POORNAPRAJNA INSTITUTE OF SCIENTIFIC RESEARCH



Annual Report 2013-2014



Recognized by Dept. of Scientific and Industrial Research (DSIR) and Manipal University Promoted and Managed by Udupi Sri Admar Mutt Education Foundation







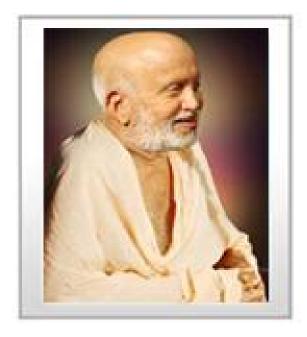








Founder's Message

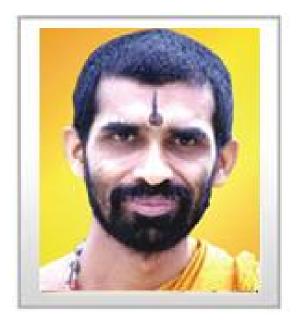


Knowledge is Power! Providing facilities to do research in the Pure Sciences has become very necessary. Our brilliant youth go outside the country to do research and settle there. Until we check this trend, India can't make real progress in any field. Hence the attempt to establish the Poornaprajna Institute of Scientific research (PPISR) under the guidance of many eminent scientists of

this country. More the investment by the nation in science and technology, 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 necessary strength to develop this institute for the benefit of the nation and the world.

> HH Sri Vibudhesha Theertha Swamiji, Founder Chairman, PPISR

Chairman's Message



The rishis in ancient India were indeed pioneering scientists, and may properly be called spiritual scientists, who investigated the laws behind this wonderful physical world we live in. Inspired by the ideal set forth by these ancient savants, my beloved Guruji and illustrious predecessor, HH Sri Vibudhesha Theertha Swamiji, conceived and constructed Poornaprajna Institute of Scientific Research (PPISR), to serve as the crest jewel among the Poornapraina family of schools and institutes founded bv him. He envisioned for scientific fundamental research to be undertaken here in the same free spirit of

curiosity that had marked the investigations of those ancient Upanishadic sages. Under the stewardship of the present administrative set-up, headed ably by Prof. A. B. Halgeri, the PPISR has witnessed in past four years a sea change in terms of improved research output, both qualitatively and quantitatively, and also in terms of infrastructural and laboratory development, assuring me that the institute will fulfill Swamiji's vision for it, thereby in good measure benefitting both Indian science and students in their service of the world community.

Through my informal and fruitful interactions with scientists and students at PPISR, I felt a need to bridge the gap between science and ancient Indian philosophy, to bring together scientists and saints, as it were. An initial step in this direction was taken by the founding of the Center for Foundational Study (CFS) last year. This year, an interesting development has been the discussions we have had to found a Center for the Advancement of Spirituality and Sciences (CASS), which will be responsible for transcribing, digitizing and archiving various manuscripts pertaining to Dvaita philosophy, as well as developing the requisite software for the same.

By the Grace of Lord Sri Krishna, may PPISR play a pioneering role in initiating this dialog between the physical and spiritual sciences!

H H Sri Vishwapriya Theertha Swamiji Chairman, AMEF

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Message from Hon. Secretary, AMEC / AMEF

Even while fulfilling his religious duties as the Pontiff of Sri Admar Mutt, Udupi, His Holiness Sri Vibudhesha Theertha Swamiji, maintained an avid interest in science interacting with scientists and sometimes even attending classes. He was keen on drawing comparisons between scientific and spiritual knowledge. Even though he founded about 30 Poorna Prajna Institutions all over the Country, Poorna Prajna Institute of Scientific Research established in Bidalur, Bangalore during 1998 is a crest jewel and the tangible symbol of love of a Saint for the Sciences. He envisioned PPISR as a forum for Scientists to pursue ninterrupted research and to provide training to young researchers



When H.H. Sri Vibudhesha Theertha Swamiji attained the Lotus Feet of Lord Sri Krishna, H.H. Sri Vishwapriya Theertha Swamiji, the present Pontiff of Sri Admar Mutt, Udupi, the President of AMEC and Chairman of AMEF, took up the task of guiding us through this journey that is both sacred and scientific. With the completion of the construction of the new Biological Wing and the nearing of the First Batch of our students towards completion of their Doctoral work, the first concrete step along the path laid by H.H. Sri Vibudhesha Theertha Swamiji has been achieved. This current year witnessed many milestones, which include PPISR crossing the 105 number of Publications in peer-reviewed journals of international repute, an achievement that is especially significant considering that it was achieved in a shorter time and with fewer faculty members when compared to many other better known institutes. While PPISR has begun its journey in pursuit of the noble vision set forth by H. H. Sri Vibudhesha Theertha Swamiji and guided most ably by H. H. Sri Vishwapriya Theertha Swamiji, it is a fact that all activities of PPISR are being funded mainly by AMEF. It is our fond hope that more members from the Corporate World and the General Public would come forward to contribute their mite to furthering this noble cause.

Bangalore 14th March, 2014 Dr. K. Srihari Professor (Rtd), UAS, Bengaluru Hon. Secretary, AMEC and AMEF This Page Intentionally Left Blank

Foreword from the Director



I have great pleasure in presenting the fourth Annual Report on account of research and academic activities of Poornaprajna Institute of Scientific Research (PPISR) for the year 2013-14. I had the privilege of taking this responsibility as the Director of this Institute four years back. We have been able to consolidate many of our academic activities in terms of establishing new scientific facilities. The journey of 4 years for me at PPISR, as a private, non-profit research organization, is an inspiring story which has its ups and down but has crossed all the hurdles and is moving ahead. In 2013-14 alone, the Institute has published more than 20

research papers in all areas of sciences and in overall, PPISR has crossed 104 publications in international peer reviewed journals which itself is a great achievement.

PPISR also strengthened industry-academic camaraderie by inviting several companies to the institute for mutually beneficial scientific interactions. Several new research projects have been initiated with sponsorship from industry and also Government agencies like VGST, DST, DBT, BRNS, etc. Currently, 15 doctoral students, 3 postdoctoral fellows, 3 project assistants are actively involved in many sponsored projects both from Government agencies as well as industry. We are also hoping that 9 students will be submitting their Ph.D. thesis to Manipal University by the end of December 2014. The Institute has made a significant achievement by successful completion of second year of sponsored research project of M/s. GTC Technology, USA. They have acknowledged our catalysis group in recognition of their dedicated research in the development of modified zeolite catalyst and also for enabling continued commercial exploration of this aromatic technology. M/s. GTC has generously supported for the extension of project for the third year.

The science outreach programmes with an aim of Today's Science for Tomorrow's scientist have been initiated with our Poornaprajna School students in Bangalore in order to create interest in basic science in young minds. Students from all five Poornaprajna Schools along with faculty members visited our campus and had interaction with our students and faculty members. Many of the students as well as faculty were quite impressed with our activities and have shown interest to pursue science as a research career. We have provided opportunities for young talented students to carry out research projects. We have also conducted Faculty Development Programme in Catalysis in association with Bangalore Institute of Technology and also Chemical Engineering Department of M S Ramaiah Institute of Technology. The participants gained knowledge in catalyst making and catalyst screening in batch mode and also industrial application of catalysis with our facilities at PPISR.

Based on our ongoing research projects, our faculty members and research scholars have all attended various National and International conferences and have won best presentation awards. Several distinguished Professors and scientists from both India and abroad visited our Institute and have given lectures. The infrastructure is being constantly upgraded to meet the academic requirement and for scientific and student activities. All these developments would not have been possible without the guidance drawn from H H Sri Vishwapriya Theertha Swamiji, excellent support from Admar Mutt Education Foundation Management and cooperation from the faculty members and students of PPISR.

Dr. A.B. Halgeri Director, PPISR

Board of Trustees

- 1. H.H.Sri Vishwapriya Theertha Swamiji (Chairman) Head of Admar Mutt
- Padmabhushana Prof. U.R. Rao, Former Chairman, Space Commission & Secretary, Dept. of Space
- 3. Sri Rajendra J. Hinduja Industrialist
- 4. Sri. V. V. Bhat, IAS, (Retd), Former Secretary to the Govt. of India
- 5. Prof. K.J. Rao FASC, FNA, FNASC Professor, SSCU, IISC, Bengaluru
- 6. Sri. B.R. Prabhakara, IAS, Former Chief Secretary Govt. of Karnataka
- 7. Sri. Laxmisha G. Acharya Industrialist
- 8. Prof. P. Rama Rao FASC, FNA, FNASC, Ex. Secretary, Ministry of S & T, GOI
- 9. Sri. K.R. Prasad, Advocate, Bengaluru.
- 10. Dr. U. Shankar Rao, Medical Director, National Hospital, Chennai
- 11. Dr. Gautham Nadig Director, Metahelix Life Sciences Pvt Ltd
- Dr. V.R. Prahalada Vice Chancellor, Defence Institute of Advanced Technology, Pune
- 13. Dr. K. Srihari (Hon. Secretary) Professor (Rtd), UAS, Bengaluru
- 14. Sri. M. Ashok Kumar, (Hon. Treasurer) Chartered Accountant, Bengaluru

Research Advisory Committee

Chairman

Dr. V.R. Prahalada, Vice Chancellor, Defence Institute of Advanced Technology, Pune

Members

Prof. T. M. Aminabhavi, CSIR Emeritus Scientist, Visiting Professor, Cambridge University, U.K

Prof. C. Sivaram, Professor, Indian Institute of Astrophysics, Bengaluru

Prof. K.R. Krishnamurthy, Chair Professor, National Centre for Catalysis Research, IIT Madras, Chennai

Prof. G. U. Kulkarni, Professor, JNCASR, Bengaluru

Padmashri Prof. N. Kumar, Emeritus Professor, Raman Research Institute, Bengaluru

Prof. A Jagannadha Rao, Professor, Rajaramanna Fellow; DST, Department of Biochemistry, IISc, Bengaluru

Prof. T.N. Guru Row, Professor, SSCU, IISc, Bengaluru

Prof. S. Ramakumar, Professor, Bio Informatics Centre, IISc, Bengaluru

Prof. A. B. Halgeri, (Member Secretary) Director, PPISR

Doctoral Advisory Committee

According to the UGC rules students registering under Manipal University for PhD degrees should have a doctoral advisory committee (DAC). Listed below are the members of DAC at PPISR for all the registered students in respective subjects who review every six months progress.

- 1. Prof. T. M. Aminabhavi, Karnataka University, Dharwad.
- 2. Prof. Y. S. Bhat, HOD, Chemistry Dept, Bangalore Institute of Technology (BIT).
- 3. Prof. B. S. Chandrasekhar, IISc, Bangalore
- 4. Prof. T. N. Guru Row, SSCU, IISc, Bangalore
- 5. Prof. B. S. Jai Prakash, Director, IEHMM, BIT campus, Bangalore
- 6. Prof. N. Kumar, Homi Bhabha Distinguished Professor, RRI, Bangalore
- 7. Prof. H. G. Nagendra, MVIT Engg. College, Bangaluru.
- 8. Prof. S. Ramakumar, Physics Dept., IISc, Bangalore
- 9. Dr. Raman Ravishankar, HPCL, Bangaluru
- 10. Prof. A. J. Rao, Biochemistry Dept., IISc, Bangalore
- 11. Dr. N. S. Raviraja, Stempeutics Pvt. Ltd., Manipal
- 12. Prof. S. A. Shivashankar, Materials Research Center (MRC), IISc
- 13. Prof. C. Sivaram, IIA, Bangalore University.
- 14. Prof. Udupi Ramagopal, PPISR, Bangalore
- 15. Prof. A. M. Umarji, SSCU, IISc, Bangalore
- 16. Prof. A. R. Ushadevi, Bangalore University
- 17. Prof. H. N. Vasan, SSCU, IISc, Bangalore

Administration

Director:	Prof. Anand B. Halgeri
Financial Advisor:	Sri P.Sreenivasa Rao
Scientific Staff:	Dr. Udupi Ramagopal
	Dr. Srikanth S
	Dr. Sujit Sarkar
	Dr. Ganapati V Shanbhag
	Dr. Nalini G Sundaram
	Dr. Ananda
	Dr. Raghu AV
	Dr. Sanjeev P Maradur
Administrative Staff:	
Administrative Officer:	Mr. Kishore L Gaikwad
Accountant:	Mr. Nagarajan R
Administrative Secretary:	Mrs. Latha Srinivasan
Support staff:	
	Mr Vishwaprakasha A (Electrical)

Mr. Vishwaprakasha A (Electrical) Mr. Praveen Kadam (Transport) Mr.Shashidara (chief cook)

Adjunct/ Honorary Faculty

Prof. S Asokan, IISc (Glasses & Sensors)
Prof. Y S Bhat, BIT (Catalysis)
Prof. T N Guru Row, IISc (Crystallography)
Prof. S A Shivashankar, IISc (Thin films)
Prof. B S Ramchandra, CFRCE, Bangalore (General relativity)
Prof. S K Srivatsa, PES University, Bangalore
Prof. Suryaprakash, IISc (NMR Studies)
Prof. T M Aminabhavi, UGC Emts Scientist (Polymers)
Prof. B S Jaiprakash, BIT/IEHMM (Catalysis)
Prof. K J Rao, IISc (Glasses & Ceramics)
Prof. K G Satyanarayana, Ex.Director, RRL (Polymers)
Prof. N J Shetty, Bangalore University (Genetics)

About the Institute

History and Mission

then

PPISR was conceptualized and founded by late HH Sri Vibudesha Theertha Swamiji, the chief pontiff of the Udupi Sri Admar Mutt to create а serene environment, questions, conducive to scientists to ponder basic scientific in much the manner that

India's ancient philosopher-The vision scientists did. for PPISR is of Swamiii interpreted to be: "To promote and nurture excellence in fundamental and applied sciences for the advancement of scientific knowledge and benefit of mankind".

The institute is situated at Bidalur, near the Bengaluru



International Airport on a sprawling area of 32 acres and is funded by Udupi Admar Mutt Education Foundation (AMEF). The foundation is a trust sponsored by the Admar Mutt Education Council (AMEC) and registered under the Karnataka Trust Act.

The AMEC is presently managing 27 Poornaprajna Education Institutions which have earned a name for themselves in providing quality education at school and college levels. A board of trustees consisting of eminent personalities was constituted to oversee the growth of PPISR. The present chairman, HH Sri Vishwapriya Theertha Swamiji has taken up the responsibility of fulfilling his Gurus dreams.

The foundation stone for the research campus was laid in 1998 by the then Prime minister of India, Sri A. B. Vajpayee. The first phase of buildings which provided office and laboratory space, also consisted of an auditorium with a capacity to seat 35 people and a modern kitchen. The building was inaugurated in May 2003 by the then deputy Prime Minister Sri L. K. Advani. The first phase of hiring of post-docs and faculty started in 2003. Initially faculty in Theoretical Sciences were hired.

Since, March 2010 Dr. Anand B. Halgeri, an eminent scientist from Reliance Petrochemicals, one of

India's top industries, took charge as Director of PPISR and achieved appraisable growth. The research campus located at Bidalur, Devanahalli attained fully functional research labs with the procurement of advanced research equipments during last three years. A Laboratory dedicated to synthesis of materials for the Materials Science has been built and inaugurated in the first year. Recently biological science facility laboratory is built for the future research and inaugurated by Sri Vishwapriya Theertha Swamiji.



There are three divisions, (A) Theoretical Sciences, (B) Materials Sciences, and (C) Biological Sciences under PPISR where research programmes of advanced nature are in progress. There are nine core faculty members working in materials science, biological sciences and in theoretical sciences in different research filed. All the faculty members are trained in advanced research labs in abroad to conduct applied research. The research laboratories are well equipped with state of the art instruments to give every advantage to the students and faculty pursuing research here. In addition to research, PPISR is conducting outreach activities to develop innovative and imaginative platform for research in young minds of school and college students.

There are distinguished professors from other renowned institutions such as IISc, RRI, BIT, Bangalore University etc, graciously helping PPISR as adjunct and honorary professors. A research advisory committee formed to review and guide the overall progress of the research undertaken by different faculty at PPISR.

The mission of PPISR is to carry out world-class quality research in both basic and applied science involving multidisciplinary collaborations nationally and internationally and thus help graduate students reach their full potential by providing research guidance and technical skills required to live and work in a complex technological society. PPISR also aims to develop teaching material for core courses in Physics, Chemistry and Biology in order to strengthen the basic foundations of science in doctoral students.

The institute is recognized by DSIR, Govt. of India, New Delhi. PPISR is also recognized as a research centre by Manipal University (MU), Manipal, Karnataka. Further all the faculty members are recognized as official PhD supervisors of MU and 12 students are registered for their PhD degrees with Manipal University.

Contact details:

- City office : Poornaprajna Institute of Scientific Research No 4,16th Cross, Sadashivnagar, Bangalore- 560 080 Karnataka, India. Phone: 080-2361 1836
- Main campus: Poornaprajna Institute of Scientific Research , Bidalur(post), Devanahalli, Bangalore - 562 110.Karnataka, India. Telephone: 080-2760 7242 Website: http://ppisr.res.in

Administrative Officer: admin@poornaprajna.org

Division Structure

FACULTY

Materials Science

Dr. A B Halgeri (Catalysis) Professor and Director

Dr. A V Raghu (Polymers) Asst. Professor

Dr. G V Shanbhag (Catalysis) Asst. Professor

Dr. Nalini G Sundaram (Nanomaterials) Asst. Professor

Dr. Sanjeev P. Maradur (Catalysis) Asst. Professor

Biological Sciences

Dr. U A Ramagopal (Structural Biology)
Associate ProfessorDr. Raghurama P Hegde (Research Associate)
Ms. Pavithra G C (Research Scholar)
Ms. Swetha L (Research Scholar)Ramalingaswami FellowMr. Sathish L (Research Scholar)Dr. K Ananda (Mycology)
Asst. ProfessorMr. Sathish L (Research Scholar)
Ms. Pavithra N (Research Scholar)

Theoretical Sciences

Dr.Sujit Sarkar (Quantum physics)
Asst. ProfessorDr. Kallol Roy (Research Associate)
Mr. Chandan G N (Research Scholar)Dr.R Srikanth (Quantum Information)
Asst. ProfessorMr. Omkar Srikrishna (Research Scholar)
Mr. Aravinda S (Research Scholar)

Mrs. Swetha Sandesh (Research Scholar, SRF)

Mr. Suhas D P (Research Scholar, SRF)

Mr. Vijay Kumar S M (Research Scholar) Mr. Janardhan H L (Research Scholar) Mr. Manjunathan P (Research Scholar) Mr. Prashant Kumar (Project Assistant) Mr. Karthik (Project assistant) Mr. Santhosh Kumar (Project Assistant)

Dr. Sowmya Palimar (Research Associate) Ms. Swetha S M (Research Scholar, SRF) Mr. Srinidhi R (Research Scholar) Mr. Pradeep Shanbogh (Research Scholar)

Mr. Dundappa (Research Scholar)

Materials Science

Introduction

Established in May 2010 by the present Director, Prof. A. B. Halgeri, with the assistance of Prof. K. J. Rao, then Chair, Executive Committee of AMEF, the department now consists of a core of five faculty members hailing from diverse background as chemistry, industrial chemistry and biochemistry. Shortly, a new materials synthesis laboratory, with several sophisticated equipment, was established in the group. Bright students passionate for research were interviewed and inducted into Doctoral Program in the Department. The mission of the department is two-pronged:



1. To forge a fruitful academia-industry partnership by innovating,

designing and developing novel multifunctional materials that have wide-ranging applications, in catalysis, nanotechnology, etc.

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

The department engages with other national academic institutions through collaborations, education training and outreach activities.

The broad areas of the department include: (1) Novel functional materials: Novel (2) micro/mesoporous materials for green chemical processes; (3) Biomass conversion to value added products; (4) X-ray crystallographic studies; (5) Crystal engineering; (6) Ceramic materials and functional glasses; (7) Liquid crystal studies; (8) Thin film studies; (9) Polymers.



Academic and Research Highlights

Catalysis group: Catalysis group of Dr. G. V. Shanbhag and Dr. Sanjeev Maradur presently consists 4 research scholars and 4 project assistants with 2 industry sponsored research programmes. The group is working on frontier areas of research such as pore engineering of microporous materials; design of new acidic, basic and bifunctional materials for eco-friendly organic transformations; biodiesel synthesis from non-edible vegetable oils such as honge, jatropha, simarouba and waste cooking oil; bioglycerol transformation into value added products such as solketal, glycerol carbonate and tertbutyl glyceryl ethers. Novel pore engineering techniques were developed for microporous materials such as ZSM-5 and zeolite beta for enhancing the shape selectivity for commercially important products such as para diethyl benzene (PDEB), 6-acetyl-2-methoxynaphthalene from respective alkylation and acylation reactions. Dr. Shanbhag and group recently published an article in RSC Advances journal where zinc hydroxy stannate was reported for the first time as bifunctional heterogeneous catalyst. Another academic programme, "metal ion exchanged zeolites as novel efficient catalysts for the synthesis of nopol by Prins reaction" also submitted for publication to an international journal.

The research work carried out by Catalysis group of PPISR has been getting recognized in National conferences and workshops. Poster Presented by Vijaykumar on "Tin (II) hydroxychloride: A Novel Solid Brønsted Acid Catalyst for Selected Condensation Reactions" at 16th National Workshop on "Catalysis for Sustainable Development" at Nagpur, Maharashtra on 4-5, February, 2014 won the best presentation award. Three other students from Materials Science also showcased their work at this workshop

Second year of GTC, USA sponsored industry project on "Novel catalyst development for aromatics technology" was successfully completed and third year project programme was initiated from 1st October. One catalyst was finalized for scale-up operations to further explore commercial exploitation of the process. The sponsored project from Shell Technology Centre, Bangalore also finished one year in August after fulfilling the tasks given by the collaborator.

Third industry project sponsored by HPCL R & D centre also completed one year in October 2013 with part of the research work was filed for joint Indian and world patent (PCT). Catalysis group also had several technical review meetings for the above projects with the top scientists of the respective collaborators which helped the group to improve the quality of research.

Functional Energy Nanomaterials Group: Dr Nalini and her group works on functional nanomaterials. Project entitled Solid state synthesis of a new n=2 Aurvillius Sillen phase for Photocatalytic Degradation of Dyes is ongoing.

A new oxychloride phase belonging to the Aurivillus-Sillen structure type has been synthesized at different temperature and different time. XPS measurement has been conducted in order to confirm CI present in the matrix. The phase shows good photocatalytic activity for the degradation of dyes in UV light. At present growing good single crystals to elucidate the crystal structure is in progress. Simultaneously, high resolution neutron diffraction data has also been obtained from the instrument SPODI at M LZ, Garching, Germany under the rapid access program. Another project Influence of the alkali metal ions on the crystal structure and photoluminescence of rare earth double tungstates synthesized by glycothermal technique is ongoing. A manuscript has been communicated on Synthesis & Characterization of Substituted Metal Acetylacetonate and Anthranillate complexes, and their application to the preparation of Nanomaterials.

Functional Polymers Group: Dr. Raghu's group actively works in the area of developing novel polymeric membranes for pervaporation applications. A BRNS sponsored project entitled "Effect of Electron Beam Irradiation on Polymeric composite Membranes for Pervaporation Separation Application" has been initiated with the hiring of JRF. A manuscript entitled "Graphene loaded Sodium alginate Nanocomposite Membranes with Enhanced Isopropanol dehydration performance via Pervaporation" has been accepted for publication in RSC Advances. A manuscript has been communicated on Pushing the limits of pervaporative dehydration of isopropanol using organically modified clay composite membranes of sodium alginate.

Following the success of our graphene filled sodium alginate membranes, we are now involved graphene oxide with chitosan polymers. The reason for choosing chitosan is, being a cationic polymer can offer electrostatic interaction along with, its regular hydrogen bonding interaction with graphene oxide. Membranes with various graphene oxide loading were prepared and characterized by FTIR, XRD, contact angle measurements, FE-SEM analysis, sorption experiments and Optical Profilometer studies in order to understand physico-chemical properties of the membranes. Performance evaluation studies of the prepared membranes for ethanol dehydration and Optimization studies are under progress

Faculty Profiles



Dr. A. B. Halgeri Professor Director, PPISR.

Educational Qualifications

1. Masters Degree in Chemistry from Karnataka University, Dharwar

2. Ph.D fin Physical Chemistry (Heterogeneous Catalysis) from Bangalore University

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

Broad areas of research

He has extensively worked on Alkylation of Aromatics using modified Zeolites as Eco-friendly catalysts. He has developed Zeolite based catalyst for Alkylation of Toluene to produce selectively para-Xylene which is raw material for polyester industry and transferred for the first time to advanced country to M/s. GTC Technology Inc. USA. Subsequently, super selective pore size engineered modified Zeolite catalyst has been successfully developed and commercialized for the manufacture of specialty chemical para-diethyl benzene (PDEB) of 10,000 MTS capacity plant at Reliance Petrochemicals Industry at Surat, Gujarat. After the merger of Indian Petrochemical Corporation Ltd (IPCL) with Reliance Industry Ltd, he had provided sustained leadership as Vice President and Head of R&D, Baroda, led a team of 150 Scientists/Engineers and coordinated the entire research and development activities for Petrochemical/Refinery catalysts, Polymer Science and Technology, Materials Science and Applied Biology groups for all Reliance Industries at different locations. He also worked as Senior Scientific Advisor at Reliance Research & Technology Centre at Navi-Mumbai.

After his post-doctoral work on Zeolite Catalysis as applied to Chemical Technology with Prof. Y. Ono at Chemical Engineering Department of Tokyo Institute of Technology during 1973-75, he returned to India, and joined in a newly established Research Centre of Indian Petrochemicals Corporation Ltd (IPCL), Baroda, Gujarat in 1976. He was involved in the development and commercialization of Zeolite based catalyst for Xylene Isomerisation process in 1985, the first petrochemical catalyst developed in India. He was also associated in the development and manufacture of several petrochemical catalysts from concept to commercialization. He has provided leadership for the development of reforming catalysts for Gasoline & BTX production, paraffin-dehydrogenation catalysts for Linear Alkyl Benzene (LAB) production (Raw material for soap manufacture), catalysts for petrochemical industry. All the above indigenously developed catalysts helped to put India in the world map of petrochemicals.

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

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

2. Hari Om Ashram Prerit Prof.S.S. Bhatnagar Endowment Research Award for Excellence in Applied Catalysis. Lifetime Achievement Award Eminent Scientist in Catalysis by the Catalysis Society of India, Indian Institute of Technology, Madras.

3. Elected as Fellow of Institute of Chemical Engineer by Indian Institute of Chemical Engineers, Kolkata.

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

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

6. Awarded as "Pride citizen of Baroda" in recognition of significant contribution for Science & Technology from Community Science Centre/Rotary Club of Baroda - 2008.

7. He has been advisory member of several professional bodies, Department of Science & Technology, CSIR, IOCL (R&D) and Reliance Industry. He has traveled widely and presented several invited lectures in both National and International symposia.

He has published over 105 Research papers in peer reviewed national and international journals and has obtained 35 Indian/International patents. He has been life member of many scientific and professional bodies both in India and abroad.

He is currently working as Director of Poornaprajna Institute of Scientific Research and coordinating the entire research activity in Theoretical Science in Physics, Mathematics, and also expanding to new areas Materials science & Biological sciences. His area of interest includes Nano catalysis, Heterogeneous catalysis, mesoporous materials, novel Zeolites, Solid Acid Catalysts, Industrial Refinery/petrochemical processes, adsorption, Eco-friendly processes, and Biodiesel/Biofuel, alternate energy feed stocks etc.

Students

- 1. Mrs. Swetha Sandesh (along with Dr. G. V. Shanbhag)
- 2. Mr. Vijay M. (along with Dr. G. V. Shanbhag)
- 3. Mr. Janardhan H. L (along with Dr. G. V. Shanbhag).

Projects

Prof. Halgeri is actively involved in the industrial projects along with Dr. G. V. Shanbhag and Dr. Sanjeev, and in particular, is responsible for getting sponsorships from the companies GTC, HPCL and Shell.

Dr. A.V. Raghu, Assistant Professor



Phone: 080-2740 8552 Email: raghu.AT.poornaprajna.org gsraghu2003.AT.yahoo.co.in Webpage: poornaprajna.org/raghu

Area of Interest

- Polymeric-graphene based nanocomposite membranes for Pervaporation Separation Applications
- Development of Polymeric Proton Exchange Membrane for Fuel Cell Applications
- Design of Hybrids Photovoltaics of Future "Inorganics in Organics"
- Development & Evaluation of Novel Polymeric Particulate Drug Delivery Systems
- Synthesis & Characterization of Novel Polymers

Curriculum vitae:

- > 2011 Present: Asst. Professor, PPISR, Bangalore, India.
- > 2008-2011: Manager, Reliance Industries Limited, Mumbai
- > 2007-2008: Postdoctoral Scientist, Department of Chemistry, University of Ulsan, South Korea
- > 2002-2007: Lecturer, Center of Excellence in Polymer Science, Karnatak University, Dharwad

Representative publications

1. D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu,* "Graphene-loaded sodium alginate nanocomposite membranes with enhanced isopropanol dehydration performance via pervaporation technique". **RSC Advances**, 2013, **3**, 17120-17130.

2. D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu^{*}, "Synthesis and characterization of novel polyurethanes based 4,4'-{oxy-1,4-diphenyl bis(nitromethylidine)} diphenol Schiff base hard segment", Polymer Engineering and Science, 2014, 54, 24-32.

3. D.P. Suhas, T.M. Aminabhavi, A.V. Raghu,* "Mixed Matrix Composite Membranes of H-ZSM5 Loaded Poly(vinyl alcohol) Used in Pervaporation Dehydration of Alcohols: Influence of Silica/Alumina Ratio" Polymer Engineering and Science, 2013, Accepted, online

4. D.P. Suhas, T.M. Aminabhavi, A.V. Raghu,* "para-Tolune sulfonic acid treated clay loaded sodium alginate membranes for enhanced pervaporative dehydration of isopropanol" Submitted to International Journal. 2014

5. A.V. Raghu*, H.M. Jeong, "Synthesis, Characterization of novel dihydrazide containing polyurethanes based on N'¹,N'²-bis[(4-hydroxyphenyl)methylene] ethanedihydrazide," Journal of Applied Polymer Science, 107, 2008, 3401-3407.

6. A.V. Raghu, H.M. Jeong, Y.R. Lee, C.M. Shin, "Preparation and Physical Properties of Waterborne Polyurethane/Functionalized Graphene Sheet Nanocomposites" Macromolecular Chemistry & Physics, 209, 2008, **2487 - 2493.**

7. K.R. Reddy, H.M. Jeong, Y. Lee, A.V. Raghu,^{*,} "Synthesis and Structural properties of MWCNTs-Core/Thiophene polymer-Sheath Composite Nanocables by a Cationic surfactant-Assisted Chemical Oxidative Polymerization" Journal of Polymer Science Part A: Polymer Chemistry, 48, 2010, **1477-1484.**

Graduate student:



Mr. D.P. Suhas, Senior Research Fellow, CSIR, Govt. of India

Mr. Suhas D. P. has been selected for CSIR-Senior Research Fellowship (SRF) (Ack. No. 124281/2k13/1) from Materials science category (MCEH-24) for the year 2014. He was selected for this prestigious fellowship in an interview held at CSIR complex New Delhi, where only 30 students were selected from a pool of 250 applicants.

Projects/Recognitions

Awards: "Seed Money for Young Scientist," VGST, Department of Information Technology, Biotechnology and Science & Technology, Government of Karnataka. Amount: Rs. 4 Lakhs (2011-2012)

Ongoing Project: "Effect of Electron Beam Irradiation on Polymeric composite Membranes for Pervaporation Separation Application" Awarded from BRNS, Mumbai, Government of India: Rs. **19,05,000/-**.

Editorial board member

1. International Scholarly Research Network (ISRN) Nanomaterials

2. International Scholarly Research Network (ISRN) Polymer Science

3. Journal of Polymer Science

Scientific reviewer for ACS Nano, Carbon, Journal of Polymer Science Polymer Chemistry Part A, Journal of Applied Polymer Science, Journal of Membrane Science, Chemical Engineering Journal, Carbohydrate Polymers, Drug Invention Today, Polymer International, Desalination, European Polymer Journal, Reactive & Functional Polymers, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Polymer Composite, Macromolecular Research, Materials Chemistry and Physics. etc., **Member of professional bodies**

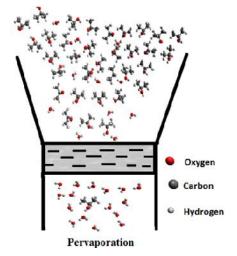
- > Life Member of the Society for Polymer Science, Dharwad Chapter, INDIA
- Establishment of laboratory in Center of Excellence in Polymer Science, Karnatak University, Dharwad.
- Resource person, Vision Group on Science and Technology, Department of IT, BT and Science & Technology & Department of Collegiate Education, Government of Karnataka.
- Resource person, Karnataka Rajya Vijnana Parishat, Government of Karnataka.

Research Highlights of our group

Research at our group primarily focuses on fabrication of novel composite membranes for pervaporation dehydration of ethanol, isopropanol and butanol, which are of industrial importance as solvents, reactants and as bio-fuels. We use polymer composites consisting of zeolites, clays, graphene, cellulose nanofibrils as fillers. We pioneered the use of graphene composite membranes for pervaporation applications. All the membranes developed by our group has shown better performance in comparison to distillation and also results are comparable with most of the best performing membranes in this field. We also work on intelligent design of fire-retardant polyurethanes.

Completed Projects:

1. Preparation and characterization of Novel Polyurethanes containing 4, 4^l-{oxy-1,4 diphenol bis (nitromethylidine)} diphenol Schiff Base Diol



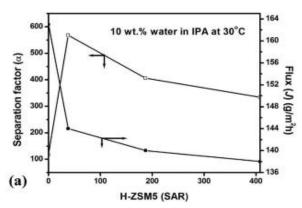
Four segmented polyurethanes (PUs) based on 4, 4^l-{oxy-1, 4 diphenol bis (nitromethylidine)} diphenol diol with different diisocyanates such as toluene 2, 4 diisocyanate, isophorone diisocyanate, 4, 4 diphenylmethane diisocyanate and hexamethylene diisocyanate have been prepared by solution method.

The structures of diol and polyurethanes have been confirmed by FTIR, NMR (¹H-NMR and ¹³C-NMR). The segmented polyurethanes were characterized by thermogravimetry (TGA), differential scanning calorimetric (DSC) and wide angle X-ray diffraction. FTIR confirmed hydrogen bonding interactions, where as TGA and DSC suggested that introduction of aromatic phenyl rings in the main chain considerably increased the thermal stability. Some of these polyurethanes could be used as fire retardants.

The results of this work are published as full length article in **Polymer Engineering and Science 2014**, **54**, **24**.

2. Mixed Matrix Membranes of H-ZSM-5 loaded Poly (vinyl alcohol) used in pervaporation dehydration of alcohols: Influence of Silica/Alumina ratio

Mixed matrix membranes of poly (vinyl alcohol) loaded with zeolite particles having different silica alumina ratio were prepared and used in dehydration pervaporation ethanol of and isopropanol. The effect of Si/Al ratio with respect to membrane performance have been investigated and based on the results it is concluded that, the SAR (silica alumina ratio) shows an inverse relation to membrane performance (flux and selectivity). The membrane characterization using XRD, FTIR, SEM, contact angle studies complement these observations. Such an increase

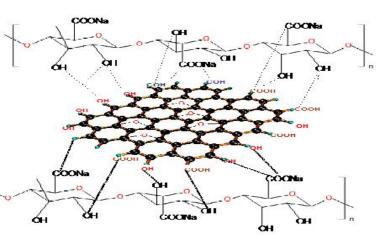


in membrane performance with increase in zeolite's alumina content is attributed to enhanced interface interaction, resulting from higher hyrophilicity of zeolites with lower SAR. Thus we have demonstrated a tunable membrane performance of PVA by incorporating H-ZSM5 particles of varying SAR. The results of this work are published as full length article in **Polymer Engineering and Science DOI:-**10.1002/pen.23717

3. Graphene-loaded sodium alginate nanocomposite membranes with enhanced isopropanol dehydration performance via a pervaporation technique

There is a lot of excitement among scientific community, on use of functionalized graphene as water selective membranes. However, the practical implications of such membranes are quite limited due to high cost involved in graphene preparation. In this view, we have prepared graphene composite

membranes with sodium alginate and tested its efficiency in pervaporation dehydration of isopropanol. These membranes display a reasonably high degree of permeance and selectivity at just 2 wt.% of functionalized graphene loading. The interaction of functionalized graphene with sodium alginate matrix was studied by a verity characterization techniques, which revel good dispersion of graphene oxide into sodium alginate matrix, resulting from favourable interface



interaction. To gain more insight into membrane behaviour, its diffusion, sorption and Arrhenius activation energy parameters were calculated. Overall we could show that functionalized graphene, could be effectively used as fillers in pervaporation membranes for dehydration application. We have received a

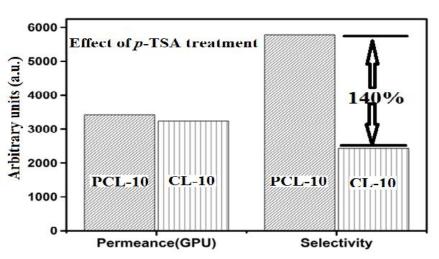
Annual Report 2013-14

good number of citations and appreciation mails after publication of this work. Published in **RSC** Advances 2013, 3, 17120

4. para-Toluene sulfonic acid (p-TSA) treated loaded sodium alginate membranes for enhanced pervaporative dehydration of isopropanol

Clay composite membranes are one of the widely studied materials for pervaporation dehydration application. In this work we have incorporated p-TSA treated clay into sodium alginate matrix and the resulting composite membranes were used in pervaporation dehydration of isopropanol. The p-TSA treatment could bring about enhancement in surface area and hydrophilicity of clay, without

compromising on its crystal structure. As a consequence the modified membranes could show 140 % increase in selectivity as compared to unmodified loaded clay membranes. Further, the membranes of this study characterized have been using a verity of physicochemical techniques. Their pervaporation performances were investigated to evaluate selectivity, permeance, thermodynamic and kinetic



interaction parameters as a function of filler loading, temperature and feed water composition. Hence, p-TSA treatment has proved to be an effective method to increase membrane performance of clay composite membranes. Communicated to an international journal

On-Going Work

1. Other Graphene composites:

After the success of our earlier work on graphene oxide/sodium alginate composites, we have undertaken steps to increase the compatibility of graphene oxide with membrane matrix and thereby enhance its performance. In this direction, we are trying graphene oxide/chitosan composites and graphene oxide/chitosan- poly (vinyl pyrrolidone) membranes. Meanwhile we have also extended our interest towards dehydration of ethanol-water and butanol-water mixtures.

2. Effect of electron-beam irradiation on membrane performance:

Recently, our group has undertaken one more interesting work concerning "effect of electron-beam irradiation on pervaporation performance of graphene composites". Here we will be exposing all of our graphene composite membranes to different dosage of electron beam and study their effect on physicochemical characteristics of composites in general and their pervaporation behaviour in particular. This project is funded by BRNS.

Dr. Ganapati V. Shanbhag

PhD (NCL, Pune), PDF (KAIST, S.Korea)

Asst. Professor, Materials Science Division Since June 2010



Curriculum Vitae

- 2010-Present: Asst. Professor, PPISR, Bangalore, India
- 2008—2010: Research Scientist, Dept. of Chemistry, Korea Advanced Institute of Science and technology (KAIST), South Korea.
- 2002—2008: Ph.D. National Chemical Laboratory, Pune India (Degree by University of Pune).
- 2000-2001: Research Associate in ICI India Ltd, Mumbai, India
- 1999-2000: Lecturer, M.M Arts and Science College, Sirsi, Karnataka, India
- 1999: M.Sc. Organic Chemistry, Karnatak University, Dharwad

Broad Areas of Research:

- 1. Design and development of shape selective catalysts for commercially important organic transformations
- 2. Novel multifunctional materials and their catalytic applications
- 3. Studies on catalytic conversion of biomass and biorefinary byproducts into fuels and value added chemicals

Total no of publications in international journals: 22

Participation in workshops, conferences and symposiums: 15

Research highlights

The Catalysis group at PPISR has expertise in pore engineering of zeolites and other microporous materials for shape-selective organic transformations and hydrothermal synthesis of zeolites and mesoporous Materials and their applications in green chemistry. The group is also working on designing eco-friendly solid catalysts for glycerol transformations to value-added products such as glycerol carbonate, acrolein, solketal, acetins etc. and biodiesel synthesis from transesterification of vegetable oils. The group especially working on designing new heterogeneous acid and base solid catalysts and their utilization in organic transformations such as Prins cyclization, Baeyer-Villiger reaction and photo catalysis.

List of students:



Mrs. Swetha Sandesh

Research Scholars



Mr. Vijaykumar S. M.







Mr. Manjunathan

Project fellows



Mr. Prashant Kumar



Mr. Karthik

Previous group members:

Research Associa Dr. Ramesh S. (1-5-2012 to 4-7-2013)





Mr. Dundappa

Mr. Santhosh Kumar

Project Fellow Mr. Satish Burla (1-7-2012 to 31-10-2013)

Representative Publications:

- Sulfated zirconia; an efficient and reusable acid catalyst for the selective synthesis of 4-phenyl-1,3dioxane by Prins cyclization of styrene. V.S. Marakatti, G.V. Shanbhag* and A.B. Halgeri, Applied Catalysis A: General 451 (2013) 71–78
- Shape selective catalysis by phosphate modified ZSM-5: Generation of new acid sites with pore modification. Janardhan HL, GV Shanbhag* and A.B. Halgeri, Applied Catalysis A: General, 2014, 47, 12-18
- 3. Zinc hydroxy stannate: a promising acid-base bifunctional catalyst .Swetha Sandesh, G V Shanbhag* and A.B. Halgeri, **RSC Advances**, 2014, 4, 974-977
- 4. Transesterification of glycerol to glycerol carbonate using KF/Al₂O₃ catalyst: The role of support and basicity Swetha Sandesh, GV Shanbhag* and A.B. Halgeri, **Catalysis Letters**, 2013, 143, 1226-1234
- Condensation reactions assisted by acidic hydrogen bonded hydroxyl groups in solid tin(II)hydroxychloride. Vijaykumar S. Marakatti, Ganapati V. Shanbhag^{*} and Anand B. Halgeri RSC Advances, 2013, 10795-10800
- Mesoporous sodalite: A novel stable solid catalyst for base catalyzed organic transformations. G V Shanbhag, M.Choi, J.Kim and Ryong Ryoo, Journal of Catalysis, Volume 264, 2009, 88-92.
- Chemoselective synthesis of -amino acid derivatives by hydroamination of activated olefins using AISBA-15 catalyst. G. V. Shanbhag, S.M. Kumbar and S.B. Halligudi, Journal of Molecular Catalysis A: Chemical, Volume 284(1-2), 2008, 16-23.
- Copper(II) ion exchanged AISBA-15: a versatile catalyst for intermolecular hydroamination of terminal alkynes with aromatic amines. Ganapati V. Shanbhag, Trissa Joseph and S. B. Halligudi*, Journal of Catalysis, Volume 250 (2), 2007, 274-282.
- Heterogeneous intermolecular hydroamination of terminal alkynes with aromatic amines, GV. Shanbhag, S.M. Kumbar, T. Joseph and S.B. Halligudi*, **Tetrahedron Letters**, Volume 47(2), 2006, 141-143.

Patents:

1) Indian patent

Title: A process for the preparation of isomers of aromatics

Application No. 2754/MUM/2013: Date of Filing: 23 August 2013

Inventors: R Ravishakar, PVC Rao, NV Choudhary, G Sriganesh (HPCL, R & D Centre, Bangalore), **G. V. Shanbhag,** V. S. Marakatti and A. B. Halgeri (Poornaprajna Institute of Scientific Research, Bangalore).

2) World patent filed (PCT)

Date of Filing: October 2013

Inventors: R Ravishakar, PVC Rao, NV Choudhary, G Sriganesh (HPCL, R & D Centre, Bangalore), **G. V. Shanbhag,** V. S. Marakatti and A. B. Halgeri (Poornaprajna Institute of Scientific Research, Bangalore).

Book Chapter:

"Supported heteropoly acids and multicomponent polyoxometalates as eco- friendly solid catalysts for bulk and fine chemicals synthesis". Book Chapter "Environmentally Benign Catalysts: For Clean Organic Reactions", Springer, USA Published in July 2013. **G. V. Shanbhag**, Ankur Bordoloi , Suman Sahoo, B. M. Devassy , and S. B. Halligudi

Research Projects:

Industrial Project 1: Design and development of a catalyst and process for selective alkylation of aromatics (sponsored by: GTC Technology, USA)

Project Coordinator: Dr. A. B. Halgeri

Principal Investigator: Dr. Ganapati V. Shanbhag

Co-investigator: Dr. Sanjeev Maradur

Project Assistants: Mr. Satish Burla, Mr. Manjunathan, Mr. Prashant Kumar, Mr. Karthik, Mr. Santhosh Kumar

The first generation catalyst based on medium pore zeolite for the selective alkylation of aromatics to produce alkylated aromatics has been finalized in May 2013. The catalyst was shown to be stable up to 300 hours of time on stream. The catalyst was also recycled for 100 hours successfully. The mechanical properties of the catalyst such as crush strength and attrition loss before and after the reaction were within the acceptable limits for commercial scale testing. Different batches of zeolite catalyst were received from the manufacturer to check if the same performance can be achieved on other batches of zeolite also. Hence extrudates with silica-alumina binder were prepared for all the batches and tested the performance. It is seen that the zeolite with higher crystal sizes gave lower conversion with high selectivity for para isomer whereas zeolite with small crystal size showed high conversion. All the reaction data were correlated with crystal sizes obtained by SEM analysis.

Large pore zeolite like beta was also screened for alkylation of aromatics at lower temperatures. It showed fast deactivation due to coke formation because of the presence of high acidity. To decrease the acidity in beta zeolite, the catalyst was dealuminated using steam and HCI to increase the SAR from 30 to 90 and checked for its performance. However, the catalyst showed similar trend of deactivation. Hence this modified beta gave inferior performance compared to medium pore zeolite catalyst.

July, 2013 was the last month for the 2nd year work of GTC sponsored project. During this month, a long time on stream run of 300 hrs was conducted with the final catalyst developed at PPISR for alkylation of aromatics process. During this run, reaction parameters such as WHSV and mole ratio were varied to check the performance of the catalyst. The performance of the catalyst remained almost the same during 300 h run which indicated the high stability of the catalyst. With this experiment, PPISR provided GTC almost all the required data for catalyst scale-up and commercialization of the process.

During this time, new ideas to extend the GTC project for third year were formulated and budget for it has been finalized. New agreement was signed between GTC and PPISR during September 2013. Clarient, a well-known Chemical industry having world-wide operations will be the part of this project. A nondisclosure agreement was signed between Clarient and PPISR during this time.

The 3rd phase of the project started from October 2013 for the period of one year. The first quarter work started with the hiring of 3 project fellows. This project is a joint collaborative project with GTC USA, GTC, China and Clarient, Germany. The project was started with catalyst testing of aromatization of Liquefied

Petroleum Gas (LPG) which we conducted at PPISR for the first time without modifying the existing equipments. The catalysts were prepared by Clarient and sent to PPISR for modification and testing. Catalyst screening was carried out by conducting a number of reactions for 50-75 h reaction time. PPISR was able to execute the reaction with high accuracy by achieving high mass balance by calculating both gas and liquid products formed during the reaction with off line GC analysis.

After two months work on aromatization, research was then shifted to development of 2^{nd} generation catalyst for alkylation of aromatics to selectively produce para isomer. The Preparation and evaluation of several novel metal modified zeolite catalysts are under progress. The effect of carrier gas like H₂ and steam had significant effect on selectivity for para isomer. Initial screening results with metal modified zeolite catalysts are promising. Optimization of process conditions and catalyst recipe is under progress.

Teleconference between GTC, USA and PPISR is held weekly twice to review the project work. GTC expressed their happiness with the research work and results generated at PPISR so far.

Industrial Project 2: Post-synthesis pore engineering and surface treatment of some solid catalysts (September 2012-August 2013) (Sponsored by: Shell Technology Center, Bangalore

Project Coordinator: Dr. A. B. Halgeri

Principal Investigator: Dr. Ganapati V. Shanbhag

Co-investigator: Dr. Sanjeev Maradur

Research Associate: Dr. Ramesh S.

Pore modification of zeolites and pore size estimation with model reactions like disproportionation were studied in detail. During previous year, pore modification procedure was optimized on medium pore zeolite and selected the best recipe of catalyst preparation. Then, disproportionation was carried at different temperature and space velocity.

Pore modified zeolite catalysts gave higher selectivity for para isomer at all reaction temperatures. Interestingly, the difference in conversion between modified and unmodified zeolites decreased with increase in temperature. At very high temperatures, zeolite gave high conversion due to dealkylation to form more benzene and higher aromatics. However, the conversion was almost the same for pore modified zeolite at 450°C. This could be due to the decrease in external surface acidity after modification. For unmodified zeolite, the conversion decreased with increase in space velocity whereas after modification, the conversion was almost constant at both space velocities. For modified catalyst, selectivity for para isomer increased with decrease in space velocity.

Monthly technical reports have been sent to Shell team every month and a Teleconference was held between Shell and PPISR every month to review the project work.

Annual comprehensive report has been submitted to Shell after finishing one year project tenure.

Industrial Project 3: Development of Zeolite Modified Catalysts for the Hydrocarbon Conversions such as light naphtha aromatization and side chain alkylation of toluene.

(Sponsored by: HPCL R&D Centre, Bangalore

Project Coordinator: Dr. A. B. Halgeri

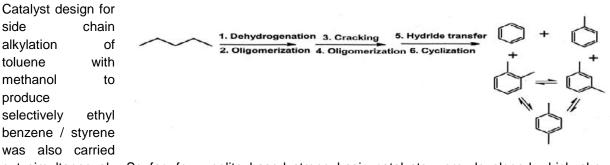
Principal Investigator: Dr. Ganapati V. Shanbhag

Co-investigator: Dr. Sanjeev Maradur

Senior Research Fellow: Mr. Vijaykumar, Mr. Janardhan

A new catalyst recipe was developed and successfully applied for light naphtha aromatization. This heterogeneous eco-friendly, bimetallic, microporous catalyst gave high yield for aromatics ~ 65 % which was achieved for the first time so far. The carrier gas effect was studied and acidity required in the catalyst was optimized by varying silica/alumina ratio of the catalyst. Furthermore, actual light naphtha from petroleum refinery obtained from HPCL R & D centre, was tested on newly developed catalyst. The catalyst showed excellent performance both on hexane (model feed) and light naphtha. The catalyst was modified by introducing small amount of metal oxide as promoter and tested. The catalysts are further modified by making extrudates by mixing with suitable binder. The catalyst in extrudate form also showed

very good performance for light naphtha aromatization. These catalysts have been submitted to HPCL R & D centre for further testing under high pressure conditions.



out simultaneously. So far, few zeolite based strong basic catalysts were developed which showed reasonably good conversion and excellent selectivity for ethyl benzene/styrene. Further work to improve the performance of the catalyst is under progress.

Joint patents were filed in India and World patent (PCT) on "Catalyst development for ring alkylation of toluene to produce xylenes with high o-xylene selectivity". A detailed study on catalyst characterization and testing of this work is under progress to have joint publication in an international journal.

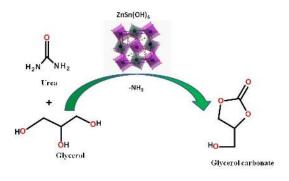
One year of the project was completed on 31-10-2013 and Annual Comprehensive Report was submitted to HPCL. Later, annual technical review meeting was held in HPCL corporate office to review the progress and decide on future work. The HPCL team applauded the overall progress made by PPISR during one year time. The project is now continued for the second year to further improve the catalyst recipe for achieving better performance.

Project 4: Zinc-tin mixed hydroxide; a novel solid bifunctional catalyst (completed)

Guide: Dr. Ganapati V. Shanbhag

Student: Ms. Swetha Sandesh

The catalytic activity of zinc tin hydroxide, a strong solid base catalyst was studied for transcarbonylation of glycerol with urea. The catalyst showed high performance among different solid base catalysts. The catalyst also showed good recyclability and structural stability after repeated runs. The strength and amount of basicity of the different catalysts were measured by Hammett indicator method, where Nile blue and phenolphthalein were used as indicators. Zinc tin hydroxide showed strong basic sites which changed



color with nile blue. Other conventional catalysts like hydrotalcite and MgO were less basic. Published in RSC Advances, 2014

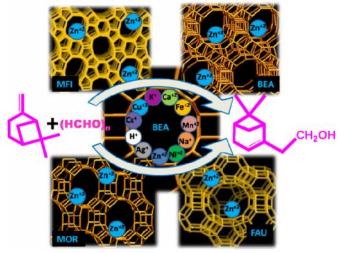
Project 5: Metal ion exchanged zeolites as novel efficient catalysts for the synthesis of nopol by Prins reaction.

Guide: Dr. Ganapati V. Shanbhag

Student: Mr. Vijaykumar SM

Nopol is optically active, primary alcohol used as aroma in soap and detergent industries. Nopol is also used as pesticide in agrochemical industry. It is synthesized from -pinene and formaldehyde from Prins reaction. The aim of this project is to design an eco-friendly and cost effective, novel solid acid catalyst for this reaction.

Among the catalysts, zeolites are widely accepted as major type of catalyst in industries and are widely used as a catalyst in petrochemical, fine speciality chemical and in many synthesis organic transformations. The zeolites have not been studied for the Prins reaction so far. To study the effect of the zeolites with different pore structure on the activity and selectivity, zeolites like HZSM-5(10 membered ring), H-Y, H-, (12-membered ring), HMOR (8*12 membered ring) were screened for the Prins reaction. The H and H-Y zeolites showed higher conversion of around 57 % and 44 % respectively, compared to H-ZSM-5(15%) and H-MOR (6.6%) zeolites. To improve the performance further, different metal ions were exchanged on beta zeolite and catalytic activity was evaluated. Among these, Zn²⁺ -beta



"Metal ion-exchanged zeolites for the green synthesis of nopol from Prins reaction"

showed high activity and selectivity. The reaction was found to be efficient in polar solvents like acetonitrile and benzenitrile. Study on the role of solvent, optimization of ion exchange method and the reaction conditions are under progress.

Manuscript under revision in Applied Catalysis A Journal

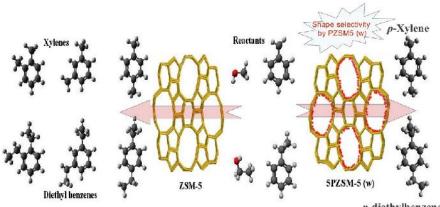
Project 6 : Pore engineering of ZSM-5 by phosphate modification: Generation of new acid sites and enhancement in shape selectivity

Guide: Dr. Ganapati V. Shanbhag

Student: Mr. Janardhan

Pore engineering of ZSM-5 was carried out with post synthesis phosphate modification and shape selectivity was evaluated for alkylation, disproportionation reactions and competitive reaction of ethylbenzene and meta-

metaxylene. Catalysts were characterized by XRD, NMR, NH₃-FTIR, MAS TPD, PZC etc. Post synthesis modification of ZSM-5 by phosphate treatment generated new kinds of acid sites with pore narrowing. Even though acid site strength changed after phosphate treatment, these active sites efficiently



p-diethylbenzene

catalyzed toluene alkylation with methanol, ethylbenzene alkylation with ethanol and disproportionation of ethylbenzene. P-ZSM-5 effectively catalyzed toluene alkylation with methanol resulting in 14.2 % toluene conversion with para-xylene selectivity of 96.1 % and almost complete conversion of methanol. Selectivity ratio of para to meta enhanced substantially from 0.6 to 32 after phosphate modification. EB alkylation with ethanol gave 20 % EB conversion with 98 % PDEB selectivity and ethyl benzene disporoportionation resulted in 7 % conversion and 99 % PDEB selectivity with P-ZSM-5 catalyst.Constraint index for modified catalysts obtained from competitive reaction of ethylbenzene and m-xylene was used to determine extent of pore narrowing by phosphate modification. Impregnated phosphates increased

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diffusion limitation and narrowed the pore opening resulting in high para-selectivity. Decrease in pore volume by phosphate modification has a direct correlation with increase in shape selectivity.

Project 7: Nano-sized beta zeolite as an efficient solid acid catalyst for acetalization of glycerol to produce solketal

Guide: Dr. Ganapati V. Shanbhag

Student: Mr. Manjunathan P.

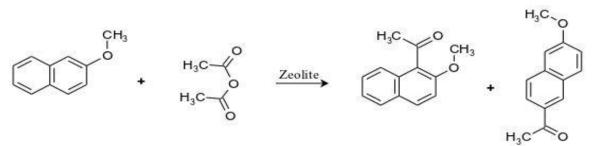
Glycerol is obtained as a byproduct during transesterification of vegetable oil or animal fat which accounts for one tenth of every gallon of biodiesel produced. Increasing availability of glycerol has made it an inexpensive and abundant raw material to synthesize value-added chemicals. In this study, acetalization of glycerol with acetone was carried out over various types of Brønsted solid acid catalysts in the liquid phase at room temperature with lower mole ratio of reactants. The chemical and structural properties of the catalyst were studied by X-ray diffraction, AAS, SEM, NH₃-TPD and FTIR-pyridine adsorption. Among various Brønsted solid acid catalysts screened, nano-sized H-Beta zeolite showed best performance at less time period with 86% glycerol conversion and high selectivity to solketal (98.5%). The effect of acidity of nano-sized H-Beta zeolite on acetalization of glycerol was studied by dealumination treatment using oxalic acid. Glycerol conversion decreased with decrease in acidity of nano-sized H-Beta. The behavior of Lewis acidic sites was studied using partial and complete Cu²⁺ ion-exchanged beta catalysts. It is observed that Lewis acidic Cu²⁺ in Cu-beta also acts as an active site for acetalization of glycerol. The different parameters such as catalyst concentration, glycerol to acetone mole ratio and reaction time were systematically studied at room temperature using nanosized-H-Beta zeolite.

Project 8: Pore engineering of ZSM-5 zeolite by phosphorous oxide modification for the shape selective transformation of 2-Methoxy naphthalene acetylation with acetic anhydride

Guide: Dr. Ganapati V. Shanbhag

Student: Mr. Janardhan

Zeolite beta was shown to be the best catalyst among solid acid catalysts to achieve high performance for acetylation of 2-methoxy naphthalene which yields 2-acetyl-6-methoxynaphthalene, pharmaceutically important intermediate used in the manufacture drug named naproxen. It also produces kinetically preferred product 1-acetyl-2-methoxynaphthalene. Zeolite beta gave ~ 60 % selectivity 2-acetyl-6-methoxynaphthalene. The aim of the project is to improve the selectivity further to 80% which would be a remarkable achievement. This can be only achieved by pore narrowing of zeolite beta which allows only the smallest isomer to come out of the pores. For this, beta zeolite was modified with phosphate



treatment as well as mild delalumination of external acid sites. Selectivity for the required isomer improved with increase with phosphate content up to 1% and then decreased. Dealumination of external acid sites also improved the performance. So far selectivity of about 75% was achieved with phosphate modification. A further study to improve the performance of this catalyst is under progress. Manuscript under preparation

Project 9: Novel organic substituted heteropoly acid catalyst for condensation of glycerol with acetone to form solketal at room temperature **(Completed)**

Guide: Dr. Ganapati V. Shanbhag

Student: Ms. Swetha Sandesh

In the last quarter, synthesis of Solketal (2,2'-dimethyl-4-hydroximethyl-1,3-dioxolane) has been performed using acetone by condensation reaction using organic-inorganic hybrid catalyst. Tetrapropyl ammonium exchanged heteropoly acid has been synthesized for the first time and reported as a solid acid catalyst. The condensation reaction of glycerol with acetone was carried out under room temperature in liquid phase batch reactor. The catalyst showed high conversion and selectivity for solketal (> 90 % yield). The heterogeneity of the catalyst was established by leaching test. The catalyst showed good recyclability up to 3 cycles. The structural integrity of the catalyst after 3 cycles was tested by XRD of spent catalyst. The spent catalyst showed the similar XRD pattern as that of fresh catalyst which confirmed the structural stability of the catalyst after repeated runs. The characterization of catalyst with XRD, FTIR, TGA, Elemental analysis and SEM has been carried out and correlated with activity. Manuscript under preparation.

Project 10: Design and development of eco-friendly novel solid base catalysts for the transesterification of non-edible oils to produce biodiesel

Guide: Dr. Ganapati V. Shanbhag

Student: Mr. Prashant Kumar (M. Tech. Project)

In the last quarter, several solid basic catalysts such as hydrotalcite, KF/ alumina, KF/ CaO etc were tested for transesterification of sunflower oil and waste cooking oil. The process or biodiesel synthesis and its analysis were standardized. This quarter, the work was focused at designing a novel catalyst which was not reported so far for biodiesel synthesis. Several catalysts have been screened for this reaction of which metal tin hydroxide showed best performance and not reported so far. This novel catalyst showed > 93 % biodiesel yield with different non-edible oils such as honge oil, waste cooking oil, simarouba oil and jatropha oil. The GC MS analysis for determining the biodiesel composition is under progress. Also biodiesel characterization to obtain its physical properties such as flash point, density, acid number, fire point and calorific value is under progress. The biodiesel produced in our lab was also submitted for checking its performance on diesel engine.

Manuscript under preparation

Project 11: Solvent free synthesis of 4-methoxyacetophenone from acylation of anisole using H-Beta as a eco-friendly solid acid catalyst **One month MSc Project work (15-5-2013 to 15-6-2013)**

Students: Mr. Nagendra Kulal and Mr. Rohan D'souza (from St. Aloysius College, Mangalore) Guide: Dr. Ganapati V. Shanbhaq

4-Methoxyacetophenone was synthesized by acylation of anisole with acetic anhydride using H-Beta heterogeneous solid acid catalyst under solvent free conditions. The catalyst was synthesized by hydrothermal method and characterized by PXRD. Different medium and large pore zeolites such as beta, mordenite and ZSM-5 were screened for this reaction. Zeolite beta with the large pores and high acidity is highly active and selective for acylation of anisole. Effect of various reaction parameters were studied in order to get the optimized conditions for the acylation of anisole. 0.25 g of H-beta catalyst showed the best catalytic activity with 2:1 mole ratio of reactants (Anisole: Acetic anhydride) at 90° C for 6 h. The catalyst showed almost same conversion even after three cycles. Under optimized conditions, 99% conversion of acetic anhydride was achieved with 100% selectivity for para acylated product. The 100% selectivity for para isomer is attributed to the micro porous structure of zeolite beta.

Dr. Nalini G Sundaram, Assistant Professor



Phone: 080-27607242 E-mail: nalini .AT.poornaprajna.org Web page: http://www.ppisr.res.in/faculty/profile_Nalini.pdf

Areas of Interest

- Rare Earth Photoluminescent nano-oxides for solid state lighting devices
- Ceramic Nanomaterials Photocatalysts for dye degradation and organic reactions
- Oxide nanoparticles and Thick films selective Gas Sensors
- Metal Organic Precursors for Optoelectronic devices

Synthesis, structural studies, polymorphism, local structure and phase transitions in multifunctional materials using Single Crystal Powder X-ray as well as Neutron diffraction techniques

Curriculum vitae

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

Awards and Scholarship

1. Awarded a project by DST, India for three years under the SERC- Fast Track Scheme For Young Scientists (FAST)

2. Senior Research Fellowship from Council of Scientific and Industrial Research (CSIR) Government of India

3. Recipient of the Joshi award for securing first rank in M.Sc. (Physical Chemistry)

Current Sponsored Projects at PPISR

1. Design and Development of Nanocrystalline Bismuth Oxychlorides for Degradation of dyes and Organic Pollutants: Sponsored by **DST,India under the Fast track scheme for Young Scientists** for three years (Jan 2012- Jan 2015)

2. Influence of Electron Beam Irradiation on the Crystal Structure and Photoluminescence of Rare Earth doped Tungstate Nanophosphors: Sponsored by **BRNS, DAE, India** for three years (April 2013-Apr 2016)

Representative publications

- 'Polymorphism in Photoluminescent KNdW₂O₈: Synthesis, Neutron Diffraction, and Raman Study', Swetha S. M. Bhat, Diptikanta Swain, Chandrabhas Narayana, Mikhail Feygenson, Joerg C. Neuefeind, and Nalini G. Sundaram, *Crystal Growth & Design*, 2014, *14* (2), pp 835–843
- A composition-dependent "re-entrant" crystallographicphase transition in the substitutional metal acetylacetonate complex(Cr1-xGax)(acac)3,', M. Srinidhi Raghavan, Piyush Jaiswal, Nalini G. Sundaram, and S.A. Shivashankar, Polyhedron 70C (2014), pp. 188-193
- Swetha. S.M., Nalini G Sundaram , 'Efficient visible light photocatalysis of Bi₄TaO₈Cl nanoparticles synthesized by solution combustion technique', *RSC Advances*, 2013, : RSC Advances, 2013, 3,14371
- Jiang, F. Bridges, N. Sundaram, D.P. Belanger, I.E. Anderson, J.F. Mitchell, and H. Zheng 'Study of the local distortions of the perovskite system La1-xSrxCoO3 using the extended x-ray absorption fine structure technique' Phys. Rev. B 80, 144423 2009
- N. Sundaram, Y. Jiang, I. E. Anderson, D. P. Belanger, C. H. Booth, F. Bridges, J. F. Mitchell, Th. Proffen and H. Zheng, 'Local Structure of La1-xSrxCoO3 determined from EXAFS and neutron PDF studies', *Physical Review Letters*, 2009, 102, 026401

Total Number of Publications in National and International Journals: 17

Research Group :

Post Doctoral Researcher:



Research Area: Development of Lanthanum based Oxide Thick films for selective Gas sensors

Dr. Sowmya Palimar, (Ph.D from NITK Surathkal)

Graduate students:



Ms. Swetha .S. M. (UGC-SRF)



Mr. Pradeep Shanbogh (JRF supported by BRNS)



Mr. Srinidhi. R (Joint SRF with Prof. Shivashankar, IISc)

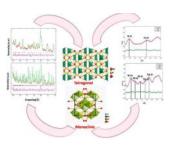
Membership of Professional bodies:

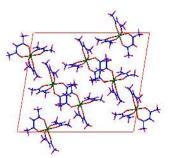
1. Member of National crystallographic Association

Completed Research Projects:

(a) Correlation of Crystal Structure and PL Activity of Polymorphs of KNdW₂O₈ Nanoparticles; Duration:2011-2013
 Primary Investigator: Dr. Nalini G Sundaram
 Research Student(JRF): Ms. Swetha S.M
 Published in Crystal Growth and Design, ACS Publications, 2014

(b) Crystal Structure of Substituted Complexes, {Ga_xCr_{1-xj}} (acac)₃ using Single crystal X-ray diffraction Techniques_; Duration:2011-2013
Primary Investigator: Prof. S.A. Sivashankar (IISc) Co-Investigator: Dr. Nalini G Sundaram Research Student(JRF): Mr. Srinidhi R. Published in Polyhedron, Elsevier Publications, 2014





(c) Efficient visible light photocatalysis of Bi4TaO8Cl nanoparticles synthesized by solution combustion technique; Duration: 2011-2013 Primary Investigator: Dr. Nalini G Sundaram Research Student(JRF): Ms. Swetha S.M Published in RSC Advances, RSC Publications, 2013

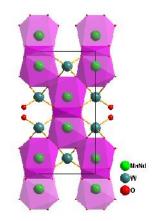
Current Research Projects

1. Solid state synthesis of a New n=2 layered Bismuth oxychloride for Photocatalytic Degradation of Dyes

A new oxychloride phase belonging to the Aurivillus-Sillen structure type has been synthesized after various trail synthesis runs at different temperature and different time. TG-DTA analysis has been carried out to understand the thermal stability and presence of phase transitions if any. XPS measurement has been conducted in order to confirm the presence of chlorine in the matrix. The phase shows good photocatalytic activity for the degradation of dyes in UV light. At present growing good single crystals to elucidate the crystal structure is in progress. Simultaneously, analysis of high resolution neutron diffraction data obtained from the instrument SPODI at M LZ, Garching, Germany under the rapid access program is in progress.

2. Influence of the alkali metal ions on the crystal structure and photoluminescence of Alkali metal doped Rare Earth Tungstate Nanoparticles

The particle size obtained from SEM for the above compositions were in the range of 30-50 nm. Emission spectra of the nanomaterials reveal that as the potassium composition increases there is a blue shift observed. Powder neutron diffraction data have been collected at POWGEN, Oakridge National Lab for all the five samples. Combined X-ray and Neutron Rietveld refinement is in progress to find the effect of Alkali metal-doping into the host matrix. Atomic absorption spectroscopy is used as tool to confirm the amount of alkali metal present in all the samples. Plotting chromaticity diagram is in progress to visualize the color rendering index.



3. Design and Development of Lanthanum Based Nanoparticles For Selective Thick Film Gas Sensors

The proposed project mainly aims to synthesize highly sensitive and selective perovskite nanoparticles leading to the development of thick film gas sensors with easy reproducibility for the Chemical Industry. Perovskite oxides are particularly attractive for selective gas sensor application as in addition to their high melting and high decomposition temperatures, these perovskites can provide micro structural and morphological stability which improves the reliability and long-term sensor performance. Moreover the perovskite structure has two differently-sized cations, which makes it well suited for variety of dopant additions. This doping flexibility allows the control of transport properties to optimize sensor performance for particular applications. Present work aims to obtain good quality of La_{1-x}A_xBO₃ (Here A=Sr, Ca Ba etc and B=Fe or Ni.) thick film sensors and to study their sensing properties to different gases such as acetone, ammonia, hydrogen sulphide, hydrocarbons and L.P.G. The results of the crystal structure analysis would provide insights into the structure-particle size-sensitivity relationship of this class of compounds and thereby help in the generation of novel gas sensing materials.

4. Rare earth doped Complex layered Photoluminescent Bismuth Oxides Nanoparticles for Up-Conversion Phosphors

Up Conversion phosphors absorb in the near infrared region and re-emit in the visible region. Therefore, a wide variety of colors, with very high brightness operation without damage to the emitters, long lifetimes and efficiencies are possible. This work aims to synthesize rare earth doped complex Bismuth oxide materials by a variety of nano synthesis techniques. The role of the rare earth as the emitter and activator will be evaluated from the electronic and crystal structure point of view.

5. Synthesis of $[(Ga_x In_{2-x})_2O_3]$ from the Acetylacetonate precursor for Optical Applications

Nanoparticles and nanostructures of different materials have been the subject of intense research recently because of wide range of physical and chemical properties they feature. Oxides in particular are of interest because of their broad range of compositional and structural characteristics, enriched further by non-stoichiometry and substitutional derivatives. These variations make it possible to tune electrical, magnetic and optical properties. An additional "handle" is through the control of the shape and orientation of fine crystallites of oxides, to obtain various and different morphologies, such as wires, tubes, rods, and belts. In this work, the precursor materials are used to synthesize substituted metal oxides .After preliminary characterization, Rietveld refinements of the powder is carried out to ascertain the presence of Ga in the mixture and then further optical properties measurements are also done.

Future Projects

1. Photoluminescent Rare earth doped Tungstate and Molybdate Nanoparticles for Biological Applications

The investigation of fundamental processes in cells and t\issues requires methods for the fast, sensitive, easy and compatible detection of the various molecular or ionic species. In this regard, one of the most popular methods to meet these challenges is the use of photoluminescence or fluorescence techniques and this is called bio-labelling. Though many types of materials have been used as bio-markers of tissues, recently, nanometer-sized up conversion phosphors are evolving as a new class of inorganic materials for bio-labelling. This is because they have promising, partly size-dependent spectroscopic features composed of a crystalline host doped with emissive lanthanide ions (localized luminescent centers). We intend to synthesize rare earth doped materials for these applications.

2. Design of Novel Bismuth based Nanomaterials for the Photcatalytic Oxidation of Glycerol into Value Added Products : Funding Agency Considered: MNRE, DST, India

The key challenge in this project is to selectively oxidize glycerol to a particular product using environmental friendly methods. In this regard, photocatalysis is one of the green processes that have been used in recent times for degradataion of dyes and also for organic reactions. This project aims to design novel Bismuth based nanomaterials as photocatalysts using various synthesis strategies in order to selectively oxidize glycerol to value added products.

Dr. Sanjeev. P. Maradur



Asst. Professor, Materials Science Since December 2012

Curriculum Vitae

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

Broad Areas of Research:

- 1. Homogeneous polyoxometalate catalysis for clean organic synthesis.
- 2. Heterogenization of homogeneous catalysis & its application on various chemical processes.
- 3. Biomass utilization/refinery to value added products.

Total no of publications in international journals: 10

Participation in workshops, conferences and symposiums: 6

Membership of Professional bodies: Member of International Zeolite Association (IZA) (2010-present) **Govt. sponsored Project:** Awarded Seed Money for Young Scientist Program from Vision Group of Science and Technology, Govt. of Karnataka for one year (Rs. 5 Lakhs)

Representative Publications:

- <u>Sanjeev P Maradur</u>, ChangHyo Kim,Kim, So, Kim, Bo-Hye, (Kim, Woo Chul, Yang, KapSeung"Development of low-cost carbon fiber technology based on lignin copolymer precursors". Synth Metals162 (2012) 453-459.
- Sanjeev P. Maradur, Changbum Jo, Dae-Heung Choi, Kyeongyeon Kim and RyongRyoo; "Mesoporous Polymeric Support Retaining High Catalytic Activity of Polyoxotungstate for Liquid-Phase Olefin Epoxidation Using H₂O₂".ChemCatChem3(2011)1435-1438.
- V. T. Magalad, A. R. Supale, <u>S. P. Maradur</u>, G. S. Gokavi, T. M. Aminabhavi "Preyssler type heteropolyacid-incorporated highly water-selective sodium alginate-based inorganic-organic hybrid membranes for pervaporation dehydration of ethanol". Chemical Engineering Journal, 159 (2010) 75-83.
- 4. <u>S. P. Maradur.</u>and G. S. Gokavi; "Heteropoly acid catalyzed synthesis of 3,4-Dihydropyrimidin-2(1H)-ones ". Catalysis Communications 8 (**2007**) 279–284.
- 5. <u>S. P. Maradur</u>. S. B. Halligudi and G. S. Gokavi; "Oxidation of aliphatic and benzylic alcohols by Oxone®, catalysed by 12-tungstocobaltate (II)". Catalysis Letters. 96 (**2004**) 165-167.

Patents:

1. Inventors: RyongRyoo, Dae-Heung Choi, **Maradur Sanjeev** "Production method of mesoporous organic polymer catalyst, mesoporous organic polymer catalyst produced using the method, and process for epoxidation of olefins using the catalyst". Registration number: 1011704860000, Dated 2012/07/26 (Granted).

2. **Inventors**: Yang, KapSeung. **Maradur Sanjeev P**.Kim, YeongCheol. "Method for preparation of carbon fibers using lignin copolymer and the carbon fibers thereby". Registration number: 1012261910000, Dated 2013/01/18 (**Granted**).

Current Projects:

Project 1: Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, potential fuel additive molecules for diesel and gasoline (**Ongoing**) Principal Investigator: Dr. Sanjeev P. Maradur

This proposed research involves the preparation of a new class of advanced structured polymers as heterogeneous catalysts which may overcome the problems and limitations of the commercial polymeric supports or the production of fuel additives from glycerol originating from biomass. Recently, mesopolymers having pure organic frameworks have been discovered. The inclusion of functional groups onto mesoporous polymers will be investigated for conversion of glycerol which is available in plenty which comes out as by-product from biodiesel industry into valuable chemicals which may find applications as fuel additives in automobile industries.

Project 2: Brønsted acid generation of alumina-supported molybdenum oxide calcined at high temperature: A promising catalyst for solketal synthesis (Collaborative Research)
Principal Investigator: Dr. Sanjeev P Maradur
Co-Investigator: Dr. Ganapati V Shanbhag
Research Students: Mr. Dundappa and Mr. Manjunathan

Metal oxides supported onto alumina shows some interesting properties after calcinations. There are many reports in the literature of supported metal oxides onto alumina which were calcined below 550°C exhibited Lewis acidity (MoO_3 , Nb_2O_5). The same materials when subjected to higher calcinations temperatures i.e. >800°C, bronsted acidity is generated onto the catalyst.

Aim of this project is to synthesize selectively solketal, a five membered ring product. Different wt% catalysts ranging from 5 to 30 wt% molybdenum onto alumina have been prepared and screened for solketal synthesis. From the initial screening, it was observed that 10 wt% catalysts gave highest selectivity for solketal (85%) at glycerol conversion at 75%. Whereas for the other catalysts and selectivity was less compared to 10 wt% catalyst. The reason for high selectivity for 10wt% catalyst is due to the creation of bronsted acidic sites which are at optimum level at this loading. Development of GC- analysis method for accurate determination of conversion and selectivity is done by preparing series of synthetic mixtures of reactant and product which mimic actual reaction conditions. A new GC program was also developed for the analysis and the standard graph of reactant/product wt v/s area has been constructed. From the std graph, we can now find out conversion and selectivity with high accuracy (up to 0.01 decimal). Characterization of the catalysts for quantification of acidity by pyridine-IR and optimization of reaction conditions. is under progress.

Project 3: Molybdenum oxide supported onto alumina calcined at high temperature: A promising catalyst for nopol synthesis **(Collaborative Research)** Principal Investigator: Dr. Sanjeev P Maradur Co-Investigator: Dr. Ganapati V Shanbhag Research Students: Mr. Dundappa and Mr. Vijay Kumar

effect of solvents on conversion and selectivity is ongoing.

The Prins reaction is an important C-C bond forming reaction in organic synthesis. It is an acid catalyzed condensation of olefin with aldehyde leading to the formation of synthetic organic chemicals like 1,3-dioxanes and unsaturated alcohol. The condensation product of -pinene and paraformaldehyde, is generally used in the agrochemical industry to produce pesticides and also in manufacturing household products such as soaps, detergents and polishes. In accordance with the concept of green chemistry, heterogeneous catalysts were widely explored and utilized in this reaction. Many of the reports for Prin's reaction are tin based catalysts and also the catalyst to substrate ratio is more in most of the cases. From green chemistry point of view, it is worth exploring a novel efficient catalyst with less toxic or non toxic in nature and which will overcome the problems associated with the already reported catalyst systems. We have initiated this project with molybdenum/alumina catalyst by varying the amount of molybdenum from 0.2 to 30 wt %.Different wt ratio of catalyst have been prepared and calcined at 800°C. Initial screening of the catalyst has been done. The maximum conversion of -pinene was seen over 10 wt% Mo/alumina catalyst and selectivity for nopol was 85%. The 10 wt% catalyst has been chosen for optimization of reaction conditions. The effect of calcination temperature on performance of catalyst,

Biological Sciences

Introduction

Focus of biological sciences division is on the research programs that explore the structure and function of proteins, protein-protein, protein-inhibitor interactions, mycology, treasure hunt in the world of fungal secondary metabolites and protein chemistry. The present Director, Prof. A. B. Halgeri with a vision to give more impetus towards diverse areas of experimental sciences, established the "Division of Biological Sciences" in 2010, following the establishment of Material Sciences Division. The division has research facility with more than 3000 sq. ft. of lab space and is equipped with all facilities for microbial studies such as isolation, identification of microorganisms, biochemical studies like anti-microbial assay and anti-oxidant assay systems. Plant and microbial secondary metabolites extraction systems are available.

Molecular biology facilities are also established for the cloning, recombinant expression, characterization and crystallization of key biomolecules. Recently, we have expanded our lab space by another 3000 sq. ft. to provide an opportunity for researchers coming from diverse areas of biology. The research activities in the department are supported by in-house funding (PPISR), as well as grants from agencies such as



Department of Biotechnology (DBT) and Vision Group On Science and Technology (VGST). Our mission is to advance knowledge of basic biological sciences and apply these understanding to improve human health, protect environment and improve our economic status. We strive to fulfill our mission every day educating and preparing the next generation of scientists in biological sciences.

Broad Areas of Research:

- 1. Understanding the fascinating world of biological molecules and their structure with atomic-levelaccuracy that gives information on form and biological function.
- 2. Studies on Endophytic fungi from medicinal plants and their secondary metabolites, bioactive compounds and enzymes.
- 3. Bioconjugation and PEGylation technology: Chemical modification of therapeutic proteins and drugs using linker chemistry and polyethylene glycol to enhance their activity and half-life.

Academic and Research Highlights:

The Biological Sciences division has made considerable progress in the last three years. The department



published several papers has in national and international journals and the faculties/students have delivered talks in national/international meetings. The microbiology group has isolated more than 100 endophytic fungi from and medicinal plants secondary metabolites were tested for their antimicrobial, anti-oxidant and anti-diabetic properties. Several positive fungi were also genetically identified by PCR method and the resulting sequences

were deposited in GenBank (33 entries). We have also purified several secondary metabolites from selected endophytic fungi which are active against either microbes or inhibitors of key enzymes such as amylase and aldose reductase. Efforts have been made towards the identification of these compounds using various techniques such as UV-Visible spectroscopy, Infrared spectroscopy, 1D and 2D NMR analysis. Interestingly, several identified compounds were much more active compared to that already available in the market.

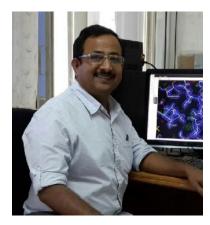
The structural biology group has successfully completed the structure of three proteins from enolase superfamily and deposited in Protein Data Bank(PDB), an international repository of protein structures. These structures represent the first few protein structures contributed to PDB from PPISR. We have also solved the structure of adenine phosphoribosyl transeferase from *Y. pseudotuberculosis* and the coordinates were deposited in Protein Data Bank with code 4MB6. Co-crystallization of APRT from *Y*.

pseudotuberculosis with its ligands adenine and adenosine monophosphate (AMP) has been carried out. Work on modification of a ligand, B7-2(CD86) present on the antigen presenting cells, has been initiated. We are also analysing data sets containing very weak anomalous signals to drive the complete structure solution of proteins. For example, sulphur atoms that are intrinsic to proteins or metal ions like calcium, potassium etc that are picked up from crystallization conditions. Analyzing 9 such cases, we have shown that the weak anomalous signals can be exploited to solve the



structures *ab initio* where automated software can fail in about 50% of the cases. Also, many new instruments have been acquired under CISEE program of VGST, Karnataka.

Faculty Profiles



Dr. Udupi A. Ramagopal

Ramalingaswami fellow (DBT) Associate Professor Poornaprajna Institute of Scientific Research

Educational and Professional Qualifications

- 2014 current, Associate Professor : 2011 2013 Assistant Professor, (Ramalingaswami Fellow DBT), Poornaprajana Institute of Scientific Research, Bangalore, India.
- 2011 Present: Visiting Faculty, Albert Einstein College Of Medicine, New York, USA. http://www.einstein.yu.edu/home/faculty/profile.asp?id=9276
- 2009-20011: Instructor, Albert Einstein College Of Medicine (AECOM), USA
- 2005-2009: Faculty Associate, Albert Einstein College Of Medicine, New York, USA.
- 2003-2005: Senior Research Associate, Department of Biochemistry, Albert Einstein College Of Medicine, New York, USA.
- 2001-2003: Visiting Fellow, National Institute of Health, USA.
- 2001: PhD, Department of Physics, Indian Institute of Science, Bangalore, India.

Broad Areas of Research

- 1. Costimulatory molecules: Biology and therapeutic intervention.
- 2. Structural study of proteins from enolases superfamily.
- 3. Structural Studies of Adenine Phosphoribosyltransferases from Pathogenic Bacteria
- 4. Testing the limits of phasing methodologies using weak anomalous signal

Awards and achievements

- 1. Ramalingswami fellow, DBT, India (2011 current).
- 2. Best thesis "Kumari L. A. Meera Award and a Gold Medal", 2001, IISc, India.
- 3. Visiting Fellow (2001 2003, NIH, USA).
- 4. Visiting Faculty (Albert Einstein College of Medicine, 2011 current).
- 5. Proposal reviewer: Macromolecular Crystallography, APS, Argonne National Laboratory, USA.
- 6. Served in the "User Executive Committee 2002-2003" of National Synchrotron Light Source, Brookhaven National Laboratory, USA.
- 7. Jeffery Award (poster award IUCr 2002, co-author).
- 8. Contributed >200 protein structures to World Wide Protein Data Bank (wwPDB).
- 9. Invited Instructor (2003-2010) at <u>RapiData</u>, a comprehensive course offered at Brookhaven National Laboratory for budding crystallographers around the world (http://www.bnl.gov/rapidata/).
- 10. Referee for Acta Crystallographica Section D, Biological crystallography.
- 11. Doctoral Advisory committee member for two students registered under Manipal University
- 12. Scientific Advisor "Genelon Life Science Ltd.", Yelahanka, Bangalore

Representative Publications:

- Ramagopal, U. A., Ramakumar, S., Sahal, D., Chauhan, V. S. 2001, De novo design and characterization of an apolar helical hairpin peptide at atomic resolution: Compaction mediated by weak interactions. <u>Proc. Nat. Acad. Sci. (USA) 98(3)</u>: 870-874. JIF (2011) = 9.8
- Ramagopal, U. A., Ramakumar, S., Joshi, R. M., Mathur, P. and Chauhan, V. S. 2002, Dehydrophenylalanine zippers: Strong helix-helix clamping through network of weak interaction. <u>Protein Engineering</u> 15(4). 331-335. JIF (2011) = 2.9
- Ramagopal, U. A., Dauter, M. and Dauter, Z. 2003. Phasing on anomalous sulfurs: What is the limit? <u>Acta Cryst</u>. D59, 1020-1027. JIF (2011) = 12.6. (Cited ~ 80 times and referred in popular book "Biomolecular crystallography" by Bernhard Rupp). (Comment: http://www.nsls.bnl.gov/newsroom/publications/newsletters/2003/03-nov.pdf)
- Klein, M. G., Shi, W., Ramagopal, U. A., Tseng, Y., wirtz, D., Kovar, D. R., Staiger, C. J. and Almo, S.C. 2004. Structure of the actin crosslinking core of fimbrin. <u>Structure</u>, 12(6), 999-1013. JIF (2011) = 6.4, (Comment:

http://www.structure.org/content/article/abstract?uid=PIIS0969212604001649)

- Ramagopal, U. A*., Thirumuruhan, RA., Fedorov, L., Dauter, Z. and Almo, S.C. 2005. Radiation-induced site-specific damage of mercury derivatives: phasing and implications. <u>Acta</u> <u>Cryst</u>. D61, 1289-1298. (*Corresponding author), JIF (2011) = 12.6
- Cao., E, Ramagopal, U. A., Fedorov, A., Fedorov, E., Yan, Q., Lary, J., Cole, J., Nathenson, S. G. and Almo, S. C. 2006. NTB-A Crystal structure: implications for homophilic interactions and signaling within the SLAM family of receptors. <u>Immunity</u>, 25(4), 559-570. JIF (2011) = 21.6
- Chattopadyay, K., Ramagopal, U. A., Mukhopadhaya, A., DiLorenzp, T. P., Brenowitz, M., Nathenson, S. G. and Almo, S. C. 2007. Novel assembly and structural properties of human GITRL: Implications for function. <u>Proc. Nat. Acad. Sci. (USA)</u>. 104(49), 19452-19457. JIF (2011) = 9.8
- Cao, E., Ramagopal, U. A[#]., Mukhopadhaya, A., Fedorov, A., Fedorov, E., Zencheck., W. D., Lary, J. W., Cole, J. L., Deng, H., DiLorenzo, T. P., Allison, J. P., Nathenson, S. G. and Almo, S. C. 2007. T Cell Immunoglobulin Mucin-3 Crystal Structure Reveals a Novel Ligand Binding Surface. <u>Immunity</u>, 26(3), 311-321. JIF (2011) = 21.6.

(Comment: http://www.immunity.com/content/article/abstract?uid=PIIS1074761307001835_)

 Chattopadyay, K., Ramagopal, U. A., Brenowitz, M., Nathenson, S. G. and Almo, S. C. 2008. Evolution of GITRL immune function: Murine GITRL exhibits previously unrecognized structural and biochemical properties within the TNF ligand superfamily. <u>Proc. Nat. Acad. Sci. (USA)</u>. 105(2), 635-640. JIF (2011) = 9.8.

News: http://stke.sciencemag.org/cgi/content/abstract/sigtrans;1/3/ec30

- Samanta, D., Ramagopal, U. A., Nathenson, S. G. and Almo, S. C. 2012, Structure of Nectin-2 reveals determinants of homophilic and heterophilic interactions that control cell-cell adhesion. <u>Proc. Nat. Acad. Sci. (USA)</u>, 109(37):14836-40, JIF (2011) = 9.8.
- Rubinstein, R., Ramagopal, U. A., Nathenson, S. G., Almo, S. C. and Fiser, A. 2013, Functional Classification of Immune Regulatory Proteins. <u>Structure (cell press)</u>, 21(5), 707-717. JIF (2011)
 = 6.4. Comment at : http://www.sciencedirect.com/science/article/pii/S0969212613001251
- Ramagopal, U. A., Dulyaninova, N. G., Varney K. M., Wilder, P. T., Nallamsetty, S., Brenowitz, M., Weber D. J., Almo S. C. and Bresnick, A. R. 2013, Structure of the S100A4/myosin-IIA complex. <u>BMC Struct. Biol.</u>, 13(1), 31. [Epub ahead of print], JIF (2011) = 2.5.

Research highlights

We are interested in structure based functional characterization of key molecules of biological and medicinal importance. We use techniques like crystallography, bioinformatics and various biochemical, biophysical techniques to study these molecules. These studies play an important role in understanding key biological processes at the molecular level that could lead to the development of novel therapeutics.

We are also interested in de novo design of self-assembling proteinaceous materials exploiting intrinsically symmetric and stable protein motifs. **Lab members:**



Dr. Raghurama P. Hegde (Research Associate)



Ms. Pavithra G. C. (Graduate Student)



Ms. Swetha L. (Graduate Student)

Sponsored Projects:

- Grant titled "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.
- 2. Ramalingaswami Fellowship titled "Costimulatory molecules: Biology and therapeutic intervention", Department of Biotechnology (DBT), New Delhi, India.

Current Projects:

1. Structural Studies of Adenine Phosphoribosyltransferases from Pathogenic Bacteria

Primary Investigator: Dr. Ramagopal U. A.

Research Student: Mrs. Pavithra G. C.

Adenine phosphoribosyltransferase (APRT), a key enzyme in purine salvage pathway, catalyzes a reaction between adenine and phosphoribosyl pyrophosphate to produce adenosine monophosphate (AMP) and pyrophosphate. Pathogenic bacteria such as Y. pseudotuberculosis, M. pneumonia, H pylori and F. tularensis that are known to cause pseudotuberculosis, gastritis/duodenal cancer and tularemia respectively depend solely on the salvage pathway for their survival. Hence, understanding the structure and function of these APRTs appears to be the key step towards the design of effective drugs to combat diseases caused by these organisms. We have selected APRTs from the above mentioned organisms for this study.

The structure of apo APRT from Y. pseudotuberculosis is successfully completed and is deposited in PDB with an ID 4MB6. To understand the mode of protein-ligand interactions at the molecular level, cocrystallization of APRT from Y. pseudotuberculosis with its ligands, Ribose-5-phosphate (R5P), adenine and adenosine monophosphate (AMP) has been carried out. X-ray diffraction data was collected from crystals of protein complexed with adenine and AMP.

2. Testing the limits of macromolecular crystallographic phasing

Primary Investigator: Dr. Ramagopal U. A.

Research Associate: Dr. Raghurama P. Hegde

One of the commonly used current methods for the resolution of phase problem in macromolecular crystallography is the use of anomalous scattering to derive phases. This conventionally required the use of heavy atom derivatives and/or production of selenomethionine derivatives. In the last decade or so there have been dramatic improvements in methods and techniques of ab initio structure solution of macromolecules. The current methods are powerful enough to use weak anomalous signals, However, many crystallographers go through the laborious process of producing heavy atom/selenomethionine

derivatives, including introduction of mutations if necessary for the derivatization. The aim of this project is to show that using the weak anomalous signals from atoms, like sulphur, in the native protein itself or anomalous scatterers picked from crystallization conditions, we can still obtain phases that can be used for model building and refinement. This would particularly be very useful in cases where molecular replacement would fail because the protein of interest does not have sufficient homology with any protein of known structure or when heavy atom derivatives for the protein cannot be obtained.

Analyzing 9 such cases, we have shown that the weak anomalous signals can be exploited to solve the structures ab initio where automated software can fail in about 50% of the cases. Using these results we would like to highlight to the macromolecular crystallography community how a careful look at a seemingly useless data can sometimes yield a protein structure.

3. Structural Study of proteins from the enolase superfamily:

Primary Investigator: Dr. Ramagopal U. A.

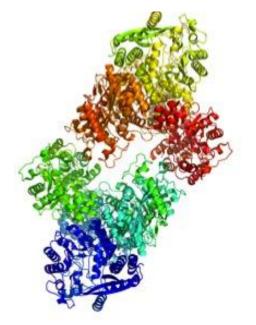
Research Associate: Dr. Raghurama P. Hegde

The Enolase superfamily consists of enzymes related by their ability to catalyze the abstraction of the proton of a carboxylic acid to form an enolic intermediate. Although each reaction catalyzed by these enzymes is initiated by this common step, their overall reactions as well as the stereochemical consequences of the -elimination reactions are diverse. Glucarate hydratase is one such enzyme catalyzing the reaction D-glucarate <-> 5-dehydro-4-deoxy-D-glucarate + H₂O as part of metabolism of D-glucarate, a natural product that can serve as a growth substrate for a number of bacteria. We were able to solve two protein structures from this family. Both the structures have been successfully completed and deposited in the Protein Data Bank (PDB), with PDB id 4HN8 for the D-glucarate dehydratase from Pseudomonas mendociana and 4HRY for the putative glucarate dehydratase from Acidaminococcus, making them the first protein structures to be deposited from PPISR. Similarly, mandalate racemase and muconate lactonising enzymes are bacterial enzymes involved in aromatic acid catabolism. These enzymes are members of the enolase superfamily. We have pursued the structure of a mandalate racemase/ muconate lactonising enzyme from Pseudovibrio sp. The structure solution/refinement is complete and the structure has been deposited in the PDB with id 4JHM. We are analyzing all the three structures of this superfamily. Biochemical and biophysical studies from our collaborators at Enzyme Function Initiative, Chicago, USA., together with these structures, we hope to functionally characterize these enzyme.

4. Structural mimicry of CTLA-4 ligand binding surface and moderate modification of B7 family of ligands

Costimulatory receptors and ligands are essential for both innate and adaptive immunity. Soluble versions of these receptors and their cognate ligands, as well as monoclonal antibodies targeted against these proteins, represent a major class of protein-therapeutics for the manipulation of immune responses to treat a wide range of infectious diseases, autoimmune diseases and malignancies. These efforts have already resulted in several proteinaceous therapeutic products, approved as biopharmaceuticals, mainly for cancer and autoimmune diseases. For example, Orencia (Abatacept) marketed by Bristol-Mayer Squibb is a fusion protein formed by the extracellular domain of CTLA-4 and the Fc region of immunoglobulins (Ig), known as CTLA-4-Ig is a drug for rheumatoid arthritis. A complimentary treatment is blocking CTLA-4 signalling using monoclonal antibodies to augment T cell mediated responses against tumors. Again, the recent FDA approval of CTLA-4 antibody known as MDX-010 and marketed as Yervoy suggest that controlling the response of these molecules is an effective strategy to control the immune response and hence to treat autoimmune diseases and cancer. We are interested in designing and characterization of peptide mimicking the ligand-binding surface of CTLA-4. Similarly, we also aim to modify the receptor-binding surface of B7 family members (receptors for CTLA-4 and CD28), which will also provide the mechanistic difference between the B7 isoforms and their role in immunological synapse. The genes coding Human B7.2 V domain, human CTLA-4 V domain were obtained and cloned in to pNIC28-Bsa4 vector.

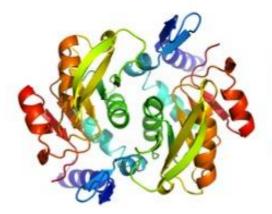
Protein structures from the lab:



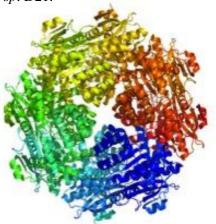


PDBID:**4HN8**,D-glucaratedehydratasefrom*Pseudomonas*mendocina ymp..

PDB ID: **4HYR**, D-glucarate dehydratase from *Acidaminococcus sp*. D21.



PDB ID: **4MB6**, APRT from *Yersiniapseudotuberculosis*



PDB ID: **4JHM** Mandelate racemase /muconate lactonizing enzyme from *Pseudovibrio sp*

Dr. Ananda K.



Asst. Professor Biological Sciences Poornaprajna Institute of Scientific Research Email: ananda@poornaprajna.org

Educational and Professional Qualifications

2011-Present: Assistant Professor, PPISR, Bangalore, India
2010-2011: Faculty Fellow, PPISR, Bangalore, India
2004-2010: Post Doctoral Fellow, Albert Einstein College of Medicine, NY, USA
2004-2004: Lecturer, P A College of Engineering, Mangalore, India
2003-2004: Project Associate, IWST, Bangalore, India
1999-2003: Administrative Supervisor, KSRTC, Govt. of Karnataka, India
1996-2001: PhD, Mangalore University, Mangalore, India.
1995-1996: Project Assistant, College of Fisheries, Mangalore, India
1993-1995: MSc, Biosciences, Mangalore University, Mangalore, India

Broad areas of interest

1. Antimicrobial, anti-oxidants, anti-diabetic compounds from endophytic fungi isolated from medicinal plants.

2. Bioconjugation of therapeutic proteins and PEGylation technology

Membership of Professional bodies

Life Member of Mycological Society of India, India

Recent Publications from the list of 25:

- Sathish, L., Pavithra, N. and Ananda K. (2014) Evaluation of antimicrobial activity of secondary metabolites and enzyme production from endophytic fungi isolated from Eucalyptus citriodora. Journal of Pharmacy Research 8(3); 269-276.
- 2.Garudachari B, Isloor AM, Satyanarayana MN, Fun HK, Pavithra N and **Ananda K.** (2013) Design and regioselective synthesis of trifluoromethylquinolone derivatives as potent antimicrobial agents. European Journal of Medicinal Chemistry 68; 422-432.
- 3.Chethan PD, Vishalakshi B, Sathish L, **Ananda K**, and Poojari B. (2013) Preparation of substituted quaternized arylfuran chitosan derivatives and their antimicrobial activity. Int J Biol Macromol. 59:158-64.
- 4.Sathish L., Pavithra N and **Ananda K**. (2012) Antimicrobial Activity and Biodegrading Enzymes of Endophytic Fungi from Eucalyptus. Int J Pharm Sci Res. 3(8): 2574-2584.
- 5.Pavithra, N., Sathish, L., **Ananda, K**. (2012) Antimicrobial and Enzyme Activity of Endophytic Fungi Isolated from Tulsi. Journal of Pharmaceutical and Biomedical Sciences. 16 (12):1-6.
- 6.Ananda, K., Manjula, B. N., Meng, F., Acharya, V. N., Intaglietta, M., and Acharya, S. A. (2012) Packing Density of the PEG-Shell in PEG-Albumins: PEGylation Induced Viscosity and COP are Inverse Correlate of Packing Density. Artif Cells Blood Substit Immobil Biotechnol. 40(1-2):14-27.
- 7. Acharya, S. A., Intaglietta, M., Tsai, A. G., Ananda, K. and Meng, F. (2011) Engineering the Molecular Shape of PEG-Hemoglobin Adducts for Supraperfusion, in Chemistry and Biochemistry of Oxygen Therapeutics: From Transfusion to Artificial Blood (eds A. Mozzarelli and S. Bettati), John Wiley & Sons, Ltd, Chichester, UK. doi:10.1002/9781119975427.ch25

PhD Students:



Mr. Sathish L.

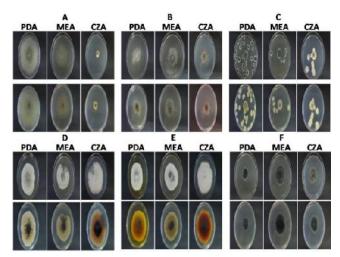


Ms. Pavithra N.

Current Projects

- 1. Antimicrobial and anti oxidants of endophytic fungi from Medicinal plants
 - Principal Investigator: Dr.Ananda
 - Research Fellow: Sathish L

During the annual report year endophytic fungi isolated last year were grown in large scale for the mass production of antimicrobial compound and antioxidant compounds. All the active fungi where identified by molecular DNA sequencing method and submitted data to the Gen Bank. The most active two fungi were selected for the detailed studies. Secondary metabolites were isolated from these two isolates and trying to identify the active compounds. Optimization of secondary metabolite production using different media, temperature, pH were perfomed and best method is selected for the further studies.



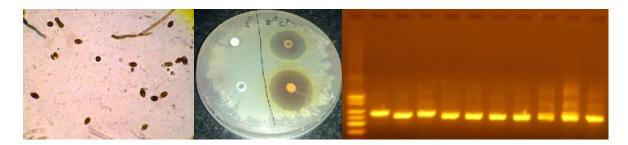
Ethyl acetate extracts were further purified using silica gel columns and active fractions were pooled for the studies. Minimum inhibition concentration of these compounds were studied using pathogenic microbes. Column purified fractions were used for the LC-MS, NMR studies etc for the purpose of identification. Pure compound separation is a challenge for us with existing research facility at PPISR. We are trying to identify the semipurified compounds using LC-MS, NMR etc. We are trying other methods such as crystallization of these compounds so that we can solve it by X-ray defraction studies. Two publications came from this project and another two to three publications are expected from this project.

2. Anti-diabetic compounds of endophytic fungi from medicinal plants used for the treatment of diabetes. Principal Investigator: Dr.Ananda

Research Fellow: Pavithra N

Hyperglycemic conditions can be controlled by the some of the inhibitors used in starch metabolism. We have selected medicinal plants used for the treatment of diabetes and isolated endophytic fungi and screened for the amylase and aldose reductase inhibitors. We have isolated more than 80 fungi and screened them for these inhibitors and few of them found positive for the inhibitors. The best active fungi were further grown in large scale and extracted secondary metabolites. All the positive fungi were identified by molecular identification and sequence submitted to Gen Bank in the name of PPISR. These endophytic fungal data can be accessed worldwide in the name of poornaprajna.

Extracted secondary metabolites were purified using column chromatography and each fraction was tested for the inhibitors. Active fractions were pooled and IC_{50} values calculated are very near to the drugs available in the market.



Further there is need of identification of these compounds. At present we are trying to identify using LC-MS, NMR etc. one publication has came from this project and two publications are under preparation. Two more publications are expected after identification of the active compounds.

3. Anticancer metabolites from endophytes of medicinal plants

Pricipal Investigator: Dr. Ananda

Endophytic fungi isolated from plants used for the cancer treatment. Grow them in fungal broth media and extract secondary metabolites. Concentrated crude extracts screened against cancer cell lines in collaboration with Genelon Pvt Ltd. There are few endophytic fungi found to be anticancer active. These are given for the further study on cancer cells for the dosimetry.

Theoretical Sciences

Introduction

The Division was established in 2005 with the induction of Dr. Sujit Sarkar in 2005, and formally recognized as such during the renewal of PPISR's recognition by Manipal University (MU) in 2010, along with the Materials Science and Biological Sciences Divisions. Per the suggestion of Prof. K. J. Rao of AMEF and the Director, Prof. A. B. Halgeri, the scope of the Divison was enlarged to include philosophical studies, apart from mainstream physics research being pursued by the existing faculty members, Drs. Sujit Sarkar and R. Srikanth. Dr.Manisha Kulkarni (specializing in number theory) was a faculty member during 2007--2011 and Dr. S. G. Bhargavi (specializing in gamma-ray astronomy) was a honorary faculty member during 2012--2013.

Mr. Omkar and Mr. Arvinda, who registered for PhD in Sep 2011 and Feb 2011 with MU, respectively, with Dr. R. Srikanth, and Mr. G. N. Chandan, who has just joined with Dr. Sujit Sarkar, are the three students with the Division. Mr. Kallol Roy, who has submitted his PhD thesis in the ECE Dept, IISc, has joined with Prof. Sujit Sarkar as DST-sponsored postdoc.

Broad areas of research:

- 1. Quantum physics of many-body systems and condensed matter physics
- 2. Non-equilibrium statistical physics
- 3. Quantum information processing & cryptography; foundations of quantum mechanics
- 4. Metamathematics and computability theory in physics

Specific problems pursued by members include: (1) Quantum criticality of geometric phase in coupled optical cavity arrays under linear quench; (2) Quantum phase transition of light in coupled optical cavity arrays: A renormalization group study; (3) Solitons and spin transport in an antiferromagnetic spin chain; (4) Counterfactual quantum certificate authorization; (5) Nonclassicality of signaling correlations; (5) Characterizing quantum noise using quantum error correcting codes; (6) Biologically inspired category theory and process calculus approach to software design with applications to cryptography and data management.

Researchers in the Division have over 77 papers in prestigious, peer-reviewed international journals over the last 8 years, presented various invited talks, and have served as referees for various journals of repute.

Research Highlights:

- 1. Studies on the applicability of cavity QED techniques to quantum walks on a network, by Dr. Sujit Sarkar.
- 2. Connecting and combining to tasks of quantum error correction and quantum state tomography in quantum information processing, in work by Mr. Omkar and Dr. R. Srikanth.
- 3. A novel usage of quantum temporal correlations for device independent cryptography, in works by Mr. Arvinda, Ms. Akshata and Dr. R. Srikanth.
- 4. Quantum Simulation in Quantum Many Body System.

Faculty Profiles



Dr. Sujit Sarkar Asst. Professor Theoretical Science

Qualification:

1. M. Sc (Kolkata University)

2. Ph. D in Quantum Many Body Physics in Strongly Correlated System from Saha Institute of Nuclear Physics.

3. Postdoctoral Experience: (A). IISc Physics Department

- (B). Bar-Ialn University
- (C). Max-Planck Institute, Germany as a Guest Scientist
- (D). The Weizmann Institute of Science.

Areas of Research Interest

(1). Quantum Many Body Physics and Quantum Field Theoretical Studies of Quantum Condensed Matter System.

- (2). Cavity Quantum Electrodynamics.
- (3). Quantum Walk and its Application in Physical System.
- (4). Non-equilibrium Statistical Physics.
- (5). Quantum Correlation Functions.

Research Group:



Dr. Kallol Roy (Post Doc)



Mr. Chandan G N (JRF)

Selected Publications:

(1). Quantum Criticality of Geometric Phase in Coupled Optical Cavity

Under Linear Quenching, (2014), Sarkar S, Physica B, marginally accepted, revised version)

(2). Josephson Relations in Superconducting Charge Qubit Lattice, Sarkar S, Annals of Physics (under review process, 2013-14).

(3). Quantum Correlation Function in Superconducting Quantum Dot Lattice, Sarkar S, Annals of Physics (under review process, 2013-14).

(4). Quantum Phase Transition of Light, Sarkar S, Journal of Mathe and Theoretical Physics, Sarkar S, (under review process, 2013-14).

(5). Emergent Majorana Fermions in Cavity QED Lattice, Sarkar S, Journal of Mathe and Theoretical Physics, (under review process, 2013-14).

(6). Quantum Simulation and Quantum Criticality of Heisenberg Spin System in Cavity QED Lattice, Sarkar S, Hu C D and Lee R K, Phys. Rev. A (under submission process, 2014).

7) Collapse and Revival of Entanglement of Two Qubits in Superconducting Quantum Dots Lattice with Magnetic Flux and Inhomogeneous Gate Voltage" Sujit Sarkar, Physica B 414, 26 (2013)

Research Projects:

(1). DST PROJECT: Geometric Phase and Quantum Phase Transition in Quantum Many Body System Principal Investigator: Sujit Sarkar

Response/Progress of Application: Project has started since October'13.

Project in a Nutshell: Total Amount: 27 Lakhs.

Time Duration of the Project: 3 Years .

Number of Students Involve in This Project: 2.

Number of Research Publication (expected): 6 in Internationally Reputed Journal.

One JRF has joined from 1st January'14 and a Postdoctoral Fellow has joined in October'2013.

Dr. R. Srikanth, Assistant Professor



Phone: 98445 93440 Coordinator, Center for Foundational Studies, PPISR Visiting scientist, Raman Research Institute, Bangalore E-mail:srik .AT.poornaprajna.org Webpage: poornaprajna.org/srik

Areas of Interest

Quantum information processing with open quantum systems: multi-qubit noise, quantum error correction.

- Quantum cryptography: Counterfactual schemes; device-independent scenario.
- Foundations of quantum mechanics: signaling effects and computational complexity in postquantum correlations.
- Meta-mathematics and computability in physics: free will, individuation and identity

Curriculum vitae

- 2009-Present: Asst. Professor, PPISR, Bangalore, India.
- 2006-2009: Faculty Fellow, PPISR, Bangalore, India.
- 2003-2006: Postdoctoral fellow, Raman Research Institute, Bangalore, India.
- 2001-2003: Postdoctoral fellow, Center for Theoretical Studies, Indian Inst. of Science, Bangalore, India.
- 1999-2001: Postdoctoral fellow, Indian Institute of Astrophysics, India.
- 1999: PhD, Dept. of Physics, Indian Institute of Science, Bangalore, India.

PhD Students:



Mr. Omkar S



Mr. Aravinda S

Representative publications

- 1. *The quantum cryptographic switch.* N. Srinatha, S. Omkar, R. Srikanth, S. Banerjee and A. Pathak. Quantum Information Processing 13, 59 (2014).
- Unification of Bell, Leggett-Garg and Kochen-Specker inequalities: Hybrid spatio-temporal inequalities. S. Das, S. Aravinda, R. Srikanth and D. Home Europhysics Letters 104 60006 (2013).
- 3. Akshata Shenoy H, R. Srikanth and T. Srinivas. Counterfactual cryptography. Europhysics Letters, 103, 60008, (2013).

- S.Omkar, R. Srikanth and S. Banerjee. Dissipative and Non-dissipative Single-Qubit Channels: Dynamics and Geometry.
 Quantum Information Processing, 12, 3725-3744 (2013).
- Balaji Rao, R. Srikanth, C. M. Chandrashekar and Subhashish Banerjee. Quantumness of noisy quantum walks: A comparison between measurement-induced disturbance and quantum discord. Phys. Rev. A 83, 064302 (2011)
- 6. R. Srikanth. Entanglement, Intractability and No-signaling. Physica Scripta 81 (2010) 065002.
- 7. R. Srikanth and Subhashish Banerjee. Complementarity in atomic and oscillator systems. Physics Letters A 374, 3147 (2010).

Graduate Students

- 1. **Omkar Srikrishna**: Operator Sum Representation for Quantum Noise due to Dissipative and Non-demolition Interaction with a squeezed Environment.
- 2. Akshata Shenoy H. (with Prof. T. Srinivas of ECE, IISc): Nonlocal, counterfactual and deviceindependent schemes for Quantum Cryptography.
- 3. S. Aravinda: Foundational Aspects of Contextuality and Nonlocality.

Projects / Patents / Recognitions

DST-sponsored project (Rs. 12 lakhs) studying the properties of entanglement and nonlocality in quantum mechanics and its possible extensions. Editor (Quanta, quanta.ws)

Reviewer (various international journals, in the field of quantum information science) Co-organizer of the Nalanda Dialogs (2009, 2010, 2012): (nalanda-dialogforum.org)

Projects

1. Characterizing noise using quantum error correcting codes

Principal Investigator: Dr. R. Srikanth Research Student: Mr. Omkar Srikrishna Collaborators: Prof. Subhashish Banerjee (IIT-Jodhpur)

Noisy quantum processes are a major hurdle to high-precision control of many-body systems in quantum information processing, and characterizing noise in quantum system is of considerable importance. All methods of characterization to date require state preparations that are separate from states used for actual information processing. Not only does this can consume additional quantum resources, but it may not cope with noise that changes in time-scales smaller than that required for a full process tomography of the noise. Here we introduce an efficient method for quantum process tomography that, by directly acting on states encoded in degenerate quantum error correcting (QECs), incorporates process tomography into (the quantum error correction that protects) the main quantum computation, thereby solving both the above practical problems. \bla For illustration, we use 4-qubit codes with maximal 2-fold degeneracy to study the inter-qubit distance dependent behavior of two-qubit amplitude damping channel.

2. Nonphysical reality of the wave function: A counterfactual quantum cryptography perspective

Principal Investigator: Dr. R. Srikanth Research Student: Ms. H. Akshata Shenoy

Counterfactual quantum cryptography, based on the idea of interaction-free measurement, allows Bob to securely transmit information to Alice without the physical transmission of a particle. From local causality, we argue that the fact of his communication entails the reality of the quantum wave packet she transmits to him. On the other hand, the travel was not physical, because were it, then

a detection necessarily follows, which does not happen in the counterfactual communication. On this basis, we argue that the particle's wave function is real, but nonphysical. In the classical world, the reality and physicality of objects coincide, whereas for quantum phenomena, the former is strictly weaker. Since classical cryptography is insecure, the security of quantum counterfactual cryptography implies the nonphysical reality of the wave function.

3. If intrinsic randomness is the answer, what's the question?

Principal Investigator: Dr. R. Srikanth Project student: S. Aravinda

The correlations that violate the CHSH inequality are known to have complementary contributions from signaling and local indeterminacy. This complementarity is shown to represent a strengthening of Bell's theorem, and can be used to certify randomness in a device-independent way, assuming neither the validity of quantum mechanics nor even no-signaling. We obtain general nonlocal resources that can simulate the statistics of the singlet state, encompassing existing results. We prove a conjecture due to Hall (2010) and Kar et al. (2011) on the complementarity for such resources. Further, we show that signaling leads to biasing of the marginals for these resources. This entails that no-signaling is a consequence of isotropic unbiasedness of the singlet statistics, by which is meant that the marginals are unbiased along any direction, and coincidence counts are determined only by the relative orientation of pairs of polarizers.

4. Counterfactual quantum certificate authorization

Principal Investigator: Dr. R. Srikanth Research Student: Ms. H. Akshata Shenoy Collaborator: Prof. T. Srinivas, IISc

In counterfactual quantum cryptography, secure information is transmitted between two spatially separated parties even when there is no physical travel of particles transferring the information between them. We propose here a tripartite counterfactual quantum protocol for the task of certificate authorization. Here a trusted third party, Alice, authenticates an entity Bob (e.g., a bank) that a client Charlie wishes to securely transact with. The protocol is counterfactual with respect to either Bob or Charlie. We prove its security against a general incoherent attack, where Eve attacks single particles. We believe that this is the first instance of a multipartite protocol in the counterfactual paradigm.

5. Free will and relativistic causality in extensions of quantum mechanics

We formulate a complementarity for the 'nonlocal resources' required to violate Bell-type inequalities, namely signaling, local randomness and free will. Our work provides a unified approach to compare and contrast two different definitions of free will in Bell tests: a measure of uncorrelatedness of experimenters' choice with the underlying hidden variable (Ghirardi and Romano 2012; Hall 2010) vs. (more stringently) that with all events outside the future light cone of measurement (Colbeck and Renner 2011; Conway and Kochen 2009). Depending on the definition of free will chosen, either quantum mechanics is unextendible, or extensions of quantum mechanics (for singlet statistics) must go hand-in-hand with modifications to relativity (e.g., wider light cone or absolute spacetime).

6. Bell degeneracy, nonlocal subspaces and dual secret sharing

Principal Investigator: Dr. R. Srikanth Project student: Akshata Shenoy Collaborators: Prof. T. Srinivas

We construct degenerate Bell operators for graph states via the stabilizer formalism, whereby more than one such state violates the associated Bell inequality to the algebraic maximum. The set of these Belldegenerate states constitute a nonlocal subspace into which a quantum secret can be encoded and shared among an authorized group of agents, or securely transmitted to a designated secret retriever through a process similar to one-way quantum computation. We point out two methods to derive such Bell inequalities, one of which is appropriate for quantum error correcting codes. The security of our cryptographic scheme stems from the monogamy of quantum correlations, and the fact that the nonlocality of the code space can be witnessed by the Bell operator. The geometric properties of graph states can be exploited to implement certain access structures for quantum secret sharing or information splitting. Our use of nonlocality allows for extracting secrecy in the device-independent cryptographic scenario, in which untrusted devices are allowed, and also in the presence of a general non-signaling adversary.

7. Model of the human mind as a causally open system

Principal Investigator: R. Srikanth

That every cognitive phenomenon in human experience has a neural correlate is as natural an assumption in neuroscience, as energy conservation is in physics. We consider some experiments in optical illusion, and consider various issues that can throw light on the implications of this assumption. Typically, these are simple experiments which require a subject to look at a picture, and involve creating an illusory static or dynamic pattern in visual perception. Interestingly, the illusion may persist even when the subject is aware of their illusoriness, a phenomenon we call mindful deception. Some neuroscientific issues provoked by such experiments are considered. First is the question of whether the illusion is physiological or psychological. Crudely, a physiological illusion can be attributed to physical effects in the optical nerve or retina (e.g., say color blindness), while a psychological illusion would involve 'higherorder' areas that take part in neural information processing devoted to interpretation. At any rate, the element of mindful deception in such experiments suggests a possible spatial (or other) separation between neural correlates for the two actions here, namely the perception of illusion on the one hand and awareness of the illusion, on the other, and thereby also a separation between a lower self (the subject of illusion) and a higher self (the discerner of illusion). Subjectively, one can induce an indefinite hierarchy of higher selves, beginning with the witness of the preceding selves (i.e., a yet higher self that witnesses the deception at one level, and of its recognition at another), and recursively constructing higher-order witnesses. This recursive self awareness may not all be within the range of normal waking consciousness, and may be partly subconscious. We consider the question of how the neural correlates corresponding to the members of this hierarchy are connected spatially with each other in the brain structure. Based on considerations raised in [1], which relate uncomputability to certain aspects of human cognition, we may ask if this hierarchy is of infinite order. Intuitively, it does seem infinite. However, by thermodynamic arguments, the brain is ultimately a finite storage and information-processing entity. This leads to the question of whether human awareness includes elements not completely representable by neural correlates in the physical brain, thereby entailing a fundamental irreducibility of cognitive phenomena.

Scientific Achievements

- 1. Second year of GTC sponsored project on "Catalyst development and process for alkylation of aromatics" was successfully completed. The project is continued for 3rd year with the collaboration of GTC, USA, GTC, China and Clarient, Germany.
- 2. One year project sponsored by Shell Technology Centre, Bangalore was successfully completed in August 2013. Annual report on the project has been submitted.
- 3. First year of the HPCL R & D Centre, Bangalore sponsored project was completed successfully on 31-10-2013 and continued for second year. Annual Comprehensive Report was submitted to HPCL.
- 4. Poster Presented by Vijaykumar on "Tin (II) hydroxychloride: A Novel Solid Brønsted Acid Catalyst for Selected Condensation Reactions" at 16th National Workshop on "Catalysis for Sustainable Development" at Nagpur, Maharashtra on 4-5, February, 2014 won best presentation award.
- 5. Dr. G.V Shanbhag was invited by Nijalingappa College, Rajajinagar, Bangalore as a resource person to deliver talk titled "Zeolites and their applications" on 25-07-2013 to their BS and MSc (Chemistry) students.
- Mr. Janardhan H L and Mr. Satish Burla attended the National workshop held in M. S. Ramaiah Institute of Technology on "Process Modelling Simulation using Aspen hysys and Aspen plus" from 12-14, August, 2013.
- 7. Mr. Vijaykumar participated in SAC-7 analytical school to be held at Manuguru . A.P organized by BARC, Govt. of India from 18 to 25th Nov 2013. He won Best presenter award in a competition conducted during the workshop.
- Mr. Manjunathan P. attended an 18 day National Orientation Program on Catalysis held at IITM, Chennai, from 1-12-2013 to 18-12-2013 organized by National Centre for Catalysis Research (NCCR) IITM Chennai.
- Dr. Shanbhag was co-organizer for 5 days National Workshop on "Recent advances in Catalysis Science & Engineering". Organized by Chemical Engineering Department of MS Ramaiah Institute of Technology (MSRIT) in association with Poornaprajna Institute of Scientific Research (PPISR) Bangalore from 27-1-2014 to 31-1-2014.
- 10. Mr. Manjunathan P. has been successfully registered for PhD degree at Manipal University. Pre-PhD registration seminar of Mr. Manjunathan was conducted at Manipal University, Manipal on 30-11-2013 which was attended by Dr. G. V. Shanbhag (Guide) and Dr. S. P. Maradur (Co-Guide).
- 11. Dr. Ramesh. S., was research associate in Shell sponsored project, left the institute for postdoctoral studies to Korea Institute of Science and Technology, South. Korea.
- 12. Mr. Satish. Burla, was project associate in GTC sponsored project left the institute to take up job at SABIC, Bangalore.
- 13. Pore engineering of ZSM-5 by phosphate modification: Generation of new acid sites and enhancement in shape selectivity" H. L. Janardhan, G. V. Shanbhag* and A. B. Halgeri, Presented poster by Janardhan at 16th National Workshop on "Catalysis for Sustainable Development" at Nagpur, Maharashtra on 4-5, February, 2014".
- 14. Nano-sized beta zeolite as an efficient solid acid catalyst for acetalization of glycerol to produce solketal", Manjunathan P., Ganapati V. Shanbhag* and Sanjeev P. Maradur, Presented poster by Manjunathan at 16th National Workshop on "Catalysis for Sustainable Development" at Nagpur, Maharashtra on 4-5, February, 2014
- 15. Dr. Shanbhag, Dr. Raghu, Dr. Maradur and Dr. Ananda organized outreach activity for Poornaprajna School, Belur on 16th November 2013.
- Dr. Maradur delivered a talk in National Seminar on "Recent Advances in Organometallic Chemistry". Department of Chemistry, Rajarshi Chatrapati Shahu College, Kolhapur on 20th to 21st December 2013.
- 17. Dr. Maradur's project proposal entitled "Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, a potential fuel additive molecules for diesel and gasoline" which

was submitted to Vision Group of Science & Technology, Govt. of Karnataka under Seed Money for Young Scientist Research Program has been awarded a grant of Rs. 6 lakhs for one year which will start from Jan 2014.

- 18. Dr. Shanbhag and Dr. Maradur organized one day instrument training as a part of 5 days Catalysis Workshop conducted by Bangalore Institute of Technology on 12-11-2013.
- 19. Dr. Maradur has established collaboration with Dr. Hongchuan. Xin, Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao, China for carrying out small angle XRD analysis.
- 20. Dr. Sujit was invited to present talks at various institutes, including Harish-Chandra Research Institute (HRI), Allahabad and Delhi University, and Dept. of Physics, National Taiwan University.
- 21. Dr. R. Srikanth was invited to present talks in various international conferences around the country devoted to the foundations of quantum mechanics and quantum information theory. Among them International Workshop on Optical and Quantum Information (Sep 1--2, 2013) held at JIIT, Noida, Quantum Information Processing and Application (Dec 2--8, 2013) held at HRI, Allahabad and the International Meet on Quantum Correlations and Logic, Language and Set Theory (Dec 9--14, 2013) being held at IIT-Rajasthan, Jodhpur.
- 22. Mrs Swetha B. V and Ms. Swetha SM were felicitated by AMEF as Best student for the year 2012-2013 during Founder's Day on 4th July 2013 for their excellent research progress and overall contribution for the growth of the institute.
- 23. Dr. A.V. Raghu has been appointed as member of editorial board for Journal of Polymer Science.
- 24. Dr. A.V. Raghu chaired the technical secession held at "International Conference of Advanced Polymeric Materials", ICAPM 2013, Kottayam, 11 -13th October 2013.
- 25. Mr. Suhas has attended Familiarization programme and Hands on training from 17-06-2013 to 28-06-2013 at Indian Nanoelectronics User's Programme (INUP) at Centre for Nano Science and Electronics (CeNSE), IISc. Bangalore.
- 26. Mr. Suhas presented his research work on "Graphene composite membranes in pervaporative dehydration of alcohols: Extending the versatility of graphene to pervaporation" at International Conference on Applied Polymeric Materials-2013, to be held at M.G. University Kottayam, Kerala.
- 27. Dr. A.V. Raghu was invited to deliver a talk at the "*National Conference on Nano Science and Nano Technology*" (NCRNT-13) held at Acharya Institute of Technology, Bangalore, on 3rd May 2013.
- 28. Ms. Pavithra N. got Best Oral Presentation Award for the talk titled "In-vitro anti-diabetic activity of endophytic fungi isolated from Ocimum sanctum and *Momordica charantia*" at National conference on Emerging trends in Bioprocessing & Simulation (Sponsored by TEQIP II) conducted on 12th -13th Sept, 2013 organized by Dept of Biotechnology, PESIT, Bangalore.
- 29. Mr. Sathish.L and Ms. Pavithra.N attended Metabolomics Satellite Meet 2013 organized by C-CAMP in collaboration with Proteomics Society India on 27th November 2013.
- 30. Dr. Ananda gave a talk on "Conservation of medicinal plants by exploring medicinal compounds from their endophytic fungi" in a national seminar on "World Heritage Tag and conservation of biodiversity" held at St.Philomina college, Puttur, D.K. on December 16-17, 2013.
- 31. Dr. Ramagopal attended the Ramalingaswami conclave organized by NCCS, Pune during 12 to 14 September, 2013 in which he presented the work being carried out in the structural biology group, PPISR.
- 32. Ms. Pavithra G. C. presented a talk titled "Structural studies of Adenine phosphoribosyltransferase from Yersinia pseudotuberculosis" on 21stNov at 42nd National Seminar on Crystallography held at New Delhi during 21-23 November, 2013.
- 33. Dr. Ramagopal was invited to give demonstration sessions on various phasing methods at Protein Crystallography Meeting, held at RajaRamanna Centre for Advanced Technology (RRCAT), Indore. India.
- 34. Dr. Ramagopal has been awarded a grant from the VGST, Govt. of Karnataka for Establishment of Centre of Innovative Science & Engineering Education for three years.

- 35. Ms. Swetha Lankipalli, a CSIR JRF awardee has joined Dr. Ramagopal to pursue her Ph.D. on T-cell costimulatory molecules.
- 36. Dr. Raghurama Hegde has submitted a project proposal titled "Structural Approach to Understand the Regulatory Mechanism of Isocitrate Dehydrogenase 1 from Mycobacterium Tuberculosis And Implications for Tuberculosis Therapy" for the VGST grant of Seed Money to Young Scientists for Research.
- 37. Dr. Ramagopal visited Department of Biochemistry, Albert Einstein College of Medicine, New York from June 29, 2013 to August 02, 2013 on a collaborative project with Prof. Steven C. Almo.
- 38. We have successfully completed the structure of apo APRT from Y. pseudotuberculosis and the coordinates for the structure is deposited in PDB with an ID 4MB6.
- 39. Mrs. Pavithra G C successfully registered for PhD under the guidance of Dr. Ramagopal at Manipal University on 30-03-2013.
- 40. DST Review Meeting: Dr. Nalini was presented the progress of her DST FAST track project for the period of two years (2012-2014) at the Group Monitoring Workshop at NIIST, Trivandrum by Dr. RajKumar Joshi at DST. There were 7 members in the committee and they declared that the progress of the project was satisfactory.
- 41. Department of Science & Technology has released the second year installment of Rs. 3,00,000 towards Dr. Nalini G. Sundaram's project titled "Design and development of nanocrystalline layered Bismuth compounds for photocatalytic degradation of dyes and organic pollutants in the visible region"
- 42. Dr. Nalini presented an invited talk titled ""Design of Nano- Materials for sustainable Photocatalytic Processes Using Solar Energy" at the Physics Department of NIE Institute of Technology, Mysore on 31st August 2013
- 43. Swetha S.M.(SRF,Materials Science division) presented her research work titled "Crystal structure, local structure and photoluminescence property of KNdW₂O₈ polymorphs" at the 12th conference of the Asian crystallographic Association (AsCA), held in Hong Kong from 7th to 10th December 2013. Her abstract was chosen for the rising star oral presentation, and she also given a travel award of \$800 including travel and registration fees by the AsCA committee. Additionally she was also granted an amount of Rs.25,000 by the Indian National Science Academy (INSA) for accommodation and other expenses to attend the conference.
- 44. The Nanomaterials group at PPISR were the first to take advantage of the mail-in program for Neutron diffraction data at the Oak ridge National Laboratory and the results were published in paper in the prestigious ACS journal Crystal Growth and Design. (Impact Factor: 4.689) http://neutrons.ornl.gov/nomad/publications/.
- 45. Dr. Sowmya has joined as Post-Doc in Dr. Nalini's group since September 2013. She is at present working on a project regarding thick and thin film La-based gas sensors and we plan to submit the project to Government funding agencies such as DST.
- 46. Mr. Pradeep has joined as JRF under the BRNS project sanctioned in April 2013. At present he is involved in the synthesis or Photoluminescent rare earth doped tungstates.
- 47. Ms. Swetha S.M. gave an oral presentation on her work titled "Synthesis and Crystal Structure of Rare Earth Tungstate Nanomaterials for Application in Solid State Lighting Devices" at the 42nd National Seminar on Crystallography conference held at Jawaharlal Nehru Centre, New Delhi from 21st -23rd November 2013.
- 48. Mr. Pradeep S attended the annual conference of ICC Dharward held at Karnataka University, Dharward from November 28th to November 30th 2013.
- 49. Dr. Nalini has been invited to deliver a Lecture in one of the Small Molecule Crystallography Sessions at the 43rd National Seminar on Crystallography to be held in IISER Mohali between 28th and 30th March, 2014 as part of the International Year of Crystallography-2014

Recent Publications

Since the inception of PPISR research activity a total of more than 115 research articles have been published with PPISR affiliation.

MATERIALS SCIENCE

- Sulfated zirconia; an efficient and reusable acid catalyst for the selective synthesis of 4-phenyl-1,3-dioxane by Prins cyclization of styrene. V.S. Marakatti, G.V. Shanbhag* and A.B. Halgeri, Applied Catalysis A: General 451 (2013) 71–78
- Shape selective catalysis by phosphate modified ZSM-5: Generation of new acid sites with pore modification. Janardhan H L, G V Shanbhag* and A.B. Halgeri, Applied Catalysis A: General, 2014, 47, 12-18
- 3. Zinc hydroxy stannate: a promising acid-base bifunctional catalyst .Swetha Sandesh, G V Shanbhag* and A.B. Halgeri, RSC Advances, 2014, 4, 974-977
- Transesterification of glycerol to glycerol carbonate using KF/Al₂O₃ catalyst: The role of support and basicity Swetha Sandesh, G V Shanbhag* and A.B. Halgeri, Catalysis Letters, 2013, 143, 1226-1234
- Condensation reactions assisted by acidic hydrogen bonded hydroxyl groups in solid tin(II)hydroxychloride. Vijaykumar S. Marakatti, Ganapati V. Shanbhag^{*} and Anand B. Halgeri RSC Advances, 2013, 10795-10800
- G. V. Shanbhag, Ankur Bordoloi, Suman Sahoo, B. M. Devassy, and S. B. Halligudi "Supported heteropoly acids and multicomponent polyoxometalates as eco- friendly solid catalysts for bulk and fine chemicals synthesis" in "Environmentally Benign Catalysts: For Clean Organic Reactions", Springer
- 7. D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu,* "Graphene-loaded sodium alginate nanocomposite membranes with enhanced isopropanol dehydration performance via pervaporation technique". RSC Advances, 2013, 3, 17120-17130.
- 8. D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu*, "Synthesis and characterization of novel polyurethanes based 4,4'-{oxy-1,4-diphenyl bis(nitromethylidine)} diphenol Schiff base hard segment", Polymer Engineering and Science, 2014, 54, 24-32.
- D.P. Suhas, T.M. Aminabhavi, A.V. Raghu,* "Mixed Matrix Composite Membranes of H-ZSM5 Loaded Poly(vinyl alcohol) Used in Pervaporation Dehydration of Alcohols: Influence of Silica/Alumina Ratio" Polymer Engineering and Science, 2013, Accepted, online
- 10. D.P. Suhas, T.M. Aminabhavi, A.V. Raghu,* "para-Tolune sulfonic acid treated clay loaded sodium alginate membranes for enhanced pervaporative dehydration of isopropanol" Submitted to International Journal. 2014.
- 'Polymorphism in Photoluminescent KNdW₂O₈: Synthesis, Neutron Diffraction, and Raman Study', Swetha S. M. Bhat, Diptikanta Swain, Chandrabhas Narayana, Mikhail Feygenson, Joerg C. Neuefeind, and Nalini G. Sundaram, *Crystal Growth & Design*, 2014, *14* (2), pp 835–843
- A composition-dependent "re-entrant" crystallographicphase transition in the substitutional metal acetylacetonate complex(Cr1-xGax)(acac)3,', M. Srinidhi Raghavan⁻, Piyush Jaiswal, Nalini G. Sundaram, and S.A. Shivashankar, Polyhedron 70C (2014), pp. 188-193
- Swetha. S.M., Nalini G Sundaram , 'Efficient visible light photocatalysis of Bi₄TaO₈Cl nanoparticles synthesized by solution combustion technique', *RSC Advances*, 2013, : RSC Advances, 2013, 3,14371

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- Ramagopal, U. A., Dulyaninova, N. G., Varney K. M., Wilder, P. T., Nallamsetty, S., Brenowitz, M., Weber D. J., Almo S. C. and Bresnick, A. R. 2013, Structure of the S100A4/myosin-IIA complex. BMC Struct. Biol.,13(1), 31.
- 15. Rubinstein, R., Ramagopal, U. A., Nathenson, S. G., Almo, S. C. and Fiser, A. 2013, Functional Classification of Immune Regulatory Proteins. Structure (cell press), 21(5), 707-717.
- Vigdorovich, V., Ramagopal, U. A., Eszter Lázár-Molnár¹, Eliezer Sylvestre¹, Jun Sik Lee^{1‡}, Kimberly A. Hofmeyer, Xingxing Zang, Nathenson, S. G. and Almo, S. C. 2013, Structure and T-cell inhibition properties of B7 family member, B7-H3. Structure (cell press), 21(5), 766-776.
- 17. Sathish, L., Pavithra, N. and Ananda K. (2014) Evaluation of antimicrobial activity of secondary metabolites and enzyme production from endophytic fungi isolated from Eucalyptus citriodora. Journal of Pharmacy Research 8(3); 269-276.
- 18. Garudachari B, Isloor AM, Satyanarayana MN, Fun HK, Pavithra N and Ananda K. (2013) Design and regioselective synthesis of trifluoromethylquinolone derivatives as potent antimicrobial agents. European Journal of Medicinal Chemistry 68; 422-432.
- 19. Chethan PD, Vishalakshi B, Sathish L, Ananda K, and Poojari B. (2013) Preparation of substituted quaternized arylfuran chitosan derivatives and their antimicrobial activity. Int J Biol Macromol. 59:158-64.

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- 20. *The quantum cryptographic switch.* N. Srinatha, S. Omkar, R. Srikanth, S. Banerjee and A. Pathak. Quantum Information Processing 13, 59 (2014).
- Unification of Bell, Leggett-Garg and Kochen-Specker inequalities: Hybrid spatio-temporal inequalities. S. Das, S. Aravinda, R. Srikanth and D. Home Europhysics Letters 104 60006 (2013).
- 22. Akshata Shenoy H, R. Srikanth and T. Srinivas. Counterfactual cryptography. Europhysics Letters, 103, 60008, (2013).
- 23. S.Omkar, R. Srikanth and S. Banerjee. Dissipative and Non-dissipative Single-Qubit Channels: Dynamics and Geometry. Quantum Information Processing, 12, 3725-3744 (2013).
- 24. Collapse and Revival of Entanglement of Two Qubits in Superconducting Quantum Dots Lattice with Magnetic Flux and Inhomogeneous Gate Voltage" Sujit Sarkar, Physica B 414, 26 (2013)

Events and meetings

1. Founder's Day Celebration

PPISR Founder's Day was celebrated on 3rd and 4th July, 2013 at Bidalur campus. The scientific program on 3rd July was inaugurated by Prof. N. Kumar, Emeritus Professor and Former Director, Raman



research Institute, Bangalore. He gave the keynote address and opened the session for scientific discussion. For the next one and half days there was series of lectures from eminent scientists in the field of materials science, biological sciences and theoretical physics. On the first day, Prof Yashonath. S,

SSCU, IISc, Bangalore and Prof Arun. M. Umarji, MRC, IISc, Bangalore gave talks during technical session of materials science which was followed by Dr Shanbhag, PPISR. The second half of the technical session was of biological sciences. Prof. K. Sankara Rao, CES, IISc, Bangalore and Dr. O. K. Remadevi, Institute of Wood Science and Technology, Bangalore gave talks followed by Dr Ananda, PPISR. On 4th July 2013, a technical session on theoretical physics started by a talk by Prof. T. Srinivas, ECE, IISc, Bangalore followed by Prof. P.R. Vishwanath, IIA, Bangalore and Dr Srikanth, PPISR



In the evening, valedictory session was chaired by Prof. U. R. Rao, Chairman, Karnataka Science & Technology Academy, former chairman, Space Commission, and Secretary, Dept. of Space, and Prof. B. Thimme Gowda, VC, Bangalore University, was the Guest of Honor. HH Sri Vishwapriya Theertha Swamiji presided over the occasion

Addressing the gathering, Prof U. R. Rao recalled his association with HH Sri Sri Vibudhesha Theertha



Swamiji . He also stressed upon the utilization of space science and technology knowledge for agriculture in our country. Technological advances in remote sensing, the Global Positioning System, information management, and farm machinery now

enable the optimization of crop control practices. Such technologies with precision farming to see if high-altitude images can map the variations

in a field and help farmers apply just the right amounts of resources only where they are needed. Prof. B. Thimme Gowda appreciated the



research progress of the institute and assured of any possible help in starting up of new courses. The dignitaries on the dais released the PPISR newsletter for the period of Jan-Jun 2013 on the occasion. HH Sri Swamiji addressed the gathering and the programme was concluded with his benediction. The large gathering on the occasion had many of the board of trustees and management members of AMEF and AMEC, other distinguished invitees and well wishers of the institute.

Annual Report 2013-14

2. AMEF Board of Trustees Meeting

a. AMEF board of trustees meeting was held at Bidalur main campus on May 25, 2013. Dr. K Srihari, Hon. Secretary, AMEF/PPISR welcomed the Chairman and all the members of the Board. Many issues related to the maintenance and development of PPISR, balance statements, ratification of resolutions passed earlier were discussed and adopted. Annual Report of PPISR for the year 2012-2013 was released by the Chairman, AMEF, H. H. Sri. Vishwapriya Theertha Swamiji. Dr. A. B. Halgeri, Director, presented the quarterly



progress report of PPISR. The Chairman and trustee members appreciated the overall progress made during this period.

b. AMEF meeting is held on 28/12/2013 at Bidalur campus and discussed about the future development plans for the PPISR. There was discussion about the new biological science building inauguration. Hon. Justice K.Santhosh Hegde was present in the meeting a invited guest and he visited labs during his visit expressed his appreciation for the achievements.



3. Annual review meetings of GTC project

Dr. Ding ZhongYi, Project Manager, GTC, USA visited PPISR on 31-07-2013 for annual project review meeting of GTC sponsored project. Dr. G V Shanbhag and Dr. Sanjeev Maradur made presentations and discussions were conducted on overall progress during 2nd phase of GTC project. Ideas and timeline for future GTC project were also discussed. GTC complemented the PPISR Team for the successful completion of the 2nd phase of the project which led to the development of 1st generation catalyst for TM process.



Dr. David Bridgeman, Global Licensing Manager, GTC, USA and Alok Saxena. Technology Mr. Manager, GTC, India visited PPISR on 08-07-2013 for the first time to understand the research facilities and capabilities of PPISR for future activities. Dr. A. Β. Halgeri presented the overview of PPISR.



Dr. G V Shanbhag and Dr. Sanjeev Maradur made presentations on the project activities. Future collaborative project programmes with GTC were discussed in the meeting.

4. HPCL Project review meetings

a) 2nd quarterly project review meeting of HPCL project was held at PPISR on 09-07-2013 to review the progress made during 2nd quarter (Feb-Apr, 2013). From HPCL R & D, Mr. G. Sriganesh, Executive Director, Dr. N V Choudhary, General Manager, Dr. P V C Rao, Dy General Manager and Dr. Ravishankar, Sr. Manager participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag and Dr. Sanjeev Maradur were present for PPISR. Students, Mr. Janardhan and Mr. Vijaykumar presented the work separately on aromatization of light naphtha and side chain alkylation of toluene respectively. The members gave several suggestions to improve the quality of the work. HPCL team expressed their satisfaction on the overall progress made during the quarter.

b) 3rd quarterly technical project review meeting of HPCL project was held at PPISR on 03-09-2013 to

review the progress made during 3rd quarter (May-July, 2013). From HPCL R & D, Dr. N V Choudhary, Dr. P V C Rao, and Dr. Ravishakar, participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag and Dr. Sanjeev Maradur were present for PPISR. The students Mr. Vijay and Mr. Janardhan presented the research data to the team. HPCL team appreciated the novel and impressive results obtained and gave their approval to file a patent.



c) Annual technical project review meeting of HPCL project was held at HPCL Corporate Office, Whitefield, Bangalore on 06-12-2013 to review the progress made during 4th quarter (Aug-Oct, 2013) and also reviewed one year progress. From HPCL R & D, Sri. G. Sriganesh, Dr. N V Choudhary, Dr. S. G. T. Bhat, and Dr. Ravishakar, participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag and Dr. Sanjeev Maradur were present for PPISR. The students Mr. Vijay and Mr. Janardhan presented the research data to the team. HPCL team applauded the overall progress made during one year and gave their approval to file another patent.

5. Doctoral advisory committee (DAC) meeting

Doctoral Advisory committee meetings were held for each doctoral student who has registered for Ph.D. degree wherein subject experts review the six-month research work and give suggestions to improve the quality of research.

1. Third and Fourth DAC meeting to review the doctoral work of Ms. Swetha SM and Mr. Srinidhi was conducted in Sadashivnagar campus on June 5th and 21st Oct 2013. Prof. S. Shivashankar, Prof. T. N. Guru Row and Prof. Arun M. Umarji of IISc, Bangalore was present in the meeting.

2. DAC meeting to review the doctoral work of Mr. Suhas in the area of Polymers was conducted in Sadashivnagar campus on 20th June and 23rd Dec 2013. Prof. Y.S. Bhat, BIT, Bangalore and Prof. Siddaramaih, Mysore University, Mysore, were present in the meeting.

3. DAC meeting of Biological Sciences students, Mr. Satish L. and Ms. Pavithra N. was conducted on 22nd June and 7th Dec, 2013 with DAC members Prof. A. J. Rao, IISc, Dr. Raviraja, Stempeutics Research Pvt. Ltd and Dr.Ramagopal U as subject experts.

4. Theoretical physics students Mr. Omkar and Mr. Aravinda successfully completed their fourth and third doctoral advisory committee meetings, respectively. Prof. N. Kumar, Emeritus Professor, RRI, Bangalore, Dr. A. R. Usha Devi, Dept. Of Physics, Bangalore University, Bangalore and Dr. B. S. Ramachandra, Director, Center for Fundamental Studies and Creative Education, Bangalore were present in the meeting.

5. 3rd DAC meeting for Ms. Swetha Sandesh, Mr. Vijaykumar and Mr. Janardhan was held at Main Campus on June 17, 2013. Prof. B.S. Jai Prakash, Director, IEHMM, Bangalore, Prof. H.N. Vasan, SSCU, IISc, Bangalore and Prof. Y.S. Bhat, BIT, Bangalore, were present as external subject experts. The experts gave several suggestions to improve the quality of the work. Overall, the committee expressed their satisfaction about the research progress of the three students so far.

6. 4th DAC meeting for Ms. Swetha Sandesh, Mr. Vijaykumar and Mr. Janardhan was held at Sadashivnagar campus on January 5, 2014. Prof. B.S. Jai Prakash, Director, IEHMM, Bangalore, Prof. H.N. Vasan, SSCU, IISc, Bangalore and Prof. Y.S. Bhat, BIT, Bangalore, were present as external subject experts. Students presented their six-month research work. The experts gave several suggestions to improve the quality of the work. The committee was happy with the progress made by students during that time.

7. 1st DAC meeting for Mr. Manjunathan P. was held at Sadashivnagar campus on 19-10-2013 to discuss his preliminary work on the PhD topic and finalizing the synopsis for PhD registration. Dr. Ravishankar, Sr. Manager, HPCL R & D Centre and Dr. Y. S. Bhat, HOD, Chemistry Dept, BIT were the experts. Mr. Manjunathan registered for PhD in Manipal University with Dr. G V Shanbhag as his Guide and Dr. Sanjeev Maradur and co-guide.

8. Mrs. Pavithra G. C. successfully presented her first six monthly DAC progress report on 21.10.2013. The DAC members appreciated the quality and the amount of work carried in the six months.

6. Faculty Development Program

A. Five days "Faculty Development Program in Catalysis Training" was conducted at BIT Bangalore in collaboration with Silicon Education World Pvt Ltd, Bangalore. Dr. Y. S. Bhat and Dr. Jai Prakash of BIT were the conveners of the workshop. As part of course schedule, two batches of the



participants visited PPISR and spent one day learning heterogeneous catalysis. The first batch visited on 21st August 2013 and the second batch on 12th November 2013. The participants gained the knowledge of catalyst making and catalyst screening in batch mode and under flow conditions.

B. PPISR and Department of Chemical Engineering, M. S. Ramaiah Institute of Technology, Bangalore coorganized a five day faculty development program on " Recent Advances in Catalysis & Engineering" under TEQUIP-II program. Participants from various institutes attended the workshop. For the first three days a series of lecturers by eminent scientists in the area of catalysis from industry as well as research institutes were



organized at M. S. Ramaiah Institute campus. As pat of course schedule, PPISR hoisted two days training program on catalyst preparation and characterization & application of catalyst to vapor phase and liquid phase reactor. The participants gained the knowledge of catalyst making and catalyst screening in batch mode and under flow conditions. On the last day, Dr A. V. Ramaswamy gave a valedictory talk on "Opportunities and Challenges in Catalysis" followed by distribution of certificates to the participants.

7. Visitors' to the Institute

Dr. D. Yogeswara Rao, Advisor, Office of the Principal Scientific Adviser to the Govt. of India visited

PPISR campus on 29th October 2013. He was impressed with the achievements of PPISR in such a short period. He also stressed to look upon research opportunities in the area of rural technologies. All the faculties and staff were present during the visit.

A group of 10 Chemistry faculty members from Mount Carmel College, Bangalore visited the campus to have a look of the

research facilities available at PPISR. The visitors were impressed to see research facilities of both Materials Science and Biological Science divisions

Dr. Bhanuprakash Reddy, Scientist E, National Institute of Nutrition, Hyderabad visited PPISR on 24/7/2013. His visit was arranged on behalf of our existing research collaboration and to discuss for further strengthening the bond. On this occasion we made a brief presentation of Institute and Biological science activities at PPISR by Biological science division.

Sponsored Research Projects

Last year highest numbers of sponsored projects were sanctioned to PPISR from Govt. agencies; BRNS, DST and VGST and industrial project GTC, USA. Currently, 9 sponsored research projects are executed at PPISR in different areas of research as follows.

- Dr. Maradur's received a grant of Rs. 6 lakhs for one year from Jan 2014 by VGST, Govt. of Karnataka under Seed Money for Young Scientist Research Program for the project proposal entitled "Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, a potential fuel additive molecules for diesel and gasoline".
- The project titled "Layered Bi based Nanomaterials for Photocatalytic Degradation of Dyes and Pollutants" sponsored by DST, Govt. of India under the SERC- Fast Track Scheme For Young Scientists is executed by Dr. Nalini G. Sundaram as Principal Investigator.
- The project titled "Influence of Electron Beam Irradiation on the Crystal Structure and Photoluminescence of Rare Earth doped Tungstate Nanophosphors" was sanctioned by BRNS, DAE, Govt. of India to Dr. Nalini G Sundaram in 2013 for the period of 3 years.
- Dr. A.V. Raghu obtained a project titled "Effect of Electron Beam Irradiation on Polymeric composite Membranes for Pervaporation Separation Application" from BRNS, Govt. of India in May 2013 for the period of 3 years.
- The infrastructure fund, "The Establishment of Center of Excellence in Science, Engineering and Medicine" (CESEE), Department of IT, BT and ST, VGST, Govt. of Karnataka) was sanctioned to Biological Sciences Division in 2013.
- Dept. of Science and Technology (DST), Govt. of India sanctioned a project titled "Entanglement, nonlocality and Superluminal Signaling in Deterministic and Indeterministic Extensions of Quantum Mechanics" to R. Srikanth of Theoretical Sciences Division in 2013 for the period of 3 years.
- A project titled "Geometric Phase and Quantum Phase Transition in Quantum Many Body System" sanctioned by DST, Govt. of India to Dr. R. Sujit Sarkar, Principle Investigator in June 2013 for the period of 3 years.
- Two years of industry project sponsored by GTC, USA on the "Design and development of solid acid catalyst for aromatics technology" completed successfully and has been extended for another year. The project is managed by Dr. G. V. Shanbhag and his group.
- Other two industrial sponsored projects from Shell Technology Centre, Bangalore and Hindustan Petroleum Corporation Ltd, Bangalore have been carried out in Materials Science Division, PPISR with Dr. G. V. Shanbhag as Principle Investigator and Dr. Sanjeev Maradur as co-investigator.



New members

1. Dr. Kallol Roy has joined as a Postdoctoral Fellow since October 2013, with Dr. Sujit Sarkar under DST project on geometric phases, and is studying applications of semantic computing, quantum computing and the petrinet formalism to biological systems. Dr Kallol has completed his PhD in the ECE Dept, IISc, Bangalore.

> 2. Dr. Sowmya Palimar has joined as Post-Doc in Dr. Nalini's group since September 2013. She obtained her PhD from NITK Surathkal before Joining PPISR. At present working on a project related to Thick and thin film La-based gas sensors.

3. Miss. Swetha Lankipalli has joined for PhD in biological science division under Dr. Udupi. Ramagopal. She is a gold medalist in M. Sc in Zoology from Sri Venkateswara University, Tirupati. Her academic achievements include CSIR JRF-2012, GATE-2012 and Andra Pradesh SET-2012.

> 4. Mr. Pradeep P. Shanbogh has joined as a JRF in BRNS sponsored project in Materials Science division under Dr. Nalini. Sundaram. He has done five years intergraded M. Sc in Chemistry from University of Mysore. Before joining PPISR, he had worked as project fellow in JNCSAR, Bangalore.

5. Mr. Dundappa B. Mumbaraddi has joined the Catalysis Group as a Research Fellow in industry sponsored project in Materials Science Division. He has done M. Sc in Inorganic Chemistry from Karnatak University Dharwad.

6. Mr. Karthik. K. has joined the Catalysis Group as a Research Fellow

in industry sponsored project in Materials Science Division. He has done M. Tech in Chemical Engineering from Dayanand Sagar College of Engineering, Bangalore

7. Mr. Prashant Kumar has joined the Catalysis Group as Research Fellow in industry sponsored project in Materials Science Division. He has done M. Tech in Chemical Engineering from Siddaganga Institute of Technology, Tumkur.

8. Mr. G.N. Chandan has joined as JRF under Dr.Sujit Sarkar in DST project

9. Mr. Santhosh Kumar has joined the Catalysis Group as a Research Fellow in industry sponsored project in Materials Science Division.















Invited Talks

Prof. S. Ramasesha, Solid state and Structural Chemistry Unit, IISC, Bangalore delivered a lecture on "Chemistry of Correlated Electrons" on April 26, 2013

Dr. Satish. A. Patil, Associate Professor, Solid state and Structural Chemistry Unit, IISC, Bangalore delivered a lecture on "Polymer based Solar Cells" on May 9th, 2013.

Prof. Yoshihiro Sugi, Gifu University, Japan and University of Queensland, Australia, delivered a lecture on "The Shape-Selective Catalysis in Alkylation of Polynuclear Aromatics" on May 28, 2013. Prof. Sugi is an internationally acclaimed scientist in Catalysis Research and the Catalysis group of PPISR was greatly benefited from his visit.

Dr. R.P. Verma, Former Executive Director, R&D, Indian Oil Corporation Faridabad and Advisor for R&D, HPCL visited PPISR and delivered a lecture "Innovations in Oil and Gas Industry" on June 5, 2013. Later, the faculty of Catalysis group discussed with him about their research activities and sought his guidance.

Dr. Prathibha Nadig, Professor, Dept of Pharmacology, Vydehi Institute of Medical Sciences and Research Centre, Bangalore gave a talk "In-vitro and in vivo screening of herbal extracts for diabetes and its complications" 25th July 2013.

Dr.Chanrdasekhar, Professor, IISc Bangalore and Former Head of Patent Division at MS Shell Technology India, delivered a series of lectures on "Intellectual Property Rights and Patents Literature". In August and October 2013.

Dr. S. Narasimhamurthy Associate professor- Pharmaceutics, University of Mississippi, USA delivered a lecture on "Technological innovations in Transdermal Drug Delivery". 25th July 2013.

Prof. Arun M. Umarji, MRC, IISc, Bangalore. gave a talk on "Nanostructurization of Transition Metal Silicides for High Temperature Thermoelectric Applications". 4th July 2013.

Prof. K. Sankara Rao, Centre for Ecological Sciences, IISc Bangalore gave talk on "Habitat building through conservation- role of Informatics". 4th July 2013.

Prof. O. K. Remadevi, Scientist-G (Rtd), Institute of Wood Science and Technology, Bangalore gave a talk on "Entomopathogens for ecofriendly pest management". 4th July 2013.

Prof. T. Srinivas, ECE, IISc,Bangalore, gave a talk on "Micro-Opto-Electro-Mechanical Sensors (MOEMS)". 4th July 2013

Dr. Divya BU, PhD in Biology from Georgetown University, Washington D.C., USA gave a talk on "Multi-sensory, multi-trophic communication between predators and prey". 16th October 2013

Prof. P.R.Vishwanath, IIA, Bangalore, gave a talk on "The World of Particles". 4th July 2013

In-house Seminars

- 1. Mr. Aravinda.S : "Mysteries of quantum mechanics", 2-4-2013
- 2. Mr. Satish.L : "DRUG DISCOVERY FROM FUNGI", 16-4-2013.
- 3. Mr. Suhas.D.P: "Graphene: "A revolution in science by a pencil line"", 30-4-2013
- Dr. Ramesh. A: "GTL TECHNOLOGY AND IT'S ROLE IN THE WORLD "ENERGY MARKETS", 14-05-2013
- 5. Dr. Sujith sarkar: "Quantum Phase Transition Light: A Renormalization Group Study", 2-8-2013
- 6. Dr. Ananda.K: "Blood is an essential body fluid: can we synthesize artificially?", 30-08-2013
- 7. Mr. Janardhan.L: "Application of theoretical chemistry as a tool for understanding catalysis",10.9.2013
- 8. Mr. Omkar.S: "Quantum error correction", 20-9-2013
- 9. Ms. Pavithra. G. C. "The enemy inside the stomach: Helicobactor pylori and its impact on human life.", 27-9-2013
- 10. Ms. Pavithra.N. "Nutraceuticals: Promising Health Product", 8-11-2013
- 11. Dr. Sowmya.P :"Vacuum Technology and Thin Film Deposition", 11-12-2013
- 12. Dr. G. V. Shanbhag : Catalysis for the Valorization of Exhaust Carbon: from CO₂ to Chemicals and Fuels. Technological use of CO₂, 24-01-2014
- 13. Dr. Udupi Ramagopal: Immunotherapy : Fraction of a penny from PPISR, 14-02-2014
- 14. Ms.Pavithra G C: Tularemia a potential bioterrorism threat 28-02-2014.

Outreach Activities

1. The institute is helping the external graduate and post graduate students to carry out their short term projects or by giving them training in research. Mr. Prashant Kumar, M.Tech. (Chemical Engineering) student from SIT, Tumkur, conducted his M. Tech. Thesis project on "Designing eco-friendly solid base catalyst for biodiesel synthesis from transesterification of non-edible oil." under the guidance of Dr. G. V. Shanbhag from October 2012 to June 2013. Two students from St. Aloysious College, Mangalore, Mr. Nagendra and Mr. Rohan conducted their one month M.Sc. project with Dr. G. V. Shanbhag on "Solvent free synthesis of 4-methoxyacetophenone using eco-friendly zeolite beta catalyst".



2. A one day training programme was conducted for 12 M.Sc. Chemistry students from Govt. Science College, Bangalore on March 22, 2013, accompanied by Prof. Gururaj of Chemistry Dept. All the research scholars and faculty of Materials Science explained their research activities and demonstrated the analytical instruments and catalytic reactors

3. Ms. Gargi Sabaraya, BSc Student from Poornaprajna College Udupi got trained in Biological Science laboratory for two weeks in the month of October 2013. She was awarded Inspire fellowship from DST,

Govt. of India and selected PPISR as her research centre for training in research project.

4. In order to create interest in basic science in young minds, PPISR has taken up an initiative of **"Today's Science for Tomorrow's Scientists**" for Poornaprajna School students. The first batch of 50 class 10th students along with 5 faculty members of Poornaprajna School Belur had visited PPISR



Bidalur campus on 16th November 2013. Students interacted with the faculties and PhD students of the institute about the ongoing research and showed a lot of interest.

5. Students of IX standard from five Poornaprajna Schools in Bangalore visited PPISR as part of the

outreach program held for 5 days in the month of January- February 2014. The motto of this program was 'Today's Science for Tomorrow's Scientist'. The objective was to motivate and inspire young students to take science as a career in the future. About 30 students from



Sadashivnagar, 90 students from Indiranagar, 90 students from Yelahanka, 90 students from Widia and 40 students from Krishnanagar poornaprajna high schools participated in this program along with teachers. Experiments were conducted in Physics, Chemistry and Biology.

In physics, demonstrations on polarization of light and liquid crystals were done. These concepts were used to explain the working of the mobile phone display, LCD TV's and other devices.



Chemistry experiments include the synthesis of the dye Fluorescein and decomposition of Hydrogen Peroxide using KI showing the importance of catalysts. To help understand Osmosis better, a colourful silica garden experiment was displayed. The importance of photocatalysis in degradation of pollutants was

illustrated by degrading methyl orange in sun light in the presence of Titanium Oxide nanoparticles. The students were also shown to all the sophisticated lab equipments such as X-ray Diffractometer, Gas Chromatograph, UV-Visible ,IR and Fluorescence spectrophotometer etc. used for various measurements.

Biology experiments included Gram's Staining and observation of Bacterial cell wall differentiation, Preparation, staining and observation of different stages found in mitotic cell division using a onion root

tip, growing and observation of small and macro molecular crystals and observation of fungal spores. Each experiment was explained in detail and demonstrated along with the question and answers.



The feedback got from the teachers and students on the outreach program were very favourable and they appreciated the Director, faculty and students of PPISR for this initiative. In addition they also requested for the organization of many more such programmes and invited our faculty and students to give a talk/demonstration at their schools.

Campus life

Vanamahosthava: World Environment Day is celebrated every year on June 5 to raise global awareness of the need to take positive environmental action. It is run by the United Nations Environment Programme (UNEP). PPISR also celebrated the day and conducted few programmes during the month of June. In this connection, Vanamahotsava, was celebrated at

Bidalur campus on **14th June 2013** by the faculty and students with a concern



to love & care for the nature as nature alone is our future sustenance. It was inaugurated by H. H. Sri Vishwapriya Theertha Swamiji by planting a coconut tree followed by Dr. Halgeri and Sri. Srinivasa Rao planted trees. About 80 trees were planted by invitees, students and staff of PPISR on this occasion inside the

campus.

Independence Day celebration: The 67th Independence Day was celebrated in PPISR campus with

high spirit and pride. The Director of the institute hoisted the National Flag at 09:30 AM. All the students and staff were present during this occasion. The Director encouraged the youth to contribute whole-heatedly in the activities of National interest and the institute. Shri. Sreenivasa Rao, financial advisor shared his experience on vigilance and financial management with all PPISR members



Sharada Pooja: Sharada Pooja and Ayudha Pooja were performed at PPISR campus on October 11th,

2013. All the books, instruments and vehicles were decorated and worshiped on this special occasion. Priest from the nearby temple performed a pooja to goddess Saraswathi and all instruments.



A **new borewell** was constructed in order to meet the growing demand of water in the campus and inaugurated by H. H.Sri Swamiji on the same day. The concept of Vanamahotsava for the nature lovers was first initiated by Hon. (Late) K.M. Munshi, the then Union Minister for Food & Agriculture in the year 1950. Unless timely action is taken to prevent & restore environmental degradation, it may go beyond human control & threaten the survival of any living organisms on this earth planet. While survival & development of human being is important, it is also equally important to preserve the nature which is the only source of oxygen and other essentials required for our living.

Inauguration of new Research Lab

PPISR is fast growing in terms of its research activities and there was a need increase the infrastructure for all the activities. In view of this, a decision was taken by AMEF to construct a 150-sitter conference

hall and biology laboratory at Bidalur campus. Inauguration of newly constructed 150-sitter conference hall and Biology laboratory at Bidalur campus was held on 31st October 2013. H.H. Sri Vishwapriya Theertha Swamiji, Chairman, AMEF preceded over the function. Gana-homa was offered during this occasion. Dr. K Srihari, Hon. Secretary, AMEF, Dr. A.B. Halgeri, Director and Sri. Sreenivasa Rao, Financial Advisor were present during the ceremony. Dr. A.B. Halgeri gave a welcome note and Dr. K. Srihari, Hon. Secretary, AMEF presided over the function. H.H. Sri Vishwapriya Theertha Swamiji gave the benediction on this occasion. The large



gathering on the occasion had many of the board of trustees and management members of AMEF and AMEC, other distinguished invitees and well wishers of the institute.



Library

The library of PPISR has over 1000 books related to Maths, Physics, Chemistry, Biology, Materials Science and other interdisciplinary subjects, apart from books of general interest, magazines and daily newspapers.

The library also contains a reasonably good collection of Indian and international journals in print and access to a reasonably large number of e-journals. All the books have been barcoded to facilitate online

access. The library is accessible at all times, and has internet access. Plans are afoot to provide wiFi access throughout the library. Recently, the library was shifted to the new Biological Science building, to make more reading space available.



Computer and internet facilities

Sufficient computer and internet facility is given to faculty members and students at PPISR. Further, a central computing facility of two GPU-based supercomputers with Intel Xeon 8 core machines with 32 GB RAM each is available. These are outfitted with multi-core DDR3-based powerful NVidia GPU's for CUDA computing. Internet access is through a dedicated 4 MBPS line provided by Mirconova, our new internet service provider.

Research facilities added during 2013-14

Fluorescence spectrophotometer

The Varian Cary Eclipse Fluorescence Spectrophotometer is a compact instrument and measures the fluorescence, phosphorescence, chemi/bio-luminescence, and time resolved phosphorescence. Specifications:

• Spectral range UV-Vis and NIR.

- Xenon flash lamp technology with room light immunity and high sensitivity.
- Both solid and liquid samples can be analyzed.



The equipments sponsored by Vision Group on Science and Technology, Karnataka.



Type-1 Water Purification System

Ice-Flaker

Cold-room

Visitors' view

Prof. Joel M. Friedman , Albert Einstein College of Medicine, New York, USA

"It was a real pleasure to visit this exacting institution which is filled with much promise. The energy of the institute is alive with creative forces. I expect great achievements to emerge from this young and growing institute".

Prof.Yoshihiro Sugi, University of Queensland, Gifu University, Japan

"I am very happy to visit you. I am also happy if we have collaboration on Zeolite catalysis. Have a nice work".

Prof. S. Ramasesha, Solid state and Structural Chemistry Unit, IISc, Bangalore

"Impressive to see the rapid development of the campus. The students and faculty are excited about their work. I wish the institute all the best in year to come".

Dr. Dattatray J. Late, Department of Materials Science and Engineering, International Institute of Nanotechnology, Northwestern University, USA

"I find this institute has bright future and growing like institute JNCAJR and other. Facilities are well experienced and good qualified. I wish all very good and bright success in their carrier".

Dr. R.P. Verma, Former Executive Director, R&D, Indian Oil Corporation, (IOC) Faridabad and Advisor for R&D, HPCL

"Extremely impressed with the Institute and its faculty. Director is giving guidance and all research projects have been found to be relevant. I wish good success in Institute's Endeavour. There is good potential to increase collaborative R&D work."

Dr. David Bridgeman, Global Licensing Manager, GTC Technology Houstan, Texas, USA

"So very pleased to visit and see such outstanding work that's been done and also consistent with positive social relevance. Thank you for your hospitality".

Dr. S. Narasimhamurthy Associate professor- Pharmaceutics, University of Mississippi, USA

"I am overwhelmed by the scientific ambiance and cordiality in this campus. I thank Director and all faculty and students and wish their all the best".

Dr. Prathibha Nadig, Professor, pharmacology, Vydehi Institute of Medical Sciences and Research Centre, Bangalore

"Poornaprajna Institute of Scientific Research is a very promising institute for budding PhD Scholars. It would be a privilege to be around such an institution".

Immanuel IT Queensland, Officer, Income Tax Department Bangalore

"Poornaprajna Institute of scientific Research is promising and upcoming institute and this is built of public in general and for common people".

Staff, Mount Carmel College, Bangalore

"Amazing work. Especially in biological block, protein crystallography. Material science is excellent! We are touched by the warm reception and ambiance. It would be definitely beneficial for our students. Anticipating many such visits".

Dr. S. Harish Kumar, MIT, Manipal

"Excellent infrastructure, best ambience for research. Very good faculty and research scholars. Thank to Dr.Halgeri for providing the opportunity. Exploring the possibilities of further research collaboration with chemical engineering dept. MIT Manipal"

Dr. D. Yogeshwara Rao, Adviser, Office of the Principal Scientific Adviser to the Govt. of India

"It is a pleasant surprise for me to see such a nice institute. It is more creditable that the institute was set up in the last 3 years. The staff are young and dynamic as well as enthusiastic to take up challenges. The institute has been able to attract good funding speaks volume of the institute growing image. I wish all the best".

Dr. C. V. Satyanaranana, Senior Principal Scientist, NCL, Pune

"I was highly impressed by the type of research carried out and the facilities that were created in a short span of time. Since, most of the staff are young and able to attract such a large number of good quality students. I foresee a great future to this Institute. In fact I predict that it will be a force bearer for many such institutes in the future. I wish all the best to the faculty and students of this institute"

Sri. N. Santhosh Hegde, former justice of the Supreme Court Of India, former Solicitor General of India and was Lokayukta for Karnataka State of India

"I got the opportunity of visiting PPISR at Bidalur. I am deeply impressed with the infrastructure provided for the researcher by the Institute. From my interaction with the staff and students I found both are very satisfied with the facilities provided. It is amazing how a religious institution can manage a research institute successfully, that too in such a short time. I am sure this institution will grow over the time and will compete with such international institutes. I wish the institute all success"

Mrs. Kirthi P Shetty, Principal PPHC, Bangalore

"We are really inspired by the simplicity and methods of explaining to our students very important concepts. Our students and me got to see wonderful instruments. I am sure this will inspire at least few of our students to take research as their future"

Dr. B.H.S. Thimmappa, MIT, Manipal

" I have visited the institute and found that this place has conducive work environment research facilities and other infrastructure developed in a short period of time. It is useful for younger researchers to continue their research in specialized areas. I wish all the people to achieve their goals"

Dr. Bipin V Vora, consultant, R&D Advisor, A Honeywell company, USA

"It was my great pleasure to visit PPISR institute in lovely setting at Bangalore. This gave me an opportunity to visit an old friend, Dr. Anand Halgeri. The institute has done excellent ground work to become a world class research institution. A very professional highly qualified staff and enthusiastic young students. I wish all the best for their continued success".

Prof. Gundu H.R.Rao, Emeritus Professor at University of Minnesota

" I was very much impressed with the way research activity has been developed in such a short time. In enjoyed meeting the young students, scientists and the senior faculty. There is great window of opportunity for developing research that can be used for providing new molecules of interests. In addition variety of commercially useful molecules as well biomaterials can developed on this flat form. I wish the PPISR all the success"

Dr. Anil C. Banerjee, Professor of Chemistry, Columbus State University, Georgia, USA

"I visited PPISR along with a group of eight students and one staff from my university on 3rd March, 2014. Students were given some exposure of research in catalysis preparation and testing as well as biology. We were very impressed with the knowledge and devotion of faculty and research students. This is a small institution made of very dedicated group. Our students got a good feeling about research and culture. We are thankful to Dr.Halgeri and his team for providing us hospitality"





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