virtual research orientation workshop (ROW) to Poornaprajna college students, Udupi.
17. Ms. Shrilakshmi S presented a talk on “Revisiting Darwinism: examples of environmental adaptations across organisms” on December 30, 2020 in the

Virtual Research Orientation Workshop-2020-21 organised for Poornaprajna college, Udupi.

18. Mr. Shankar was invited to give a presentation at the PES Institute of Technology, Bengaluru on the topic titled “*Rational modification of immune checkpoint receptors of PD-1 inhibitory pathway for cancer immunotherapy*” on 12th November 2020 via Microsoft Teams.
19. Mr. Shankar Kundapura determined the high-resolution crystal structure (1.26Å) of lipoprotein LpqH from *Mycobacterium tuberculosis* and deposited the structure to Protein Data Bank (<http://www.wwpdb.org/>). The entry code for new structure is 7FDS.

19. INVITED LECTURES (Webinar)

1. Title: Principles & Applications of 3D printing.
Speaker: Dr Vikas Garg, o-Founder & CTO, Prayasta 3D Inventions Pvt Ltd, Pune
Date: Jan 04, 2021
2. Title: Introduction to process intensification
Speaker: Dr. M. Pimplapure
Date: Feb 15, 2021
3. Title: Introduction to IPR
Speaker: Mr. Varunraj Limaye and Dr. Venkatesh Seshan from K&S Partners, Mumbai.
Date: 8th October 2020
4. Title “Understanding Space, Time and causality: Modern Science and Ancient Indian Traditions “
Speaker: Prof Sisir Roy:
Date: Dec 01, 2020
5. Title: “Microbial Communication and Bacterial Intelligence”
Speaker: Professor Sisir Roy
Date: Dec 08, 2020
6. Title: Introduction to Patents and its applications
Speakers: Dr. Venkatesh and Mr. Varun of K&S Partners Mumbai
Date: Dec 10, 2020
7. Title: “Electron Microscopy for microstructure analysis – basics and applications”
Speakers: P. S. Sankara Rama Krishnan, School of EEE, Nanyang Technological University, Singapore,
Date: Dec 12, 2020

20. IN-HOUSE SEMINARS (Webinars)

1. Title: Physics and Material Science of Bionic Ear (Cochlear implant)
Speaker: D. H. K. Murthy
Date: Jan 22, 2021

2. Title: Viral protease as a drug target
Speaker: Ms. Salima Parveen
Date: Feb 10, 2021

3. Title: Recent Advances in Electrochemical Sensors for the Non-Invasive Detection/Real Time Monitoring of Drug Molecules
Speaker: Ms Chethana A
Date: Feb 25, 2021

4. Title: A study of quantum Berezinskii–Kosterlitz–Thouless transition for parity-time symmetric quantum criticality
Speaker: Prof Sujit Sarkar
Date: Mar 25, 2021

5. Title the Nobel Prize Physics 2020
Speaker: Mr. Rahul
Date: Oct 16, 2020

6. Title: “The physics of the Big Bull”
Speaker: Mr. Vinod Rao
Date: Nov 30, 2020

7. Title: “Importance of catalyst composition and reaction conditions”
Speaker: Dr R Vetrivel
Date: Nov 06, 2020

8. Title: CRISPR-Cas9: Genetic scissors that can reach where a surgeon’s scissors can’t Nobel prize in chemistry, 2020
Speaker: Ms. Swetha Lankipalli
Date:Nov 20 2020

9. Title: “Porous materials for CO2 capture, storage and catalytic applications”
Speaker: Ms Chaithra M
Date: Dec 29, 2020

10. Title: Desired Chemical Modification of Therapeutic Proteins: Challenges and Prospects
Speaker: Dr. Ananda K.
Date: September 4,2020.

21. EVENTS AND MEETINGS

Solar Power Plant Implementation and Inauguration

Karnataka Bank Ltd, under the CSR green initiative scheme, provided financial support of Rs 25 lakhs for installation of solar power plant at PPISR bidalur campus. In this context, one of the representatives from Karnataka Bank Sri Srinivasa Deshapande, Head, CSR, Karnataka Bank, Head Office Mangaluru visited PPISR and discussed about proposed area for installing the solar panels and prepared a proposal for a solar plant to be set up at our Bidalur Campus. The 48 kWp solar plant was planted with the help of M/s Avyaya Technologies Private Limited, Bengaluru. We were able to successfully install the photovoltaic solar power plant at our Bidalur Campus. This facility was inaugurated by Shri Mahabaleswara Rao, MD and CEO, Karnataka Bank Limited in the august presence of H H Sri Vishwapriya Theertha Swamiji on February 20, 2021

National Science Day:

National Science Day in commemoration to recall the great discovery of Prof.C V Raman was celebrated at PPISR on march 4, 2021. The programme started with the welcome address and inaugural speech by Director, Dr A B Halgeri. This was followed by the popular science talks by our doctoral students in all three divisions of sciences. Sri Sudjhindra Haldodderi, former scientist DRDO, former DGM- hal, and popular science writer was invited as the chief guest and he addressed all faculty members and students. Dr. Ramagopal gave the concluding remarks. Overall, this programme benefitted all the doctoral students of PPISR.

One Day programme on Introduction to Python

A One-day programme on Introduction to Python was organized at PPISR on Jan 10, 2021. Dr. Shreekant Jere conducted hands on class as a part of this programme and all students actively participated in this programme.

Virtual Research Orientation Workshop-2020-2021 for PPC undergraduates

Poornaprajna Institute of Scientific Research, Bengaluru and Poornaprajna college and post graduate centre, Udupi organized a 3-day workshop on orientation: research & development from 30-12-2020 to 01-01-2021 under Science Association and Internal Quality Assurance Cell via google meet. The programme was inaugurated with the blessings of His Holiness Sri Vishwapriya Theertha Swamiji, president, Udupi Sri Admar Mutt Education Council, Bengaluru. Dr. A. B. Halgeri, Director, PPISR, was invited as the chief guest for this programme. Dr. R. Srikanth Associate Professor, Theoretical Science was the coordinator for this webinar. This programme was well received by Poornaprajna College students and over all the programme was a grand success.

Project review meeting

1. A review meeting with Project Steering Committee sponsored by Hindustan Petroleum Corporation Ltd on “Catalyst and process development for CO₂ hydrogenation reaction” was conducted virtually on March 10, 2021. Dr. Ganapati Shanbhag made a presentation on the experimental part, whereas Dr. R. Vetrivel presented the DFT part of the work. From HPCL: Head R & D, S. Bharathan, G. M. B. Ramachandrarao,

Dr. G. Valavarasu, Dr. Santhosh Kotni and from PPISR, Dr. A. B. Halgeri, Dr. G. V. Shanbhag, Dr. R. Vetrivel, Dr. S. P. Maradur attended the meeting. The HPCL committee asked several questions and made some recommendations for the future work. Overall, the committee expressed satisfaction with the progress made in this project. 1st Annual Comprehensive report of this project was submitted to HPCL by PPISR.

2. A review meeting of the project sponsored by Hindustan Petroleum Corporation Ltd on catalyst and process development for CO₂ hydrogenation reaction was conducted with the Project monitoring committee of HPCL virtually on November 23, 2020. Dr. Ganapati Shanbhag made a presentation on the experimental part, whereas Dr. R. Vetrivel presented the DFT part of the work. The committee asked several questions and made some recommendations for the future work. Overall, the committee expressed their satisfaction with the progress made in this project.
3. The second-year review meeting of the CESEM project sponsored by VGST, Govt. of Karnataka was conducted virtually on December 2, 2020. Dr. Ganapati Shanbhag, Project coordinator presented the research conducted during the past one year. The review committee made several comments and suggestions and overall happy with the progress made in the project with three publications in reputed international journals.

HPCL Technical Review Meeting

Technical Review meeting was held on 2nd December 2020 in order to discuss the proposal on Development of cost-effective process for the synthesis of mesoporous alumina". Dr Maradur & Dr Shanbhag from PPISR, Dr. K Raja, Dr. N V Choudray, Dr. Arun Basrur and Dr. P Satyanarayana Murthy from HPCL Green R&D were present during the meeting.

Second DFT workshop organized by PPISR

Second two-day's workshop on Density Functional Theory (DFT) for computational catalysis was conducted by PPISR in a virtual mode as a part of HPCL collaborative project. The training on DFT was given to the researchers by Dr. R. Vetrivel, Hon. Professor, PPISR.

Honoring PhD awardees

In recognition of the excellent performance in research at PPISR with publications in highly reputed international journals, Dr. Vasudeva Rao, Dr. Archana K. M and Dr. Kavitha Navada, who received their degree in 2020; were honored by AMEF Chairman, HH Sri Vishwapriya Theertha Swamiji during the AMEF Board of Trustees meeting, which was held on December 5, 2020 at PPISR Sadashivnagar Campus.

PPISR Activity Forum

Recently students of PPISR initiated 'PPISR Activity Forum' which serves as a platform to nurture and showcase the hidden talents of all the members of PPISR in various fields. Various creative programs are being organized every month which includes paintings, sketches, write-ups, poems etc.

22. Poornaprajna Analytical Centre (PAC)

In order to strengthen technological infrastructure to carry out advanced research in various science disciplines under one roof and make their services available for the faculty and students to carry out globally competitive R & D in basic and applied sciences, PPISR has procured several analytical instruments namely Powder X-ray Diffractometer, Fourier Transform Infrared Spectroscopy (FTIR) Ultra Violet-Visible Spectroscopy (UV-VIS), Atomic Absorption Spectroscopy (AAS), Fluorescence Spectrophotometer, Temperature Program desorption (TPD) Analyzer and Surface Area Analyzer etc., that are necessary for general analysis. The aforementioned instruments are available for use mainly by the Scientists and the Research students at PPISR and our collaborators. This facility is also extended to all researchers from academic institutions and industries, to characterize their samples at nominal charges under the guidance of highly qualified PPISR staff. The following instruments are available for external users.

1	<p>Powder X-ray Diffractometer (PXRD) The D2 PHASER – table top X-ray Powder Diffractometer from Bruker is ideal for qualitative, quantitative and structure analysis of polycrystalline samples.</p>	
2	<p>Fourier Transform Infrared Spectroscopy (FTIR) The Bruker-alpha FTIR spectrophotometer is a compact instrument and measures the infrared spectrum, which represents the molecular absorption and transmission of a sample.</p>	
3	<p>Fluorescence Spectrophotometer The Varian Cary Eclipse Fluorescence Spectrophotometer is a compact instrument and measures the fluorescence, phosphorescence, chemi/bio-luminescence, and time resolved phosphorescence.</p>	
4	<p>Ultraviolet – Visible Spectroscopy The UV-Visible spectrophotometer from Perkin Elmer can be routinely used in <u>analytical chemistry</u> for the <u>quantitative</u> determination of different analytes such as <u>transition metal ions</u>, <u>highly conjugated organic compounds</u>, and biological macromolecules.</p>	

5	<p>Atomic Absorption Spectroscopy</p> <p>This instrument from Perkin-Elmer is used for the qualitative and quantitative determination of chemical elements employing the absorption of optical radiation (light) by free atoms in the gaseous state. In analytical chemistry, the technique is used for determining the concentration of a particular element (the analyte) in a sample to be analyzed.</p>	
6	<p>Temperature Program desorption (TPD) Analyzer</p> <p>BEL's new fully-automated catalyst analyzer, enables comprehensive catalyst study by using the techniques;</p> <ol style="list-style-type: none"> 1) Temperature programmed desorption (TPD) 2) Temperature programmed reduction (TPR) <p>BELCAT II will be the strong tool for the catalyst evaluation.</p>	
7	<p>Surface Area Analyzer</p> <p>BELSOPR-miniII is a compact, volumetric adsorption measurement instrument used for specific surface area and pore distribution measurement. Up to 3 samples can be measured simultaneously and independently with dedicated software, which makes operation of the instrument straightforward.</p>	
8	<p>Thermo Gravimetric Analyzer (TGDTA/DSC)</p> <p>STA6000 (Perkin Elmer) is Simultaneous Thermal Analyzer for simultaneous measurement and analysis of weight change and heat flow</p>	



Karnataka Bank Pvt. Ltd., Sponsored a 48kWp Solar Power Plant which was installed at the Bidalur campus, PPISR and was Inaugurated by Sri. Mahabaleswara M S, MD & CEO of Karnataka Bank



AMEF BOARD OF TRUSTEES MEETING



FOUNDER'S DAY CELEBRATION



PPISR Activity Forum meeting



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