

## Message from the Secretary, AMEF

In addition to discharging his religious and spiritual obligations as the Pontiff of Sri Admar Mutt, His Holiness Sri Vibudhesha Theertha Swamiji, Udupi, was an educator and a research facilitator in science. He had a clear model for the synergy of basic education and scientific research, whereby the scientists of PPISR were free to pursue their research objectives and train young researchers, while the Poornaprajna schools would be nourished by and support PPISR. With the submission of the PhD thesis by the first batch of our nine research students, part of Sri Swamiji's dream has been fulfilled. The outreach program, which has now become established since its inception two years ago, and the most recent edition of which took place earlier this year, has now become an excellent forum where students of Poornaprajna schools interact with our scientists of PPISR.



After the completion of the new biological wing last year, construction has now begun on an extended hostel facility, in anticipation of an expansion of our student strength. I am now emboldened to think that we are now in a position where we can march forward with a steady step further along the path indicated by HH Swamiji.

Upon HH Sri Vibudhesha Theertha Swamiji attaining the Lotus Feet of Lord Sri Krishna, the task of guiding us through this journey that is simultaneously sacred and scientific was most graciously taken up by HH Sri Vishwapriya Theertha Swamiji, the presiding pontiff of Sri Admar Mutt, Udupi, the president of AMEC and Chairman of AMEF.

Milestones witnessed the past year include an additional 28 publications in international peer-reviewed journals by PPISR scientists, with which our total number crosses the 132 publications.

My heartfelt thanks and congratulations to Prof. A. B. Halgeri, the Director, and his team of researchers and their students, who, despite being fewer in number, have, in my opinion outperformed many other larger and better known institutes.

In the pursuit of the lofty vision set forth by H H Sri Vibudhesha Theertha Swamiji, and guided most ably by H H Sri Vishwapriya Theertha Swamiji, PPISR has been funded mainly through the Admar Mutt Education Foundation (AMEF). I fervently hope that more well-wishers from the general public and the corporate world would contribute their mite to furthering and nurturing this noble cause.

**Dr. K. Srihari**

(Hon. Secretary, AMEC and AMEF),

Professor (Rtd), UAS, Bengaluru

March 19, 2015

## Foreword by the Director



I have great pleasure in presenting the fifth Annual Report on account of research and academic activities of Poornaprajna Institute of Scientific Research (PPISR) for the year 2014-15. We have been able to execute a significant progress in our academic activities by submitting doctoral thesis of first batch of **nine research scholars** to Manipal University who were pursuing research in the area of Materials Science, Biological Science and Theoretical Sciences. This is the first step of our achievement to realize the dreams of our Founder Chairman H H Sri VibudheshaTheerthaSwamiji.

PPISR has successfully completed two industry sponsored projects namely M/s GTC US LLC and also HPCL R&D. The most significant achievement of PPISR is the development of catalyst and process on Toluene Alkylation has been licensed by M/S. GTC US LLC to new China refinery. The entire credit goes to faculty members, students and project engineers of catalysis group by taking up this challenging task and executing it successfully. Based on the above achievement, PPISR has signed an agreement with GTC US LLC for a new collaborative project on “Natural gas conversion to value-added chemicals.” During this period, our faculty members have been awarded a grant under Centre of Excellence in Science, Engineering and Medicine (CESEM) by Vision Group on Science & Technology, Government of Karnataka. The Department of Science & Technology has also technically approved for extramural research funding for a period of three years. Several new projects have been initiated with sponsorship from DBT, DST, VGST& BRNS.

In 2014-15 alone, the Institute has published more than 25 research papers in all areas of sciences and in overall, PPISR has crossed 138 publications in international peer reviewed journals which itself is a great achievement. Based on our ongoing research projects, many of our students and faculty members have presented research papers at 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 science outreach programmes with an aim of Today’s Science for Tomorrow’s scientist have been successfully conducted 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. The infrastructure is being constantly upgraded to meet the academic requirement for carrying out scientific activities and this year H H Sri VishwpriyaTheerthaSwamiji had laid foundation stone for the construction of a new Hostel Building at the Bidalur campus on the occasion of Founder’s Day Celebration.

At a glance through this Annual Report, we believe you will realize that PPISR is on the right path in realizing Paramapoojya Sri SriVibudheshaTheerthaSwamiji’s dream of creating a vibrant and flourishing institutional environment for scientists and research students. On the whole the entire year 2014 was much more productive and successful with the unstinted support and blessings from H H Sri VishwapriyaTheerthaSwamiji and also enthusiastic support from the management of Admar Mutt Education Foundation and Trustee members, and also with the support of all faculty members and students of PPISR.

**Dr. A. B. Halgeri,  
Director**

## Board of Trustees

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**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). The functions of the doctoral advisory committee is to review research progress of doctoral also making suggestions in further improving the quality of the research. 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, CSIR Emeritus Scientist, Visiting Professor, Cambridge University, U.K
2. Prof. Y. S. Bhat, HOD, Chemistry Dept, Bangalore Institute of Technology (BIT) Bangalore.
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, Bangalore.
8. Prof. S. Ramakumar, Physics Dept., IISc, Bangalore.
9. Dr. Raman Ravishankar, HPCL, Bangalore.
10. Prof. A. J. Rao, Biochemistry Dept., IISc, Bangalore.
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12. Prof. S. A. Shivashankar, Material Research Center (MRC), IISc, Bangalore.
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17. Prof. H. N. Vasan, SSCU, IISc, Bangalore.
18. Prof. Prof. Chandrabhas Narayana, JNCSAR, Bangalore
19. Prof. Giridhar . Madras, Dept of Chemical Engineering, IISc, Bangalore
20. Prof. Andal Narayanan, Raman Research Institute, Bangalore
21. Udupi Ramagopal, PPISR, Bangalore

## Organization

<b>Director:</b>	Prof. Anand B. Halgeri
<b>Financial Advisor:</b>	Sri P.Sreenivasa Rao
<b>Scientific Staff:</b>	Dr. Udupi Ramagopal
	Dr. Srikanth R
	Dr. Ananda
	Dr. Sujit Sarkar
	Dr. Ganapati V Shanbhag
	Dr. Nalini G Sundaram
	Dr. Sanjeev P Maradur

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Mr. Kishore L Gaikwad	Senior Administrative Officer
Mr. Nagarajan R	Accounts Officer
Mrs. Latha Srinivasan	Administrative Secretary

### Support staff:

Mr. Vishwaprakash A  
Mr. Praveen Kadam  
Mr. Shashidara

### 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 (Liquid Crystals)  
Prof. Suryaprakash, IISc (NMR Studies)  
Prof. T M Aminabhavi, CSIR 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)

## About the Institute

### History and Mission

PPISR was conceptualized and founded by late HH Sri Vibudsha Theertha Swamiji, the then chief pontiff of the Udupi Sri Admar Mutt to create a serene environment, conducive to scientists to ponder basic scientific questions, in much the manner that India's ancient philosopher-scientists did. The vision of Swamiji for PPISR is 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 30 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 eight 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 laboratories abroad to conduct basic as well as 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 also conducting outreach activities for high school students with the aim of “**Today’s Science for Tomorrow’s Scientists**”in order to develop innovative and imaginative platform for research in young minds.

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 conducts course works in core areas of 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 PhD supervisors of MU, Manipal and The first batch of 9 students submitted their doctoral thesis to MU, Manipal. Currently, 7 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>

Sr. Administrative Officer: [admin@poornaprajna.org](mailto:admin@poornaprajna.org)

## Key Scientific Accomplishments during 2014-2015

### Catalysis Group

#### **A breakthrough for PPISR-GTC collaborative project: GTC licenses TolAlk technology to a China refinery**

An Industrial project sponsored by GTC Technology USA is going on in Materials Science Division since four years on the development of catalyst and process for aromatics technology. This successful collaboration with US Company has brought a lot of credibility to PPISR.

Research collaboration of GTC with PPISR started way back in 2010 when new faculties had just joined in materials science. Then onwards PPISR has become a nodal center of R&D for GTC. This catalyst and its development work for toluene alkylation from lab to pilot scale was conducted at PPISR since 2011. The vast experience of Director, Dr. A. B. Halgeri on the catalyst development and process commercialization and also past collaboration with GTC has made them to approach PPISR for a collaborative project. In 2011, the first delegation scientists from GTC, USA, Süd-Chemie, Germany and SCIL visited PPISR (22-25, June 2011), for face to face meeting to review the project visited PPISR. Dr. ZhongYi (GTC), Dr. Köhler, Dr. Olivier (Süd-Chemie, Germany), Dr. Sabde (SCIL) and Dr. Prasad Rao (consultant to GTC) attended the 4 days meeting along with Dr. Halgeri and Dr. Shanbhag from PPISR. In addition to the research work, the matters related to filing patent and FTO were also discussed. A fully automated micro-reactor catalyst testing unit was procured and installed at the institute during first week of April 2011 initiating the research. Over the years PPISR in collaboration with GTC scientists could able to develop first generation catalyst and process development for aromatic production technology. This technology with novel process operation was announced worldwide by GTC in December 2012 and this was a happiest moment for the scientist involved in development of the technology. PPISR-GTC association continued further in coming up with second generation catalyst for selective production of aromatics of interest. This work is soon going to be filed for patent.

In the recent past, **“GTC licenses novel toluene alkylation technology at new China refinery”**

It was very pleased to know that GTC licenced a toluene alkylation technology to a china based company. Being an academic institute full of PhD students and various academic programs, working on a time bound industrial project focused on certain goals is a challenge by itself. Also, competing with proven technologies and making the process commercially viable was an uphill task. The credit at large goes to Dr. Ganapati Shanbhag, Dr. Sanjeev Maradur and their team of project students and project engineers for taking up this challenge, for constantly pursuing the work and making it a success. The regular support by the team of GTC, USA on both scientific and technical aspects is highly acknowledged. Also, continuous support by AMEF management to the Catalysis Group to achieve its goal is worth mentioning.



PPISR-GTC collaboration continued for fifth year starting from November 2014 with Dr. Halgeri, Director, and PPISR signing an agreement with GTC for this new collaborative project. Dr. Ganapati Shanbhag is the Principal Investigator and Dr. Sanjeev Maradur as co-investigator of the project. There were discussions on the technical requirement and literature on the new project related to the catalyst and process development for the aromatics technology with the routes other than alkylation. Synthesis of aromatic compounds from cheaper feed stocks obtained from refineries is an important area of research and the scientists are continuously working on developing new alternative and cost effective technologies involving mainly novel catalyst design and process development to achieve this goal.

### **HPCL sponsored project**

Based on the credentials of Catalysis Group of PPISR and Director Dr. A. B. Halgeri, HPCL R & D Centre Bangalore sanctioned a project to PPISR on "Catalyst development for hydrocarbon conversion to value-added products" in October 2012. This project involved the catalyst development for aromatization of light naphtha and side chain alkylation of toluene to produce ethyl benzene/ styrene. This two-year collaborative project with R & D Centre, Hindustan Petroleum Corporation Ltd, Bangalore was successfully completed in October 2014 with the filing of two Indian and world patents (PCT) and communication of two joint publications to internationally reputed journals. Based on the excellent performance of Dr. Ganapati Shanbhag and his two students Mr. Janardhan H L and Mr. Vijaykumar Marakatti, HPCL R & D Centre has asked to submit another 2 year project proposal. This project not only gave PPISR the credit but also good industrial exposure to PhD students involved in this project.

### **Nano Materials group**

- The proposal titled "***Influence of Compositional Phase Transition on the Sunlight driven Photocatalysis observed in Rare Earth (RE=Eu, Tb) substituted Bi<sub>2</sub>WO<sub>6</sub> Nanoparticles***" was awarded beamtime from February 9<sup>th</sup> to 12<sup>th</sup> at the Elettra Synchrotrone, Trieste. Dr. Nalini and Mr. Pradeep carried out experiments at the MCX beamline of the Elettra beamline at Synchrotron Trieste during the cycle January – July 2015. Dr. Jasper Plaiser, the beamline scientist and his post doc Dr. Abdellatif helped collect data at the beam line. Their travel was supported by DST-India under the Indo-Italian S&T POC. Local hospitality cost for visiting Trieste, Italy was borne by the Italian MAE/ Synchrotrone Trieste as per agreed financial norms of the Indo-Italian S&T POC.
- Dr. Nalini was invited by Prof. Umarji, Chairman, MRC, IISc, to conduct a 5 days hands on workshop on "X-ray Rietveld Refinement" using the program GSAS-EXPGui at MRC from February 25 – March 3 2015. The workshop was conducted successfully by Dr. Nalini Sundaram and her group. This was a unique program where in all the participants ran through the technique simultaneously following the instructions. The transfer of knowledge was very high and practically useful. The first day (27<sup>th</sup> February) was attended by about 30 students. The second day attracted more than 40 students and all of them stayed put till the last day (March 3<sup>rd</sup>). Some young faculty and Prof. Umarji attended the workshop. A high tea was arranged by Professor. Umarji on the last day to consolidate the successful completion of the workshop.



# First Batch of Nine Doctoral Students submitted their PhD thesis to Manipal University, Manipal

## Materials Science

1. Title of the Thesis: **Carbonaceous, Nanostructured Metal Oxides Obtained From Metalorganic Precursors through Inert-Ambient, Sealed-Tube Pyrolysis**

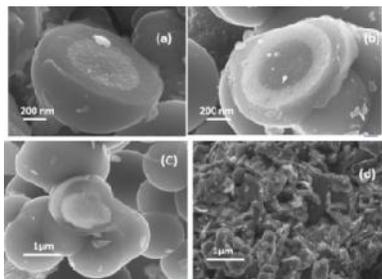
Name of the Student: Mr. Srinidhi Raghavan

Date of Registration for Ph.D: 4<sup>th</sup> November 2011

Date of Submission: 24<sup>th</sup> November 2014



Mr. Srinidhi Raghavan joined PPISR as a joint student of Dr. Nalini, PPISR and Prof. Shivashankar, IISc. The focus of his work was on the synthesis of metal oxides and metal oxide nanoparticles from the corresponding metalorganic complexes, and on the investigation of the properties of nanostructured metal oxides. Mr. Srinidhi used a novel and simple technique for the



synthesis of metalorganic complexes, specifically substituted acetylacetonate complexes of Ga, Cr, and In. These have been characterized comprehensively using a number of techniques and, later, purified and produced in ample quantity by scaling up the synthesis procedure. In particular, single crystals of the complexes have been grown and detailed structural elucidation has been undertaken resulting in a publications in international peer reviewed journals. In addition, adducts of these complexes have also been prepared and characterized. The second aspect of

the work to be undertaken is the synthesis of  $(Cr_{1-x}Ga_x)_2O_3$  and  $(Ga_{1-x}In_x)_2O_3$ , for various values of  $x$ , from the different complex compositions prepared and characterized in the earlier part of the effort. This will be carried out through a. An integral part of this work will be the investigation of the detailed characterization of the oxides, and a study of some dielectric and optical characteristics of the oxides, and of their catalytic/sensing capabilities.

2. Title of the Thesis: **Investigation of smart oxide nanomaterials for photoluminescent and photocatalytic applications**

Name of the Student: Ms. Swetha S. M.

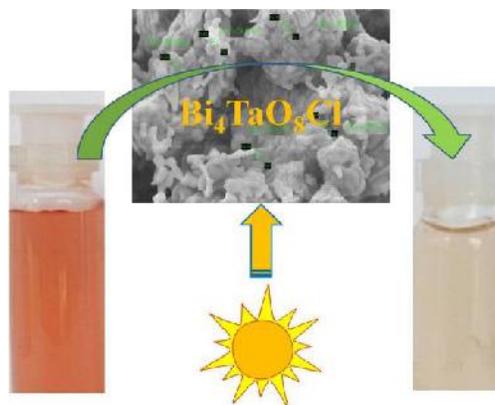
Date of Registration for Ph.D: 4<sup>th</sup> November 2011

Date of Submission: 4<sup>th</sup> January 2015



Ms. Swetha Bhat, my first student and joined Dr. Nalini's group in the Materials Science Division at PPISR in September 2010. She was awarded the Junior Research fellowship (JRF) and subsequently the Senior Research Fellow (SRF) by the Government of India. Swetha initiated research work in two important and current areas of Photoluminescent and Photocatalytic nanomaterials using environmental friendly synthesis methods. During this period she also registered for her Ph.D with Manipal University. Her thesis entitled "**Investigation of smart oxide nanomaterials for photoluminescent and photocatalytic applications**" focuses on the syntheses of mixed metal complex oxide nanoparticles and their detailed local and crystal structure study by X-ray, neutron powder diffraction and pair

distribution function. She was able to synthesize for the first time, polymorphs of rare earth tungstate materials using a low temperature fast solution combustion technique. Swetha investigated structural influence on photocatalysis and photoluminescence by analyzing data obtained at various international facilities such as Oakridge National Lab, Argonne National Lab, U.S.A, FRM II, Germany etc. She was able to gain an insight to understand the fundamental aspects of impact of nano size and crystal structure to tune the properties. Furthermore she was able to establish key factors such as bandgap, particle size as well as local structure responsible for the enhanced photocatalytic activity. In appreciation of this work Swetha won the best oral presentation award at the 41st National Seminar on Crystallography (NSC) organized at CLRI, Chennai by the Indian Crystallography Association. Further for her research on photoluminescent materials, she was awarded for 'Rising Star Oral Presentation Award' and Swetha presented the same at AsCA13 which was held in HKUST, Hong Kong. This work has resulted in 5 publications in international Journals like RSC and ACS publications. This detailed study of synthesizing mixed metal oxide nanomaterials and crystal structure analysis of energy materials could benefit to design new materials and also to realize the observed properties exhibited by the nanomaterials.



3. Title of the Thesis: **Novel eco-friendly catalysts for biodiesel synthesis and conversion of byproduct glycerol into value-added products**

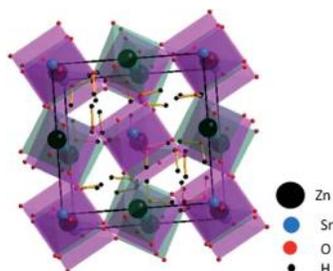
Mrs. Swetha Sandesh

Date of Registration for Ph.D: 10<sup>th</sup> December 2011

Date of Submission: 09<sup>th</sup> February 2015



Mrs Swetha Sandesh was the first student to join Materials Science Department under the guidance of Dr. A. B. Halgeri and co-guidance of Dr. Ganapati Shanbhag. Mrs. Swetha's topic of research is "**Novel eco-friendly catalysts for biodiesel synthesis and conversion of byproduct glycerol into value-added products.**" She worked on designing novel solid base catalysts for transesterification of non-edible oil to produce biodiesel. She also worked on new catalytic material metal hydroxyl stannate as a strong base and bifunctional catalyst for glycerol transformation to glycerol carbonate and biodiesel synthesis. She studied the catalytic transformation of glycerol into solketal and acetins. She studied solid base catalyst KF on alumina and established the influence of basicity and support on glycerol carbonate synthesis. He



reported for the first time a novel organic inorganic hybrid catalyst (tetrapropylammonium heteropoly tungstate) as an efficient catalyst for solketal synthesis from glycerol. Cs salt of heteropoly acid also shown to be the best catalyst for acetin synthesis better than all the reported catalysts so far. During her research work, she got experience in handling catalytic reactors, AAS, GC, XRD, FTIR, UV-Vis instruments etc. She won a **Best Oral presentation award** at a National symposium in

Kuvempu University on “Social Relevance of Chemical Sciences” in March 2011 for her work on designing novel catalyst for bioglycerol transformation into glycerol carbonate by transesterification. Her work has been published in many reputed international journals such as RSC Advances (Publisher RSC, London, Impact Factor: 3.7), Journal of Molecular Catalysis A (Elsevier, Impact Factor: 3.67) and Catalysis Letters (Springer, Impact Factor: 2.3). Another 3 manuscripts are under review in reputed journals.

4. Title of the Thesis: **Design of solid acid catalysts for Prins reaction and toluene methylation**

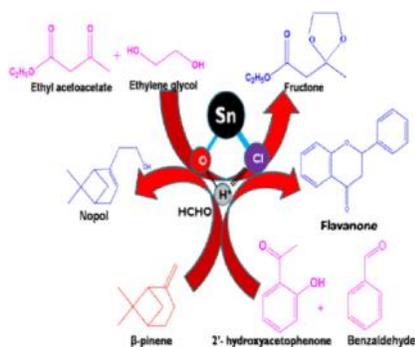
Vijaykumar Marakatti

Date of Registration for Ph.D: 10<sup>th</sup> December 2011

Date of Submission: 28<sup>th</sup> January 2015



Vijaykumar S. Marakatti joined PPISR in July 2010 under the guidance of Dr. Ganapati Shanbhag and co-guidance of Dr. A B Halgeri. He initially worked in an industry project on “Design and development of catalyst and process for shape selective synthesis of substituted aromatics” for one year. During this period, he registered for PhD programme in Manipal University in December 2011. Title on his thesis is **“Design of solid acid catalysts for Prins reaction and toluene methylation”**. In his doctoral programme, he worked on novel Sn(OH)Cl catalyst which is reported for the first time as Brønsted solid acid catalyst for organic transformation. He also studied the metal ion exchanged zeolite catalyst and sulphated zirconia as catalysts for the synthesis of nopol and dioxane derivative respectively and discovered the dependence and importance of Lewis acidity for Prins reaction. His studies also showed the importance of solvents and relation between solvent acidity/basicity (in terms of acceptor/donor number) with catalytic activity. In his work, he showed high activity and selectivity for Prins reaction products for the designed catalysts compared to conventional solid acid catalysts. He also conducted vapour phase toluene alkylation with methanol to produce selectively *ortho* xylene by alkaline earth metal ion exchanged zeolites and explained the selectivity through hard-soft-acid-base (HSAB) principle. This work was a part of a collaborative programme with HPCL R & D Centre, Bangalore. During his research, he published his work in reputed international journals such as Applied Catalysis A (Elsevier, IF = 3.67), RSC Advances (RSC, IF = 3.7), Catalysis Science and Technology (RSC, IF = 4.7). He also co-inventor in a patent filed by HPCL jointly with PPISR. Mr. Vijaykumar received **best poster presentation** award for “Tin (II) hydroxychloride: A Novel Solid Brønsted Acid Catalyst for Selected Condensation Reactions” in the National Workshop on Catalysis, CSIR-NEERI, Nagpur, Maharashtra on 4-5, Feb 2014 sponsored by Catalysis Society of India. He submitted his thesis to MU in January 2015.



5. Title of the Thesis: **Studies on pore modified zeolite catalysts for aromatization and aromatic substitution reactions**

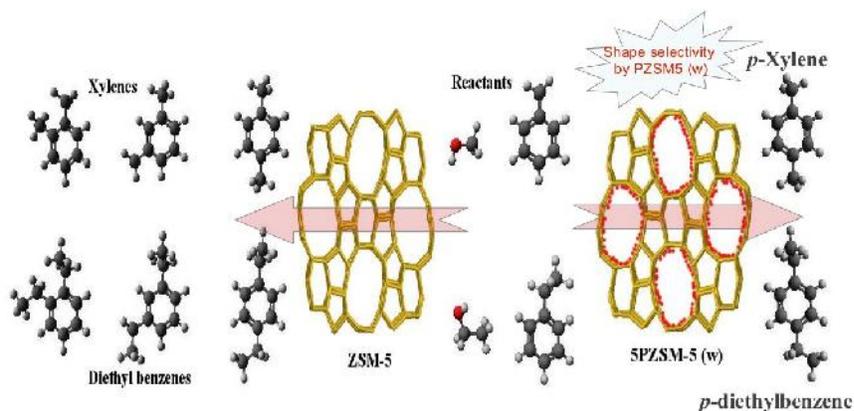
Mr. Janardhan H L

Date of Registration for Ph.D: 10<sup>th</sup> December 2011

Date of Submission: 06<sup>th</sup> February 2015



Mr. Janardhan H L conducted his doctoral research under the guidance of Dr. Ganapati Shanbhag and co-guidance of Dr. A B Halgeri from November 2010 and submitted his thesis in February 2015 to Manipal University. During his research work at PPISR, he worked initially in an industry sponsored project on “*Design and development of catalyst and process for shape selective synthesis of substituted aromatics*”. Later, he worked on the thesis topic “**Studies on pore modified zeolite catalysts for aromatization and aromatic substitution reactions**” in which he studied *development of modified zeolite catalysts for reactions viz.* conversion of light naphtha to aromatics, vapor phase toluene methylation, ethylbenzene alkylation with ethanol and liquid phase 2-methoxynaphthalene acylation reactions. He worked on pore engineering of zeolite by phosphate modification and applied these catalysts for shape selective organic transformations. He established the correlation between shape selectivity and pore size/volume of the modified catalyst. Also, he observed the generation of new acid sites *via* phosphate modification and their role in increasing the catalytic activity.



During his PhD, he gained expertise in the field of materials synthesis, modification, characterization and catalytic evaluation in liquid and vapor phase reactors. He has a thorough knowledge in heterogeneous catalysis including novel catalyst design, interpretation and correlation of catalyst

properties with activity, reaction kinetics, modelling and simulation studies. He has got first author publications published in internationally reputed journal Applied Catalysis A (Elsevier, Impact Factor: 3.67) and few others are under review in other journals and also a co-inventor in patent filed jointly with Hindustan Petroleum Corporation Ltd in a collaborative project. He has presented his work in several National/International conferences and he **received a best poster presentation award** at Manipal Institute of Technology, “National Symposium on Chemistry and Humanity” in Manipal, July, 2011 for his work on pore engineering of zeolite catalyst for PDEB synthesis.

6. Title of the Thesis: **Polymeric Composite Membranes for Pervaporation Separation of Alcohol-Water Binary Mixtures**

Mr. Suhas D. P.

PhD Guide: Dr. A. V. Raghu

PhD Registration: November 2011

PhD Thesis submission: December 2014



Mr. Suhas D.P. joined PPISR in June 2010, initially he worked in the area of “Liquid Crystals” under the guidance of Prof. B. K. Sadhashiva. Later, he worked on the thesis topic “**Polymeric composite membranes for pervaporation separation of alcohol-water binary mixtures**” under the guidance of Dr. A.V. Raghu and co-guidance of Prof. T.M. Aminabhavi, in which he has developed different composite membranes for pervaporation dehydration of aqueous alcohol mixtures. His first work was on preparation and characterization of novel segmented polyurethanes based on 4,4' - {oxy -1,4-diphenyl bis(nitromethylidene)} diphenol, which was published in Polymer Engineering and Science (publisher Wiley, Impact Factor = 1.44). Later, he has established the tuning property of zeolite composite membranes by varying their silica alumina ratio, which was published in Polymer Engineering and Science (publisher Wiley, Impact Factor = 1.44). For the first time he has reported, the use of functionalized graphene sheets as effective fillers in improving the performance of sodium alginate based membranes towards isopropanol dehydration (published in RSC Advances Impact Factor 3.8). He established the effectiveness of organic acid treated clay over clay, as effective filler in improving the performance of sodium alginate based membranes (published in Applied Clay Science, publisher Elsevier, Impact Factor 3.0). He has also worked on functionalized graphene sheets loaded chitosan based membranes for ethanol and isopropanol dehydration, which is published in Industrial Engineering and Science (publisher American Chemical Society, Impact Factor 3.0).

During his stay in PPISR he has gained expertise in membrane preparation, characterizations and testing. He has through knowledge in computational studies on membrane performance *viz.*, sorption parameters, diffusion coefficient, Arrhenius parameters etc., Based on his research proposal and subsequent interview he was selected for **Senior Research Fellowship (SRF)** by CSIR, Govt. of India. His work was presented in various national and international conferences. He has published five papers as first author and communicated two articles in reputed international journals.

## Biological Sciences

7 Title of the Thesis: **Studies on bioactive compounds from endophytic fungi of *Eucalyptus* and *Simarouba* plants**

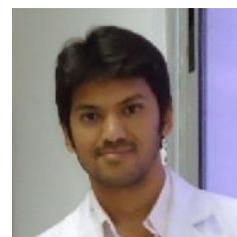
Mr. SATHISH L.

PhD Guide: Dr. ANANDA

PhD Registration: November 2011

PhD Thesis submission: January 2015

Mr. Sathish L joined PPISR as first student of Biological Sciences in August 2010 when not even minimum research facility was available for mycology research. Dr. Ananda and Mr.Sathish initiated research along with the building up of department’s research facility. Three medicinal plants were for the study and 110 endophytic fungal isolates were isolated. Out of that, 30 endophytic fungi were from leaves and



twigs of *Eucalyptus globulus*, 60 from leaves and twigs of *Eucalyptus citriodora* and 20 from leaves and twigs of *Simarouba glauca*. All these isolates were subjected to preliminary screening for antimicrobial activity and 3 isolates (PEGT001, PEGT002 and PEGL001) from *E. globulus*, 3 isolates (PECL011, PECT017 and PECL014) from *E. citriodora* and 2 isolates (PSGL001 and PSGT001) from *S. glauca* showed inhibition against most of the tested organisms. All the eight positive endophytic fungal isolates were grown in large scale for the secondary metabolites extraction and tested for antimicrobial and antioxidant activity. DNA sequences of eight endophytic fungi are deposited in GenBank and obtained accession numbers. Two fungi from *E.globulus* PEGT001 and PEGT002 were identified as *Alternaria alternata* and *A. arborescence*, PEGL001 was identified as *Guignardia* sp. Fungal isolates PECL014, PECL011 and PECT017 from *Eucalyptus citriodora* belongs to *Preussia* sp., *Aspergillus* sp. and *Chaetomium* sp. respectively. Two isolates PSGL001 and PSGT001 were from *Simarouba glauca* belongs to *Curvularia* sp. and *Phomopsis* sp., respectively.

Based on the preliminary studies, PEGT002 was selected to study employing different parameters for the optimal production of bioactive compounds. Fungi grown in rice media and malt extract media showed good antimicrobial activity, while extracts from Potato dextrose broth showed moderate activity, no antimicrobial activity observed from PDB (pH 3), new media, czapek dox and PDB supplemented with tyrosine extracts. From this study malt extract was selected as the best media for the production of bioactive compounds. Secondary metabolites production optimization studied by varying different parameters such as media, pH, temperature etc. Two endophytic fungi PEGT001 and PEGT002 having highest antimicrobial and antioxidant activity were selected for the detailed study. Two endophytic fungi PEGT001 (*Alternaria alternata*) and PEGT002 (*Alternaria arborescence*) found to be the best bioactive compound producing fungi. Large-scale production and purification of bioactive compounds showed very promising antimicrobial and antioxidant activities, which are comparable to the antimicrobial and antioxidant of the known drugs. The biological activities of PEGT001 and PEGT002 can be enhanced by employing further purification process. The results of present study clearly indicate the potential of PEGT001 and PEGT002 endophytes to be used as antimicrobial and antioxidant drugs. The active compounds predicted for drug-likeness by Osiris software and rule of five resulted in Tetrahydroxyflavone appeared to be the perfect drug-like molecule with antimicrobial, antioxidant and anti-cancer activity.

8 Title of the Thesis: **Screening and characterization of alpha amylase inhibitors and aldose reductase inhibitors from endophytic fungi of medicinal plants**

Student: PAVITHRA. N

PhD Guide: Dr.Ananda

PhD Registration: November 2011

PhD Thesis submission: January 2015

Ms. Pavithra N has been selected based on the interview conducted at PPISR and joined as research scholar during December 2010. Her study focussed on isolation of endophytic fungi from medicinal plants such as Tulsi, bittergourd and menthya, isolated endophytic fungi was screened for alpha amylase and aldose reductase inhibitors. A total of 84 endophytic fungi from Tulsi, 11 from bittergourd and 11 from Menthya were isolated. Seven endophytic fungi from Tulsi, three from bittergourd and seven from Menthya were found to be active against porcine pancreatic alpha amylase and alpha glucosidase. Five endophytic fungi from Tulsi, and three from bittergourd showed aldose reductase inhibition. Only three endophytic fungi isolated from Menthya showed moderate aldose reductase inhibition. Two important fungi namely *Trichoderma atroviride* and *A.carthami* were extensively studied for the compounds responsible for enzyme inhibition activity. In the present study dihydronorwogonin from



*A.carthami* (Tulsi) and Pyrrolo 1, 2 a pyrazine hexahydro from *T.atroviride* (Bittergourd) are found to be the most probable alpha amylase and aldose reductase inhibitors. Both active compounds had anticancer activity also. Presence of dihydronorwogonin has been reported for the first time in endophytic fungi. Dihydronorwogonin and Pyrrolo 1, 2 a pyrazine hexahydro reported for the first time as an alpha amylase and aldose reductase inhibitors.

## Theoretical Sciences

9. Title of the Thesis: **Quantum Noise due to Dissipative and Non-dissipative Interaction with a Squeezed Environment, Quantum Error Correcting Codes and Characterizing Quantum Dynamics.**

Mr. Omkar

PhD Guide: Dr. Srikanth R.

Date of Registration for Ph.D: 4<sup>th</sup> November 2011



Mr. Omkar holds the special place of being both the first PhD student of PPISR as well as the first residential student. He was working with Dr. R. Srikanth as a Visiting Student at the Raman Research Institute, and when the PhD stream was opened at PPISR, joined us at Dr. R. Srikanth's invitation. Quantum systems are typically delicate and noisy. Characterizing their behavior forms a major part of today's research in theoretical and experimental quantum information science. Omkar's thesis work was devoted to applying certain geometric and error correction techniques to characterizing quantum noise. In one work that was part of his thesis, Kraus operators were constructed for various channels via the Choi isomorphism, and their various properties studied. The studied channels include those associated with dissipative and non-dissipative interactions of one-qubit and two-qubit noise. A generalization of the Kraus operator formalism was introduced, called the operator sum-difference representation, which was shown to be applicable not just to completely-positive, but also not-completely-positive channels, and indeed to any linear map.

As another problem he studied, quantum error correcting codes were used for the purpose of characterizing noise. This required introducing a novel class of stabilizer codes for which the correctable errors form a group, and can thus correct arbitrary errors on the qubits of a known subsystem. The resulting quantum process tomography technique, "quantum error correcting code based characterization of quantum dynamics" (QECCD), is implementable using current experimental techniques. The method permits an *online* characterization of quantum dynamics, in that arbitrary logical states in the code space of the stabilizer code, that may appear during fault tolerant quantum computation, can be used for concurrent characterization of noise.

A quantum error correcting that it broadened so that we only require the recovered state to be error-free up to a logical Pauli operation within code space is an ambiguous stabilizer code (ASC), a new type of stabilizer code introduced as part of the thesis work, and which generalizes the concept of a degenerate codes, which is the special case where the only residual logical operation after recovery is the trivial one. An ASC cannot be used for error correction, or even, strictly speaking, for error detection. The motivation for introducing ASCs is the characterization of quantum dynamics. In comparison to QECCD, the present method using ASCs requires a smaller size of quantum states. This can be helpful from an experimental perspective, in spite of the cost of increased number of operations.

## Achievements of faculty and students during 2014-15

- Dr. Ananda received research grant for his project titled “Effect of electron beam radiation on endophytic fungi producing ligninase enzyme” for three years from BRNS, DAE, Govt. of India.
- Dr.Nalini’s research proposal titled “Design of Lanthanum based Perovskite Nanoparticles for The Development of Thick Film Gas Sensor” to the DST committee for extramural funding at IIT Kanpur on September 18th 2014. This proposal is sanctioned for funding (40 Lakhs) for three years.
- Dr. Ganapati Shanbhag has been awarded a three year project titled “Chemical fixation of CO<sub>2</sub> by converting into value added chemicals using metal - modified ordered nanoporous silicate catalysts” towards creation of Centre of Excellence in Science Engineering and Medicine (CESEM) programme by Vision Group on Science & Technology (VGST), Govt of Karnataka.
- Dr. Srikanth has been selected by the Editor of the journal “Quantum Information Processing” (QIP) as one of the Top Reviewers for 2014.
- Doctoral Student in Theoretical Sciences, Mr. Aravinda ‘s abstract “Essence of nonclassicality: more effects than cause” was been chosen for **oral presentation** in the 12<sup>th</sup> Biennial International Quantum structures Association (IQSA) meeting: Quantum Structures 2014, **held on 23-27 June 2014 in the Czech Republic, Europe**. This conference was organized by the Faculty of Science, Masaryk University and Department of Algebra. The organizers of the conference awarded 920 Euros for Aravinda’s travel and other expenses. Additionally, his registration and accommodation fees were also been waived.
- Doctoral Student in Materials Science, Mr. Suhas D P has been awarded the **CSIR Senior Research Fellowship (SRF)** for the year 2014-2016. He was selected for this prestigious fellowship through an interview held at CSIR complex New Delhi, where only 30 students were selected from a pool of 250 applicants.
- Mr. Pradeep Shanbogh won the second prize for the poster titled“- Sunlight driven Photocatalytic Degradation of Congo-Red by RE substituted Bi<sub>2</sub>WO<sub>6</sub>" at the Two Day workshop on “Crystallography in The Sciences” organized by Bangalore University in lieu of the International Year of Crystallography 2014, on October 16th and 17th 2014.
- Nine doctoral students have submitted their thesis to Manipal University. The first batch coming out of PPISR is an important milestone for an institute of its kind.

## Division Structure

### FACULTY

### STUDENTS

#### Materials Science

Dr. A B Halgeri (Catalysis)  
Professor and Director

Mrs. Swetha Sandesh (SRF, Submitted Thesis)

Dr. G V Shanbhag (Catalysis)

Dr. Prakash Chandra (Research Associate)

Asst. Professor

Mr. Vijay Kumar S M (Submitted Thesis)

Mr. Janardhan H L (Submitted Thesis)

Mr. Manjunathan P (Research Scholar)

Mr. Santosh Kumar (Project Assistant)

Mr. Saikiran (Project assistant)

Dr. Nalini G Sundaram (Nanomaterials)

Dr. Sowmya Palimar (Research Associate)

Asst. Professor

Ms. Swetha S M (Submitted Thesis)

Mr. Srinidhi R (Submitted Thesis)

Mr. Pradeep Shanbogh (Research Scholar)

Ms Archana (Research Scholar)

Mrs Uma (M. Tech. Project Fellow)

Dr. Sanjeev P. Maradur (Catalysis)

Mr. Sathyapal (Research Scholar)

Asst. Professor

Mr. Kempanna (Project Assistant)

Mr. Manish Kumar (M. Tech. Project Fellow)

#### Biological Sciences

Dr. U A Ramagopal (Structural Biology)

Dr. Raghurama P Hegde (Research Associate)

Associate Professor

Ms. Pavithra G C (Research Scholar)

Ramalingaswami Fellow

Ms. Swetha L (Research Scholar)

Dr. K Ananda (Mycology)

Mr. Sathish L (Submitted Thesis)

Asst. Professor

Ms. Pavithra N (Submitted Thesis)

Ms. Kavita (Research Scholar)

#### Theoretical Sciences

Dr. Sujit Sarkar (Quantum physics)

Mr. Chandan G N (Research Scholar)

Asst. Professor

Mr. Nepal Banerjee (Research Scholar)

Dr. Srikanth R(Quantum Information )

Mr. Omkar Srikrishna (Submitted Thesis)

Asst. Professor

Mr. Aravinda S (Research Scholar)

## Materials Science Division



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. A new materials synthesis laboratory, with several sophisticated equipment, has been established in the group. Bright students passionate for research were interviewed and inducted into Doctoral 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; (2) Novel 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 is one of the frontier areas of research in science involving interdisciplinary subjects. Catalyst is a heart of a chemical reaction and many important sectors like petroleum refining and petrochemical, fine chemical, fertilizer and energy have been greatly benefited by catalysis research. Catalysis group at PPISR is actively doing advanced research in

different areas such as novel catalyst design, alternative fuels, fine and specialty chemical synthesis. Dr. Ganapati Shanbhag and Dr. Sanjeev Maradur are steering the group with 5 research scholars, 4 project assistants and one M. Tech Project student from Chemical Engineering Dept, Manipal University. Overall, 3 sponsored research projects are underway; two industry and one govt sponsored projects. Recently, the project proposal of Dr. Shanbhag titled “Chemical fixation of CO<sub>2</sub> by converting into value added chemicals using metal-modified ordered nanoporous silicate catalysts” has been approved for Centre of Excellence in Science Engineering and Medicine (CESEM) programme by Vision Group on Science & Technology (VGST), Govt of Karnataka. The industry project sponsored by GTC Technology Inc, USA has been successfully completed its 3rd year and the technology developed by PPISR in association with GTC has been announced worldwide by GTC in major petrochemical magazines. Second industry project sponsored by HPCL R & D Centre of two years duration was completed successfully in November 2014. The excellence of work in this project was reflected in terms of two PCT patents filed by HPCL and two research publications communicated to international journals of repute. The group is also working on frontier areas of research of academic importance such as synthesis of mesoporous materials, green catalytic processes for alkylation of aromatics, gas to liquid (GTL), light naphtha aromatization, biomass conversion etc. The group has got expertise in 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; bioglycerol transformation into solketal, glycerol carbonate, acrolein, tert-butyl ethers and acetins. Three students have submitted their PhD Thesis to Manipal University, Manipal.

#### **Functional Energy Nanomaterials Group:**

Presently, research on energy materials especially in the nanoscale is the hot area. The group works on cutting edge problems of designing nanomaterials for energy storage and energy conversion. At PPISR, Dr. Nalini’s group study a broad range of materials systems such as, Photoluminescent materials for solid state lighting devices, Photocatalytic materials active under visible light for degradation of dyes and other contaminants, Nanomaterials for gas sensor applications and Cathode materials for energy storage. The vibrant group comprising of Dr. Nalini ,4 students, one post doc and one M.Tech student working on different areas pertaining to the energy sector. That the group has made progress in their research by leaps and bounds is shown by their recent achievements such as the funding and acceptance of their research proposal for data collection at Trieste, Italy; Publications in peer reviewed journals and also invitation to present their work at the Asian Crystallography association at HongKong. Presently there are two government funded projects that are in progress. The group also collaborates with institutes such as IISc, JNCASR, UCL and also has academic linkages with ORNL, U.S.A, UCL, London etc. Two of the students have submitted their thesis.

**Functional Polymers Group:** Polymer research group worked on developing novel polymeric membranes for pervaporation applications. 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.

## Faculty Profiles

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



#### Educational Qualifications

1. Masters Degree in Chemistry from Karnataka University, Dharwar
2. Ph.D in Physical Chemistry (Heterogeneous Catalysis) from Bangalore University
3. Post-Doctoral researcher under UNESCO fellowship on Zeolite Catalysis at Department of Tokyo institute of Technology

#### 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 purification of Hydrocarbons in PET plant, development of hydrogenation/dehydrogenation 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

Three students have submitted their PhD Thesis to Manipal University, Manipal.

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. Nalini G Sundaram, Assistant Professor



### Areas of Interest

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

Phone: 080-27607242

E-mail: nalini .AT.poornaprajna.org

Webpage: <http://www.ppisr.res.in/nalinis.html>

### 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

- Design and Development of Lanthanum Based Nanoparticles For Selective Thick Film Gas Sensors by DST, India under the Extra mural grants for Individuals for three years (2015-2018)

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

## Completed Sponsored Projects at PPISR

- 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)

## Representative publications

1. **Invited** article titled 'Fullerenes Revisited: Materials Chemistry and Applications of C60 Molecules' Pradeep P. Shanbogh Nalini G. Sundaram, **Resonance**, February 2015, 20 (02), (p.123)
2. Photocatalysis of Bi4NbO8Cl hierarchical nanostructure for degradation of dye under Solar/UV irradiation, Swetha S M Bhat and Nalini Sundaram **New J. Chem.**, 2015, DOI: 10.1039/C4NJ01814A
3. Controlled inversion and surface disorder in zinc ferrite nanocrystallites and their effects on magnetic properties, Ranajit Sai, Suresh D. Kulkarni, Swetha S. M. Bhat, Nalini G. Sundaram, Navakanta Bhat and S. A. Shivashankar, **RSC Adv.**, 2015, **5**, 10267-10274
4. 'Photoluminescence tuning of Na1-xKxNdW2O8 (0.0 <math>x</math> <math>\leq</math> 0.7) nanoparticles: synthesis, crystal structure and Raman study' Swetha S. M. Bhat, Ashfia Huq, Diptikanta Swain, Chandrabhas Narayana and **Nalini G. Sundaram**, **Phys.Chem.Chem.Phys.**, 2014, 16, 18772

Total Number of Publications in National and International Journals: 21

## Research Group

### 1. Post Doctoral Researcher:

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



#### Research Area:

Development of Lanthanum based Oxide Thick films for selective Gas sensors

### Graduate students:

#### 1. Mr. Pradeep Shanbogh (JRF supported by BRNS)



#### Research Area

Rare earth doped Complex Bismuth oxide Nanoparticles for Photoluminescent and Photocatalytic Applications

#### 2. Ms. Archana. K. M (JRF Supported by PPISR)



#### Research Area

Development of Complex Oxide Nanomaterials for Energy Conversion and Energy Storage Applications

## Membership of Professional bodies:

1. Member of National crystallographic Association

## Some Completed Research Projects 2014-2015:

### **(a) Photoluminescence Tuning of $\text{Na}_{1-x}\text{K}_x\text{NdW}_2\text{O}_8$ ( $0.0 \leq x \leq 0.7$ ) Nanoparticles; Synthesis, Crystal Structure and Raman Study**

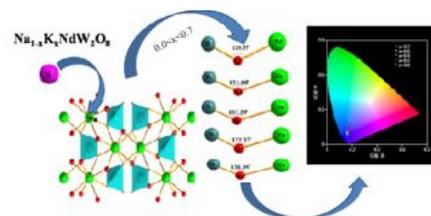
; Duration: 2011-2013

Primary Investigator: **Dr. Nalini G Sundaram**

Research Student(JRF): Ms. Swetha S.M

Published in *Physical Chemistry Chemical Physics*

RSC Publications, 2014



### **(b)**

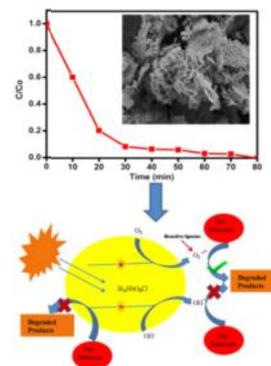
### **Photocatalysis of $\text{Bi}_4\text{Nb}_2\text{O}_{12}$ hierarchical nanostructure for degradation of dye under Solar/UV irradiation**

Primary Investigator: Dr. Nalini G. Sundaram

Research Student: Ms. Swetha. S. M.

Published in *New Journal of Chemistry*,

RSC publications, 2015



### **(c) Controlled inversion and surface disorder in zinc ferrite nanocrystallites and their effects on magnetic properties**

Primary Investigator: **Dr. Nalini G. Sundaram**

Research Student: Ms. Swetha. S. M.

Published in *RSC Advances*, RSC Publications, 2015

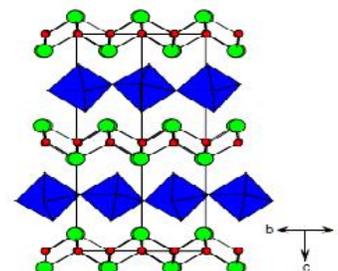
## Current Research Projects

### **1. Synthesis of $\text{Bi}_{2-x}\text{RE}_x\text{WO}_6$ ( $\text{RE} = \text{Nd, Eu, Tb}$ ) Nanoparticles for their Photoluminescent and Photocatalytic Activity**

Primary Investigator: **Dr. Nalini G. Sundaram**

Research Student: Mr. Pradeep shanbogh

Aruvillius phases with layered perovskites are shown to be good photocatalysts and better luminescent materials.  $\text{Bi}_2\text{WO}_6$  is the basic structure in the layered perovskite structure, which exhibits polymorphism, hence crystallographically also very interesting to explore the structure-property relationship. Nanoparticles of rare earth ion substituted  $\text{Bi}_2\text{WO}_6$  were synthesized by varying



temperature, pH and composition. The obtained nanoparticles were characterized by PXRD, PL and photocatalytic activity of the materials are being studied

## **2. Design of Lanthanum based Perovskite Nanoparticles for the Development of Thick Film Gas Sensor**

Name of the Primary Investigator: **Dr. Nalini G. Sundaram**

Name of the Postdoctoral Fellow: Dr. Sowmya Palimar

The synthesized single phase  $\text{La}_{1-x}\text{Ca}_x\text{FeO}_3$  ( $x=0.2, 0.4, 0.6$  and  $0.8$ ) nanoparticles, have further been characterized using a variety of techniques SEM, XRD, XPS, Zeta Potential etc. Further gas sensing studies were carried out as part of the INUP collaborative project at CeNSE IISc, where calcium substituted lanthanum ferrite nanoparticles pressed in to disc shaped pellets showed very good response and recovery time for  $\text{SO}_2$ . Sulphur dioxide ( $\text{SO}_2$ ) is a highly toxic gas which is released during various reactions in chemical and petrochemical industries. This gas poisons the victim by inhalation through lungs and the threshold limit of this gas is 5 ppm. Thus there is a great demand to develop low concentration  $\text{SO}_2$  gas sensor. To establish selectivity further gas sensing study was performed with methane. We observed  $\text{La}_x\text{Ca}_{(1-x)}\text{FeO}_3$  pellets showed a significantly good response to  $\text{SO}_2$  gas at a lower temperature with remarkably good response and recovery time, whereas at this temperature a significantly low response was seen for higher ppm of  $\text{CH}_4$ .

## **3. Design of $\text{Bi}_{2-x}\text{Gd}_x\text{WO}_6$ ( $x = 0.2, 0.4, 0.5, 0.6, 0.8$ and $1$ ) Nano photocatalysts for Degradation of Organic Pollutants.**

Name of the Primary Investigator: **Dr. Nalini G. Sundaram**

Name of the Research Student: Mr. Pradeep Shanbogh

Name of the M.Tech Project Student: Mrs. Uma

Aruvillius phase layered perovskites are shown to be good photocatalysts and better luminescent materials.  $\text{Bi}_2\text{WO}_6$  is the basic structure in the layered perovskite structure. Synthesis of  $\text{Bi}_{2-x}\text{RE}_x\text{WO}_6$  ( $\text{RE} = \text{Gd}$ ) was considered for the above project. In this quarterly period we have synthesized  $\text{Bi}_{2-x}\text{Gd}_x\text{WO}_6$  ( $x = 0.2, 0.4, 0.5, 0.6, 0.8$  and  $1$ ) at neutral pH by conventional Hydrothermal method. These materials were characterized by powder X-Ray Diffraction measurement. Photocatalytic activity of these nanoparticles was carried out for degradation of Congo-red under sunlight. A preliminary result shows that, increased photocatalytic activity has been observed for the lower substitution of  $\text{Gd}^{3+}$  ion.

## **4. Synthesis and Local Structure of Relaxor Ferroic Behaviour of $\text{FeTiBO}_6$ ( $\text{B} = \text{Ta}, \text{Nb}$ )**

Name of the Primary Investigator: **Dr. Nalini G. Sundaram**

Name of the Postdoctoral Fellow: Dr. Sowmya Palimar

$\text{FeTiBO}_6$  ( $\text{B} = \text{Ta}, \text{Nb}$ ) were successfully synthesized by solid state reaction. XRD pattern confirmed the formation of single phase pure  $\text{FeTiBO}_6$  ( $\text{B} = \text{Ta}, \text{Nb}$ ) with Rutile structure. Rietveld refinement data is to be collected for the above samples and an ORNL proposal for local structure analysis is being written.

## **5. Design, Crystal structure and Photoluminescence of $\text{Li}(\text{RE})\text{W}_2\text{O}_8$ ( $\text{RE} = \text{Yb}, \text{Tb}$ )**

Name of the Primary Investigator: **Dr. Nalini G. Sundaram**

Name of the Research Student: Ms. Archana. K. M

The alkali rare earth double tungstate materials with general formula  $\text{ARE}(\text{WO}_4)_2$ , A-Alkali metal ion and R-rare earth ion are found to be multifunctional used as solid state luminescent hosts and undergo high temperature polymorphic phase transition that results in a different luminescence properties. Currently, tetragonal and monoclinic polymorphs of  $\text{LiYbW}_2\text{O}_8$  nanoparticles were

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

#### **6. Design of Transition Metal Oxide -SnO<sub>2</sub> Based Nanocomposites for Highly Selective Gas Sensors**

Name of the Primary Investigator: **Dr. Nalini G. Sundaram**

Name of the Research Student: Ms. Archana. K. M

Tin oxide has been proven to be a highly gas sensitive material for detection of both reducing and oxidizing gases. However it has a few disadvantages such as low selectivity, low stability and higher operating temperature. Hence our approach is to couple n-type semiconducting SnO<sub>2</sub> to V<sub>2</sub>O<sub>5</sub>, Nb<sub>2</sub>O<sub>5</sub> and Ta<sub>2</sub>O<sub>5</sub> to derive a nanocrystalline composite as a selective gas sensing material. SnO<sub>2</sub> was prepared by conventional different surfactant assisted hydrothermal and Co-precipitation methods. SnO<sub>2</sub> was characterized by p-XRD. Preparation of SnO<sub>2</sub>-V<sub>2</sub>O<sub>5</sub>, SnO<sub>2</sub>-Nb<sub>2</sub>O<sub>5</sub> and SnO<sub>2</sub>-Ta<sub>2</sub>O<sub>5</sub> nanocomposite work is under

## Future Projects

### **1. Sodium and Lithium ion Based Cathode Materials for High Capacity Batteries**

The aim of the project is to employ novel approaches for synthesis of nanostructured cathode materials to enhance both ionic and electronic conductivity. The key challenge in this project is to increase Energy Density i.e. make more Li/Na ions available for the electrochemical reaction

### **2. Photoluminescent Rare earth doped Tungstate and Molybdate Nanoparticles for Biological Applications**

The investigation of fundamental processes in cells and tissues 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.

### **3. Bandgap Engineering of Rare Earth Doped Bismuth Heterostructures for Dye Degradation and Photochemical Reactions**

*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 degradation 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.

## Research Highlights

1. The proposal titled “*Influence of Compositional Phase Transition on the Sunlight driven Photocatalysis observed in Rare Earth (RE=Eu, Tb) substituted Bi<sub>2</sub>WO<sub>6</sub> Nanoparticles*” was awarded beamtime from February 9<sup>th</sup> to 12<sup>th</sup> at the Elettra Synchrotrone, Trieste. Dr. Nalini and Mr. Pradeep were supported by the Indo-Italian S&T agreement for travel to Italy for data collection
2. **DST Meeting:** Dr. Nalini presented her research proposal titled “Design of Lanthanum based Perovskite Nanoparticles for The Development of Thick Film Gas Sensor to the DST committee for extramural funding at IIT Kanpur on September 18<sup>th</sup> 2014 and the proposal has been technically approved by DST, India for extramural research funding for three years from April 2015
3. **Thesis Submissions:** Ms. Swetha.S.M.Bhat and Mr. Srinidhi Raghvan submitted their Ph.D thesis to Manipal University through PPISR, in January 2015 and November 2014 respectively.

## Dr. Ganapati V. Shanbhag, Assistant Professor



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### Areas of Interest

#### **1. Catalyst design for biofuel synthesis**

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

#### **2. Novel catalytic materials**

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

#### **3. Chemical fixation of CO<sub>2</sub> by converting into valuable chemicals.**

Industrial and automobile effluent gas, CO<sub>2</sub> conversion to hydrocarbons over catalysts has been shown very little research and development attention so far, as other technologies has been much cheaper and efficient in yielding hydrocarbons. However, nowadays, with the increasing awareness of the impact CO<sub>2</sub> is having on the environment, a lot of attention is being directed at the methods to mitigate the effects CO<sub>2</sub> as a greenhouse gas. Electricity generation from coal flue gas from chemical industries and running automobiles contribute to a great extent in generating CO<sub>2</sub>. Hence it is necessary to convert CO<sub>2</sub> from industrial flue gas into valuable chemicals instead of leaving it into atmosphere. However, CO<sub>2</sub> being an inert gas, its activation and conversion into valuable chemicals is a challenge and require a design of catalyst to make these processes feasible.

## 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. CSIR-National Chemical Laboratory, Pune India
- 2000-2001: Research Associate, ICI India Ltd (MNC), Mumbai, India
- 1999-2000: Lecturer, M.M Arts and Science College, Sirsi, Karnataka, India
- 1999: M.Sc. Organic Chemistry, Karnatak University, Dharwad, India

## Recognitions

- Received a **Meritorious Award** for Excellence in Research from AMEF during Founder's day July 6, 2012 in recognition of contribution towards research and development at PPISR.
- **Editorial board member** of an international journal "**Journal of Catalyst and Catalysis.**"
- Member of the **Syllabus revision committee for Chemistry** for Siddaganga Institute of Technology (SIT), Tumkur.
- **Referee for international journals** viz. Applied Catalysis A, Catalysis Science and Technology, Catalysis Communications and Journal of Chemical Sciences.
- **Resource person** for Refresher Course Programme for PU college Lecturers sponsored by VGST, Govt of Karnataka.
- **Co-inventor** in the 2 World **patent (PCT)** applications filed by HPCL R & D Centre, Bangalore evolved as a result of a collaborative project.
- **Three best oral/poster presentation awards** to the group for the research papers presented at National symposiums/workshops, 1. Kuvempu University on "Social Relevance of Chemical Sciences" in March 2011 (student: Mrs. Swetha Sandesh) 2. Manipal Institute of Technology, "National Symposium on Chemistry and Humanity" in Manipal, July, 2011 (Student: Mr. Janardhan H L) and 3. National Workshop on Catalysis, CSIR-NEERI, Nagpur, Maharashtra on 4-5, Feb 2014 (Student: Mr. Vijaykumar Marakatti).
- Received '**plaques**' from **GTC Technology Inc. USA** in 2012 and 2014 in recognition of the milestones achieved by the group in developing a modified zeolite catalyst for aromatics technology.

## Current Sponsored Projects at PPISR

### 1. **Design and development of a catalyst and process for the synthesis of aromatics by new catalytic routes**

(Sponsored by: **GTC Technology, USA**)

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

Project fellows: Mr. Santosh Kumar, Mr. Saikiran, Mr. Kempanna

Starting Date: November 2014

A new agreement between PPISR and GTC was signed in November 2015 for starting a new project on “design and development of a catalyst and process for the synthesis of aromatics by new catalytic routes”. During this period, two new project assistants were recruited for this project and a new reactor was set up for this process. The technical aspects of the work and timeline for this project was discussed and finalized during the visit of Dr. Ding Zhongyi, Project Manager of GTC USA in November 2014. Initial catalyst preparation and testing was carried out with a newly designed reactor system.

**Status:** Ongoing

## **2. Design and development of a catalyst and process for selective methylation of benzene/ toluene to produce *p*-xylene**

*(Sponsored by: GTC Technology, USA)*

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

Research Fellows: Mr. Prashant Kumar, Mr. Santosh Kumar, Mr. Karthik K and Mr. Dundappa

The 2<sup>nd</sup> generation catalyst development for toluene alkylation with methanol was continued using modified zeolite catalyst. The main aim of this work was to achieve high selectivity of ~90 % for *p*-xylene with good conversion and good methanol utilization under pressure conditions. Several catalysts with different compositions have been prepared and tested in a 3 g vapor phase reactor. One catalyst recipe was finalized which gave high selectivity for PX under atmospheric conditions. We also conducted mechanical property testing of selected catalysts. The catalyst showed high crush strength of 7 kg and low attrition loss. Hydrothermal ageing test of the catalyst was also carried out. The catalyst showed similar physicochemical properties after hydrothermal ageing test which means the catalyst is hydrothermally stable much above the reaction temperature. Further, a series reactor set-up was designed for the existing CTU, to test the catalytic activity of the optimized novel catalyst recipe under two reactor system to increase the productivity and catalyst life. After setting up the two reactor system, reaction was carried out under different conditions. The aromatics production improved substantially in two-reactor system. Annual comprehensive report has been prepared and submitted to GTC.

**Status:** Completed

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

Principal Investigator: Dr. Ganapati V Shanbhag

Co-Investigator: Dr. Sanjeev P Maradur

Research Students: Mr. Vijaykumar and Mr. Janardhan

*(Sponsored by: HPCL R&D Centre, Bangalore)*

Light naphtha fraction is obtained from crude distillation of petroleum and also as natural gas condensate. Presently, light naphtha is converted into isomerates and aromatics by isomerization

and reforming, respectively. However, it is observed that C5 fraction in light naphtha is difficult to reform. One of the plausible routes to convert low-valued C5 fraction directly into high-valued products such as aromatics which could be used as MS blend or petrochemical feedstock/ solvent is aromatization route. Aromatization reaction was carried out in a fixed bed, vapor phase reactor using *n*-hexane as the model feed for light naphtha. An optimized catalyst composition was further used for aromatization of *n*-pentane, *n*-heptane and light naphtha from refinery. Zeolite ZSM-5 was modified with zinc and gallium by co-impregnation method. High aromatic yields were obtained over modified ZSM-5 catalysts due to dissociative chemisorption of alkanes resulting in dehydrogenation/ aromatization. The effect of acid sites on aromatization was studied by varying SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio (SAR) of ZSM-5 and correlated with the temperature programmed desorption of ammonia (NH<sub>3</sub>-TPD) studies. The metal modified ZSM-5 catalyst produced aromatics in high yields (64.8 % for light naphtha), especially high quantities of toluene with toluene/benzene ratio. From the aromatization studies, it could be envisaged that a proper balance of acid sites with dehydrogenation function is required to achieve maximum aromatic yield. The observations supported the dual site mechanism of alkane aromatization on oxide-loaded zeolite catalysts.

The toluene methylation to produce xylenes is one of the important and well studied reactions over medium pore zeolites (ZSM-5, ZSM-11). In case of these shape selective catalysts, the geometric factor is a critical parameter in governing the selectivity of xylenes. However, shape selectivity is ruled out over large pore zeolites as their pore size is much bigger than molecular dimensions of xylenes. However the only factor that could explain the change in selectivity is acid strength of zeolites. Effect of alkaline earth cations on the acid-base hardness and softness in X-zeolite and their influence on the xylene selectivity in toluene methylation were studied. The basic strength and polarizing ability of metal ions are the main factors for controlling soft and hard surface sites of the catalysts. The difference in *p/o* ratios of xylene isomers observed over alkaline earth metal ion exchanged zeolite X could be explained by Hard-Soft-Acid-Base (HSAB) principle.

Two patents were filed by HPCL and two manuscripts have been submitted to reputed journals. Biannual comprehensive project report has been prepared and submitted to HPCL.

**Status:** Completed

#### **4. Chemical fixation of CO<sub>2</sub> into value added products using metal modified ordered nanoporous silicate catalysts**

Project Coordinator: Dr. Ganapati Shanbhag

A project proposal submitted by **Dr. G. V. Shanbhag** was sanctioned by Vision Group of Science and Technology (VGST), Govt of Karnataka in December 2014 under the category, "Centre of Excellence in Science Engineering and Medicine" (CESEM) for 2014-2015 with a total funding of **60 lakhs for 3 years**.

**Status:** Project sanctioned, funding awaited.

### **Academic Projects**

#### **5. Superior performance of mesoporous tin oxide compared to nano and bulk SnO<sub>2</sub> in activation of carbonyl group**

Research guide: Dr. Ganapati V Shanbhag

Research Students: Mr. Vijaykumar Marakatti

Mesoporous tin oxide is synthesized by hydrothermal method at room temperature using cetyl trimethyl ammonium bromide as template. The mesoporous tin oxide was further characterized by Low angle XRD, SEM, BET surface area analysis and Py-FTIR. The application of mesoporous tin oxide as acid catalyst was generalized by considering the reaction involving the carbonyl group activation. The mesoporous tin oxide was found to be a promising catalyst in conversion of  $\beta$ -pinene to nopol, carbonylation of glycerol to glycerol carbonate, acetalization glycerol to mono, Di and triglycerides. The catalytic activity of mesoporous tin oxide in these reactions was found to be high compared to nano and Bulk SnO<sub>2</sub>. Further application to different reactions are under investigation.

**Status:** Manuscript under preparation

## **6. Acetylation of glycerol to glycerol acetins using Cs exchanged phosphotungstic acid**

Research guide: Dr. Ganapati V Shanbhag

Research Students: Mrs. Swetha Sandesh

Glycerol acetins are industrially important products obtained during the acetylation of glycerol with acetylating agents like acetic acid and acetic anhydride. The reaction goes well with the strong acid catalysts. Cs exchanged phosphotungstic acid (Cs/PWA) is well known solid acid catalyst having high acid strength was first time used for this reaction. The reaction was performed using two different acetylating agents like acetic anhydride and acetic acid. With acetic anhydride the reaction was performed under room temperature and with acetic acid 65 °C reaction temperature. In this study the different solid acid catalysts were compared with Cs/PWA catalysts such as amberlyst-15 resin, montomorllite K10, sulphated zirconia and zeolite beta catalysts. Among all the catalysts tested, Cs/PWA showed highest glycerol conversion of 100 % for acetic anhydride reactant and 98% of glycerol conversion for acetic acid as a reactant. The synthesized catalyst was characterised by using various techniques like XRD, FTIR, and morphological properties were determined by SEM. Optimization of reaction conditions like mole ratio, catalysts weight percent and temperature were studied to get high yield of glycerol acetins.

**Status:** Manuscript is communicated to peer reviewed journal

## **7. Metal ion-exchanged zeolites as a highly active solid acid catalyst for synthesis of glycerol carbonate from glycerol and urea**

Research guide: Dr. Ganapati V Shanbhag

Research Students: Mr. Vijaykumar Marakatti

The application of metal ion exchanged zeolites as highly active and selective catalyst for the synthesis of glycerol carbonate from glycerol carbonylation is reported. The catalyst were prepared by ion exchange method and characterized by XRD, py-FTIR, AAS, NH<sub>3</sub>TPD, N<sub>2</sub> sorption and SEM. The Na, H and Zn form of different zeolites were screened for the reaction. The Zn-FAU zeolite exhibited high glycerol carbonate yield compared to other Zn-zeolites such as Zn-ZSM5, Zn-MOR and Zn-beta. The acidity of Zn-HY zeolite was correlated with the amount of zinc and catalytic activity of the reaction. As the amount of zinc content increased in HY zeolite, glycerol conversion and selectivity for glycerol carbonate increased due to increase in Lewis acidity. Among different

metal ion exchanged HY zeolite, Zn<sup>2+</sup> showed higher catalytic performance. The degree of zinc loading, reaction temperature, catalyst amount, mole ratio and catalyst reusability were investigated.

**Status:** Manuscript under preparation

### **8. Shape-selective synthesis of *para*-diethylbenzene over pore engineered ZSM-5: a kinetic study**

Research guide: Dr. Ganapati V Shanbhag

Research Student: Mr. Janardhan H L

Alkylation of ethylbenzene (EB) with ethanol was carried out in a fixed bed, continuous, down-flow, tubular reactor, at atmospheric pressure and H<sub>2</sub> as a carrier gas in vapor phase. A detailed kinetic study over pore engineered ZSM-5 zeolite by phosphate modification and in extrudate form was conducted. The reaction was performed at EB : ethanol mole ratio of 4:1 and with varying contact time at temperatures of 613, 633 and 653 K. Due to the induced shape-selectivity in ZSM-5 by phosphate modification, *para*-diethylbenzene (PDEB) was formed as a major product and side products like benzene, *meta*-diethylbenzene (MDEB) and other isomers were formed in minor quantity. Langmuir-Hinselwood-Hougen-Watson (LHHW) method for dual site mechanism with the assumption of surface reaction controlling was applied to derive the rate equations. Activation energies for the ethylation of EB, dealkylation of EB and isomerization of PDEB were found to be 117.2, 186.0, 298.6 kJ/mol respectively. Adsorption energetics showed that EB is weakly adsorbed, whereas ethanol is strongly adsorbed over the catalyst surface. Activation energy of PDEB formation was found to be lower than that of MDEB. Considering that the alkylation takes place mostly inside the zeolite channels, the results support restricted transition state selective mechanism for EB alkylation with ethanol over phosphate modified ZSM-5. Based on the proposed kinetic model, calculated values of EB conversion and PDEB formation were found to be in good agreement with the experimental results.

**Status:** Manuscript is communicated to peer reviewed journal

### **9. Room temperature synthesis of solketal from acetalization of glycerol with acetone: Effect of crystallite size and the role of acidity of beta zeolite**

Research guide: Dr. Ganapati V Shanbhag

Research Students: Mr. Manjunathan P.

Room temperature synthesis of solketal from acetalization of glycerol with acetone was carried out over various types of Brønsted solid acid catalysts in the liquid phase. Among the catalysts screened, H-Beta zeolite showed the best performance in less time period with 86 % glycerol conversion and 98.5 % selectivity to solketal. The chemical and structural properties of modified and unmodified beta catalysts were studied by X-ray diffraction, AAS, SEM, NH<sub>3</sub>-TPD and FTIR-pyridine adsorption. The H-Beta catalyst with lower crystallite size (average 135nm) gave better conversion and solketal selectivity compared to H-Beta with higher crystallite size (average 450 nm). The effect of acidity of the catalyst on acetalization of glycerol was studied by modified beta catalysts of varying acidities. Glycerol conversion decreased with decrease in total acidity of beta

catalysts. Strong to weak acidity ratio of the catalysts was found to have a direct correlation with catalyst performance.

(Work is published in *J. Mol Catal. A journal*)

#### **10. Novel Brønsted acidic mesoporous tin oxide as an efficient catalyst for the selective transformation of glycerol to acetals: Effect of the role of Brønsted and Lewis acidity**

Research guide: Dr. Ganapati V Shanbhag

Research Student: Mr. Manjunathan P

Certain metal oxides like tin oxide show moderately strong acidic properties which can be utilized for acid catalyzed reactions. The catalytic properties of tin oxide can be enhanced by introducing mesoporosity which improves the surface area, number of active sites per gram of catalyst, Mesoporous tin oxide was found to be highly active catalyst for these reactions compared to Al-SBA-15, Al-TUD-1 and Al-MCM-41 due to its higher Brønsted acidic nature. The effect of acidity of mesoporous tin oxide towards the reaction was studied with different calcination temperature. The catalytic performance decreases with decrease in Brønsted acidic sites of the catalyst. The different parameters such as catalyst concentration, glycerol to acetone mole ratio and reaction time were systematically studied using the active catalyst. Further characterization of catalyst like surface area, pore size, acidity, thermal stability is under progress.

**Status:** Work under progress

#### **11. Zinc-tin mixed oxide as novel solid acid catalyst for glycerol carbonylation with urea**

PhD supervisor: Dr. Ganapati V Shanbhag

Research Student: Mr. Manjunathan P

A catalyst zinc-tin mixed oxide was prepared by a novel method and applied for glycerol carbonylation with urea. Different Zn and Sn contents were optimize to get high acidity. It is found that  $Zn_2SnO_3$  is more active compared to other compositions and it is more active than other solid acid catalysts tested for this reaction. However, it is found that some amount of Zn is leaching out into the reaction medium as ZnO and hence activity is decreasing with every recycle. Further studies are carried out to rectify this issue and make it a better catalyst. Also, relevant characterization of catalyst is going on.

**Status:** Work under progress

### **Representative publications**

1. Utilization of renewable resources: Condensation of glycerol with acetone at room temperature catalyzed by organic-inorganic hybrid catalyst, Swetha Sandesh, A.B. Halgeri, Ganapati V. Shanbhag, *Journal of Molecular Catalysis A: Chemical*, In Press (2015)
2. "Room temperature synthesis of solketal from acetalization of glycerol with acetone: Effect of crystallite size and the role of acidity of beta zeolite", Pandian Manjunathan, Sanjeev P. Maradur, A.B. Halgeri, Ganapati V. Shanbhag, *Journal of Molecular Catalysis A: Chemical* 396, 2015, 47-54

3. "Phosphate modified ZSM-5 for the shape-selective synthesis of *para*-diethylbenzene: Role of crystal size and acidity", Janardhan L. Hodala, Anand B. Halgeri, Ganapati V. Shanbhag ***Applied Catalysis A: General***, 484, 2014, 8-16
4. "Metal ion-exchanged zeolites as solid acid catalysts for the green synthesis of nopol from Prins reaction." V. S. Marakatti, A.B. Halgeri and Ganapati V. Shanbhag\*, ***Catalysis Science and Technology*** 4, 2014, 4065-4074.
5. "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
6. "Zinc hydroxy stannate: a promising acid-base bifunctional catalyst"  
Swetha Sandesh, G V Shanbhag\* and A.B. Halgeri, ***RSC Advances***, 2014, 4, 974-977
7. "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
8. "Transesterification of glycerol to glycerol carbonate using KF/Al<sub>2</sub>O<sub>3</sub> catalyst: The role of support and basicity", Swetha Sandesh, G V Shanbhag\* and A.B. Halgeri, ***Catalysis Letters***, 2013, 143, 1226-1234
9. "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

<b>Research Group</b>			
<b>Ph.D. Students</b>			
			
<p><b>Mrs. Swetha Sandesh</b> Senior Research Fellow (CSIR)</p>	<p><b>Mr. Vijaykumar Marakatti</b> Senior Research Fellow (Project)</p>	<p><b>Mr. Janardhan H. L.</b> Senior Research Fellow (Project)</p>	<p><b>Mr. Manjunathan P.</b> Senior Research Fellow (Project)</p>
<b>Project Fellows</b>			

 <p><b>Mr. Santosh Kumar Jalannavar</b> M. Tech. (Chem. Eng.) January 2014-till date</p>	 <p><b>Mr. Saikiran Maleppagari</b> M. Tech. (Chem. Eng.) November 2014-till date</p>	 <p><b>Mr. Kempanna S. Kanakikodi</b> MSc (Chemistry) November 2014-till date</p>
<p><b>Past Project fellows worked in industry sponsored projects</b></p>		
 <p><b>Mr. Prashant Kumar R K</b> M. Tech. (Chem. Eng.) October 2013-Oct 2014 <b>(presently at SABIC, Bangalore)</b></p>	 <p><b>Mr. Karthik N. C.</b> M. Tech. (Chem. Eng.) September 2013-January 2015 <b>(presently at SABIC, Bangalore)</b></p>	 <p><b>Mr. Dundappa B Mumbaraddi</b> MSc (Chemistry) September 2013 to Aug 2014</p>

## Research Highlights

### A. Papers presented in Conferences

- a) **Swetha Sandesh** presented a poster on “Eco-friendly heterogeneous base catalyst for efficient syntheses of biodiesel and acetin, a fuel additive from transesterification reactions” authored by Swetha Sandesh, Ganapati V. Shanbhag\* and A.B. Halgeri in **international conference titled “GREEN SUMMIT 2014”** organized by FKCCI with Government of Karnataka on 2-4 June, 2014.
- b) **Mr. Manjunathan P.** delivered oral presentation at "**International Conference on Recent Advances in Engineering Sciences (ICRAES-2014)**" on the title “Molybdenum oxide/alumina as an efficient solid acid catalyst for acetalization of glycerol with acetone to produce solketal” at M.S. Ramaiah Engineering college, Bangalore authored by Dundappa Mumbaraddi, Manjunathan P, Ganapati V. Shanbhag, Anand B. Halgeri and Sanjeev P. Mardaur\*.
- c) **Mr. Janardhan H L** Participated in workshop on **Chemical bond to chemical plant – computational and material challenges in gas conversion technologies** was held at **JNCASR** from 25 to 28 Aug, 2014 followed by post conference summer school from 1 to 5 Sept 2014.

d) **Mr. JanardhanH L** gave Oral presentation on “Shape selective synthesis of *p*-diethylbenzene over phosphate modified ZSM-5: a Kinetic study” at 22<sup>nd</sup> National Symposium on Catalysis (CATSYMP-22) I from January 7-9, 2015, CSIR-CSMCRI Bhavnagar, Gujarat.

e) **Mr. Manjunathan P** presented a Poster on “Synthesis of solketal from acetalization of glycerol with acetone at room temperature: Effect of crystallite size and acidity of beta catalyst” at 22<sup>nd</sup> National Symposium on Catalysis (CATSYMP-22) I from January 7-9, 2015, CSIR-CSMCRI Bhavnagar, Gujarat.

## Review meetings:

### 1. GTC project review meetings

a) **Dr. Ding. ZhongYi** of GTC USA visited PPISR on 2 & 3, November 2014 to review the completed project and to discuss the start of the new project for 2014-2015.

There were discussions on the technical requirement and literature on the new project related to the catalyst development for aromatics synthesis. A new non disclosure agreement (NDA) between GTC and PPISR was signed on this occasion. Dr. ZhongYi expressed happiness over the progress of the concluded project in which PPISR successfully developed a 2<sup>nd</sup> generation catalyst for aromatics conversion. Incidentally, later, GTC made announcement on licensing and transfer of aromatics process technology to a company in China. The process will soon be commercialized in China and PPISR will be involved in future in technical service for commercialization.

b) **Annual technical review meeting** of GTC sponsored project was conducted at PPISR with **Dr. Ding. ZhongYi**, Technology Manager, GTC USA at PPISR on June 8-9, 2014. Dr. A B Halgeri, Dr. G V Shanbhag and Dr. S P Maradur attended the meeting. Dr. Shanbhag made a presentation on the annual work progress made on toluene methylation process. Dr. ZhongYi was satisfied with the work progress made during 2013-14 project. In appreciation of the project work successfully completed during previous year (2012-13), Dr. ZhongYi handed over a plaque to the PPISR team. It was decided to fabricate a series reactor to the existing single reactor to test the catalyst under multiple reactor system.

c) **Dr. Venkata Ramanujam**, Technology Process Manager GTC, USA visited the campus on 10<sup>th</sup> June 2014 to discuss the future projects with PPISR. Dr Sanjeev Maradur made a presentation on resin technology. Dr. Venkata had technical discussions with Dr. S P Maradur and Dr. G V Shanbhag.

### 2. HPCL Project review meeting

Final technical project review meeting of HPCL project was held at HPCL Corporate Office, Bangalore on 18-11-2014 to review the progress made during last quarter and overall progress in two years from 2012 to 2014. From HPCL R & D, Dr. N V Choudhary, General Manager, Dr. P.V.C. Rao, Dy General Manager, R & D, Dr. Ravishankar, Senior Manager and Dr. Sunil participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag and Dr. Sanjeev Maradur were present from PPISR. The students, Mr. Vijaykumar and Mr. Janardhan presented the research data to the team. Based on the excellent progress made during last two years, HPCL has shown interest in working a

collaborative project with PPISR in near future and invited to submit a new project proposal. A proposal will be finalized soon.

The 6<sup>th</sup> and 7<sup>th</sup> combined quarterly technical project review meeting of HPCL project was held at HPCL Corporate Office, Bangalore on 22-07-2014 to review the progress made during two quarters from February to July 2014. From HPCL R & D, Mr. Sri Ganesh Gandham, Executive Director, HPCL, Dr. P.V.C. Rao, Dy General Manager, R & D, Dr. Ravishankar, Senior Manager and Dr. Sunil participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag and Dr. Sanjeev Maradur were present from PPISR. The students Mr. Vijaykumar and Mr. Janardhan presented the research data to the team. HPCL team appreciated the overall progress made in this project.

### **3. Pre-PhD Colloquium of Swetha, Vijaykumar and Janardhan**

Pre-PhD colloquium of three students; Swetha, Vijaykumar and Janardhan was conducted on November 20, 2014 in the auditorium of PPISR main campus under the presence of 3 external experts; Dr. B S JaiPrakash, Dr. Y S Bhat from BIT and Dr. Vasana from IISc Bangalore. Other faculty and students of PPISR were also present. The students gave presentation on their entire Ph.D. work systematically. Experts and other audience gave many suggestions which would help them to make a better thesis. Experts showed satisfaction over the overall thesis work and gave a nod to complete the thesis.

### **4. Student review meetings**

a) Prof. K R Krishnamurthy, Chair Professor, NCCR, IIT, Madras and member of RAC reviewed Materials Science students' PhD progress on 5<sup>th</sup> September 2014 and gave his valuable suggestions to improve the quality of the work.

b) Dr. Prahlada, Member of Board of Trustees and Chairman RAC reviewed research projects of students on September 26, 2014. All PhD students presented their research work and Dr. Prahlada gave valuable suggestions to them.

### **Award**

GTC Technology USA sponsored industrial project is in progress in Materials Science Division for the last three years. The developmental work on first generation catalyst for aromatic technology was successful and developmental work on second generation catalyst is going on. This successful collaboration with US Company has brought a lot of credibility to PPISR. Dr. Ding ZhongYi, Project Manager, GTC, USA, visited the campus on 8-9th June 2014 for technical discussions on ongoing work and future work on aromatic technology for the next year. Dr Shanbhag and Dr. Maradur made presentations of the work done till date.

GTC complemented the PPISR team's efforts by awarding a plaque in bringing up success so far in the sponsored program. The plaque states that *"Presented to Dr. A. B. Halgeri, Dr. G. V. Shanbhag-PI Dr S. P. Maradur Co-PI. Mr. Satish Burla Research Fellow and MrManjunathan P. Research Fellow in recognition of their successful development of first generation zeolitebasedcatalyst for aromatics production and looking forward to a long term relationshipwith PPISR. GTC Technology US, LLC, is grateful for the full support of PPISR management and looks forward to our long-term relationship"*.

## Dr. Sanjeev P. Maradur, Assistant Professor



### Areas of Interest

- Synthesis of mesoporous materials (Mesoporous silica (KIT-6), Mesoporous Polymers) and their catalytic applications.
- Value addition of biomass platform chemicals
- Development of new synthetic methodologies
- Heterogenization of homogeneous catalysis & its application on various chemical processes.

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### Curriculum vitae

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

### Awards and Scholarship

- Seed Money for Young Scientist Research Award from Vision Group on Science and Technology, Govt of Karnataka 2014-2015 “*Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, potential fuel additive molecules for diesel and gasoline*”.
- Senior Research Fellowship of the Indian Institute of Technology-Bombay, Jul’2006-Jan’2007.
- Project Fellowship of the Shivaji University Kolhapur, Aug’2003-Jun’2006.

### Current Sponsored Projects at PPISR

- Co-Investigator in GTC-USA sponsored project on “Natural gas conversion technology” 2014-2015.

## Completed Sponsored Projects at PPISR

- Seed Money for Young Scientist Research Award from Vision Group on Science and Technology, Govt of Karnataka 2014-2015 “*Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, potential fuel additive molecules for diesel and gasoline*”.

## Board/Membership

- Member, The International Zeolite Association (IZA) (2010-present).
- Life Member of Catalysis Society of India.

## Representative publications

1. “Room temperature synthesis of solketal from acetalization of glycerol with acetone: Effect of crystallite size and the role of acidity of beta zeolite” P. Manjunathan, **S. P. Maradur**, A. B. Halgeri and G. V. Shanbhag, J. Mal. Catal. A: Chem. DOI: 10.1016/j.molcata.2014.09.028.
2. **Sanjeev P Maradur**, 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 Metals 162 (2012) 453-459.
3. **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 H<sub>2</sub>O<sub>2</sub>*”. ChemCatChem 3 (2011) 1435-1438.
4. V. T. Magalad, A. R. Supale, **S. P. Maradur**, 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.
5. **S. P. Maradur**, and G. S. Gokavi; “*Heteropoly acid catalyzed synthesis of 3,4-Dihydropyrimidin-2(1H)-ones*”. Catalysis Communications 8 (2007) 279–284.
6. **S. P. Maradur**, 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.

Total Number of Publications in National and International Journals: 14

## Patents

- **Inventors:** RyongRyoo, Dae-Heung Choi, **MaradurSanjeev** “*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**).
- **Inventors:** Yang, KapSeung. **MaradurSanjeev 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**).

# Research Group

## Graduate student

### 1. Sathyapal Churipard. R (JRF Supported by PPISR)



#### Research Area:

Synthesis and functionalisation of mesoporous polymers for catalytic applications

### 2. Mr. Manish Kumar (M. Tech Project student, Chem Eng. Manipal University, Manipal)

Mesoporous polymers as catalyst for etherification of glycerol with *t*-butyl alcohol to *t*-butyl ethers of glycerol, a potential fuel additive

## Current Research Projects

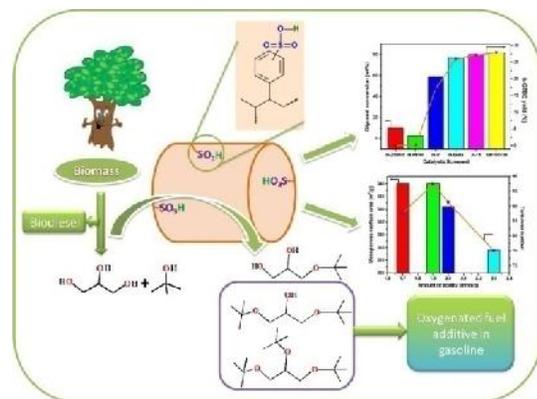
**Project 1:** Design of novel mesoporous polymers as catalyst for the synthesis of glycerol derivatives, potential fuel additive molecules for diesel and gasoline

Principal Investigator: Dr. Sanjeev P. Maradur

Co-Investigator: Dr. Ganapati V Shanbhag

Research Students: Mr. Manjunathan, Mr. Sathyapal and Mr. Manish Kumar

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

Principal Investigator: Dr. Sanjeev P Maradur

Co-Investigator: Dr. Ganapati V Shanbhag

Research Students: Mr. Sathyapal 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 ( $\text{MoO}_3$ ,  $\text{Nb}_2\text{O}_5$ ). The same materials when subjected to higher calcinations temperatures i.e.  $>800^\circ\text{C}$ , bronsted acidity is generated onto the catalyst. Aim of this project is to synthesize selectively solketal, a five membered ring product. Thus the synthesized catalysts have been screened for catalytic activity. And a manuscript is under preparation.

**Project 3:** Molybdenum oxide supported onto alumina calcined at high temperature: A promising catalyst for nopol synthesis

Principal Investigator: Dr. Sanjeev P Maradur

Co-Investigator: Dr. Ganapati V Shanbhag

Reserach Students: Mr. Dundappa and Mr. Vijay Kumar

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  $\beta$ -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.

Manuscript preparation is under progress

## Future Projects

### 1. Removal of chloroaromatics impurity from hydrocarbon feed stream by adsorption

Principal Investigator: **Dr. Sanjeev P. Maradur**

Reserach Students: Mr. Kempanna and Mr. Sathyapal

The removal of halogens, and particularly chemically-combined halogens, such as organochlorides, from hydrocarbon feed streams is highly desirable in order to prevent potential catalyst deactivation as well as equipment corrosion. If chemically-combined chlorines, such as organochlorides, are not removed from the hydrocarbon streams, the presence of organo-chlorides in the resultant hydrocarbon products, particularly gasoline or other fuels, can cause corrosion of processing equipment and engine parts, as well as other detrimental effects.

The main objective of the project is to identify and evaluate a suitable adsorbent for the removal of chloride impurity which is in the form of organic chloride and more particularly halo aromatics from hydrocarbon feed containing mixtures of toluene, xylenes, and other alkylated aromatics. Another objective of this project is to determine the efficiency and life time of the identified adsorbent in terms of adsorbent capacity and ease of regeneration of the adsorbent for reuse.

### 2. Academic Research: Metal Organic Frameworks (MOF's)

Metal-organic frameworks are one of the most important developments in recent nanoporous material science and we have seen an explosion in the numbers of scientific papers dealing with MOFs in recent years. Metal-organic frameworks (MOFs) are a class of crystalline materials that consist of coordination bonds between transition-metal cations and multidentate organic linkers. The structure of MOFs is characterized by an open framework that can be porous (porous

materials). MOFs can be used for gas storage, purification and separation, as well as catalysis and sensing applications. The first MOF was produced in 1998 and since then, their potential for industrial applications has attracted a lot of interest. The strong chemical bonds that hold a MOF together is what allows the structure to remain firm but also to be incredibly empty inside. A single gram of a MOF can have a surface area equivalent to a football pitch. One of the major applications for metal organic frameworks is storing gases. The porous material can trap and store carbon, offering a potential technology for carbon capture and storage. As well as carbon storage, MOFs may be able to play a part in industrial separation processes for gases, vapours and liquids as well as catalysis. Currently we are exploring the possibility of utilizing these MOF's in the area of separation/ adsorbents and catalysis.

## Research Highlights

1. Dr. Venkata Ramanujam, Technology Process Manager GTC, USA had visited the campus on 10<sup>th</sup> June 2014. Dr Maradur made a presentation on resin technology. Dr. Venkata had technical discussions with PPISR team and also discussed future short term projects that GTC is going to sponsor apart from the ongoing activities.
2. Dr. G V Shanbhag and Dr. S P Maradur were awarded a plaque by Chief Guest Dr. P Rama Rao in appreciation for the successful completion of the GTC Sponsored project 2012-2013

## Biological Sciences Division



Research programs in the biological science division explore the structure and function of biologically and medicinally important proteins, mycology, treasure hunt in the world of fungal secondary metabolites and protein chemistry. We study protein-protein, protein-inhibitor interactions and exploit this understanding to design of therapeutically important proteins or design small molecule drugs against these proteins. Similarly, search for secondary metabolites from endophytic fungi with potential anti-microbial, anti-cancer and anti-diabetic properties is another key area of research in biological sciences. 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 6000 sq. ft. of lab space and is equipped with all facilities for microbial studies like 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. 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), Board for Research In Nuclear Science (BRNS) 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.

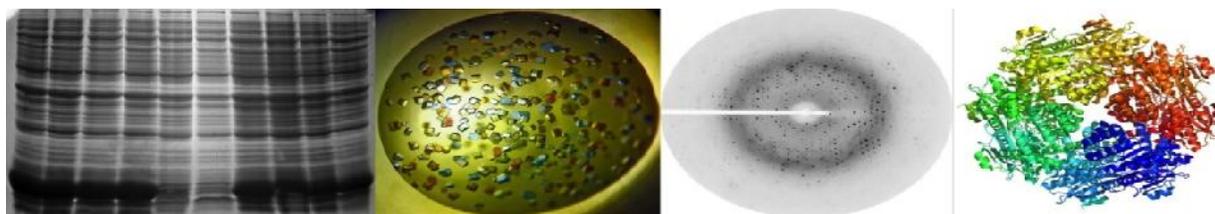
### Areas of Research:

1. Structural and functional characterization of key molecules of biological and medicinal importance, their complexes and also exploitation of these understandings towards creation of therapeutic molecules.
2. Endophytic fungi from medicinal plants and their secondary metabolites, bioactive compounds, enzymes from endophytic fungi.

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.

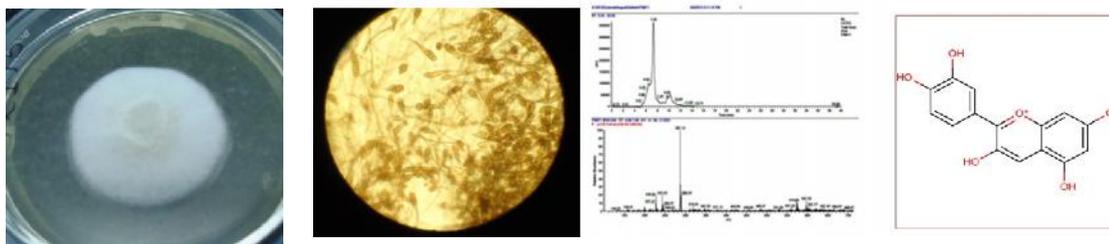
## Academic and Research Highlights:

The Biological Sciences division has made considerable progress in the last four years. The department has published several papers in national and international journals. Two students from microbiology group have submitted their PhD theses to Manipal University, which represents a major milestone for the division, as well as PPISR. Many new instruments have been acquired from the second installment of CISEE program of VGST, Karnataka.



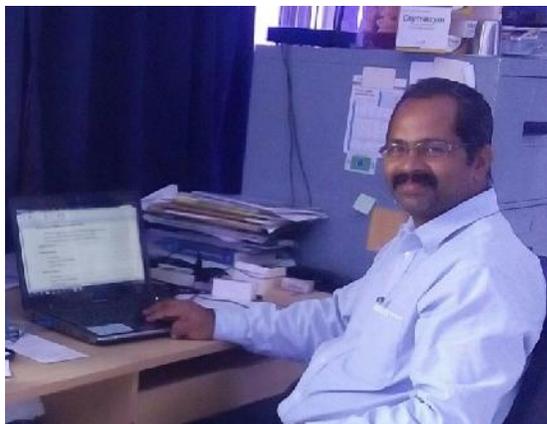
Structural biology group successfully completed the structures of apo form and several complexes of APRTs from *Y. pseudotuberculosis* and *F. tularensis*. Overall, the group has submitted four structures to Protein Data Bank, an international repository of protein structures with PDB-ID's 4MB6, 4HN8, 4HYR and 4JHM. These structures represent the first few protein structures contributed to PDB from PPISR. We have also successfully cloned B7-2 (CD86), a costimulatory molecule on the antigen presenting cells and its ligand CTLA-4 on T-cell. We have also created several mutants of B7-2 molecule as potential therapeutic agents against autoimmunity and cancer. Similarly, we are also working on the modification of T-cell immunoreceptor with Immunoglobulin and ITIM domains (TIGIT), another costimulatory molecule implicated in cancer and autoimmunity. A manuscript based on the analysis and exploitation of weak anomalous signal is in the final stage of revision and will be sent for publication soon.

In the microbiology group, discovery of novel compounds from endophytic fungi for the treatment of diabetes, cancer and compounds with antioxidant properties are under process. Research work of two scholars in the lab, on endophytic fungi generated very valuable data which could lead to many more opportunities for further explorations. Compounds responsible for the bioactivity were purified and identified using advanced techniques. There are a few compounds of which some are showing in-vitro activity very similar and some show better activity as compared to the drugs available in the market. The microbiology group is also studying the effect of radiation on fungi producing ligninase enzymes. Initial studies have shown some promising results which has applications in the field of bioremediation.



## Faculty Profiles

### Dr. Ananda K., Assistant Professor



#### Areas of Interest

- Antimicrobial, anti-oxidants, anti-diabetic compounds from endophytic fungi isolated from medicinal plants.
- Radiation effect on endophytic fungi producing secondary metabolites and enzymes
- Bioconjugation of therapeutic proteins and PEGylation technology

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#### Curriculum vitae

- 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

#### Membership of Professional bodies

Life Member of Mycological Society of India, India

#### Current Sponsored Projects at PPISR

##### 1. Anticancer metabolites from endophytes of medicinal plants

Principal Investigator: Dr. Ananda

Medicinal plants used for the cancer treatment will be selected and endophytic fungi are isolated from these plants. The endophytic fungi grown in media and secondary metabolites extracted are tested for the anticancer activity.

## 2. **Effect of electron beam radiation on endophytic fungi producing ligninase enzyme**

PI:Dr.Ananda, Student: Kavitha KN

Endophytic fungi isolated from selected plants were initially tested for the presence of ligninase enzymes. Endophytic fungi positive for ligninase are used for the dye degradation test. Five types of synthetic dyes were selected for the study and two fungi are found to be the best dye degraders. Further detailed experiments are planned for these two endophytic fungi. The lignin degrading fungi are exposed to the radiation and again analysed for the variation in enzyme production.

## Completed Sponsored Projects at PPISR

### 1. **Antimicrobial and anti oxidants of endophytic fungi from Medicinal plants**

Principal Investigator: Dr.Ananda

Research Fellow: Sathish L

### 2. **Anti-diabetic compounds of endophytic fungi from medicinal plants used for the treatment of diabetes.**

Principal Investigator: Dr.Ananda

Research Fellow: Pavithra N

## Representative publications

1. Pavithra,N., Sathish,L., Pushpalatha, H., Bhanuprakash Reddy, G., Kavya, S., Janardhana, PB., **Ananda, K.**(2014): Pyrrolo (1, 2-a) pyrazine 1, 4-dione, hexahydro an antidiabetic and anti-cancer compound extracted from a endophytic fungi *Trichoderma atroviride* (under review)
2. Pavithra N., Sathish L., Suneel Kumar A., Venkatarathanamma, V., Pushpalatha H., Bhanuprakash Reddy, G., **Ananda K.** (2014): *In-vitro* Studies on  $\alpha$ -Amylase,  $\alpha$ -Glucosidase and Aldose Reductase Inhibitors found in Endophytic Fungi Isolated from *Ocimum sanctum*, *Current Enzyme Inhibitor* 10(2)129-136.
3. N. Pavithra, L. Sathish, Nagasai, Babu, V. Venkatarathanamma, H. Pushpalatha, G. Bhanuprakash Reddy, **K. Ananda** (2014) Evaluation of  $\alpha$ -Amylase,  $\alpha$ -Glucosidase and Aldose Reductase inhibitors in ethyl acetate extracts of endophytic fungi isolated from anti-diabetic medicinal plants. *Int J Pharm Sci Res.* 5 (12) 5334-5341
4. Garudachari B, Isloor AM, Satyanaraya MN, **Ananda K**, Fun H-K. (2014) Synthesis, characterization and antimicrobial studies of some new trifluoromethyl quinoline-3-carbohydrazide and 1,3,4-oxadiazoles. *RSC Advances.* 2014;4(58):30864-30875
5. 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.
6. 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.

7. 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.
8. 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.
9. 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.
10. **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.
11. Remadevi, O.K., Rao,K.S., **Ananda, K.**, Veeranna,R., Tarakanadha, B., (2011) Status of insects and fungi intercepted from wood imported into India. *Journal of the Indian Academy of Wood Science.* 8(2):139–142.
12. 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

## Research Group



Ms. Pavithra N.



Mr.Sathish L.



Ms. Kavitha

## Research Collaboration

1. Dr. Arun M Isloor, NITK, Surathkal collaboration for the antimicrobial assay of synthetic compounds

## Govt. Sponsored project:

Received research grant for the project titled “Effect of electron beam radiation on endophytic fungi producing ligninase enzyme” for three years from BRNS, DAE, Govt. of India

## Dr. Udupi A. Ramagopal., Ramalingaswami fellow (DBT), Associate Professor



### Areas of Interest

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

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### Curriculum vitae

- 2014 – current, Associate Professor : 2011 – 2013 Assistant Professor, (Ramalingaswami Fellow - DBT), Poornaprajna 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>
- 2009-2011: 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.

### 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 ~ **230** protein structures to World Wide Protein Data Bank (wwPDB).
9. Invited Instructor (2003-2010) at *RapiData*, a comprehensive course offered at Brookhaven National Laboratory for budding crystallographers around the world (<http://www.bnl.gov/rapidata/>).
10. Referee for *ActaCrystallographicaSection 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:

1. **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. **Proc. Nat. Acad. Sci. (USA)** 98(3): 870-874. **JIF** (2011) = **9.8**
2. **Ramagopal, U. A.**, Dauter, M. and Dauter, Z. **2003**. Phasing on anomalous sulfurs: What is the limit? **ActaCryst.** **D59**, 1020-1027. **JIF** (2011) = **7.3**. (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> )
3. **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. **ActaCryst.** **D61**, 1289-1298. (\***Corresponding author**), **JIF** (2011) = **7.3**
4. 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. **Immunity**, 25(4), 559-570. **JIF** (2011) = **21.6**
5. Chattopadhyay, K., **Ramagopal, U. A.**, Mukhopadhyaya, A., DiLorenzo, T. P., Brenowitz, M., Nathenson, S. G. and Almo, S. C. **2007**. Novel assembly and structural properties of human GITRL: Implications for function. **Proc. Nat. Acad. Sci. (USA)**, 104(49), 19452-19457. **JIF** (2011) = **9.8**  
(**Comment:** <http://www.immunity.com/content/article/abstract?uid=PIIS1074761307001835> )
6. Chattopadhyay, 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. **Proc. Nat. Acad. Sci. (USA)**, 105(2), 635-640. **JIF** (2011) = **9.8**.  
News: <http://stke.sciencemag.org/cgi/content/abstract/sigtrans;1/3/ec30>

7. 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. **Proc. Nat. Acad. Sci. (USA)**,109(37):14836-40, **JIF (2011) = 9.8**.
8. 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. **JIF (2011) = 6.4. Comment at :**  
<http://www.sciencedirect.com/science/article/pii/S0969212613001251>
9. **Ramagopal, U. A.**, Dulyaninova, N. G., Varney K. M., Wilder, P. T., Nallamsetty, S., Brenowitz, M., Weber D. J., Almo S. C. andBresnick, A. R. **2013**, Structure of the S100A4/myosin-IIA complex. **BMC Struct. Biol.**,13(1), 31. [Epub ahead of print], **JIF (2011) = 2.5**.
10. Bhowmick, T., Ghosh, S., Ramagopal, U. A., Day, D., Ramakumar, S., Nagaraja, S. 2014, Structure based inhibition provides an insight into the HU mediated regulation in Mycobacterium tuberculosis. **Nature Communications**, 5, 4124. **JIF (2013) =10.7**

## Research highlights

Proteins are the key molecules of life. They work 24/7 and are responsible for all the processes that take place in any living organism. For example, when we breathe, walk or even sleep, there are different proteins working in an optimal concentration and speed depending upon the need. Most drugs we take are manipulators of functions of these proteins. Understanding the structure of proteins is essential for understanding the basic biology as well as to design drugs against these proteins. Our lab tries to see these molecular machines and how they interact with their ligands, in atomic details, in an attempt to understand the mechanism of action of these proteins and also attempts to design small molecule drug against these molecules. We use techniques like crystallography, bioinformatics and various biochemical, biophysical techniques to study these molecules.

## Lab members:



**Dr. Raghurama P. Hegde**  
**(Research Associate)**

Raghurama Hegde is working on three projects: (i) Structural Study of proteins from the enolase superfamily. (ii) Testing the limits of macromolecular crystallographic phasing and (iii) Modification of immune receptors as potential immunotherapeutic agent against cancer and autoimmunity. We have determined the crystal structures of three proteins from the enolase superfamily involved in bacterial metabolism. Complexes of these proteins with their ligands are expected to throw more light into the mechanism of action of these proteins and we have attempted to prepare complexes of these proteins and find their structures. In the second project using X-ray diffraction data with weak anomalous signal we show how we can use the signals, from serendipitous anomalous scatterers observed in crystals and from native sulphurs, obtained using X-ray energies away from their absorption edges, for *ab initio*

phasing. We are also working on design and modification of immune receptors that are expected to be potential lead molecules to cure auto-immunity and cancer.



**Mrs. Pavithra G. C.**  
**(Graduate Student)**

Mrs. Pavitra is working on adenine phosphoribosyltransferase is a glycosyltransferase that catalyzes the reaction between adenine and PRPP to synthesize adenosine monophosphate (AMP) with the release of pyrophosphate (PP). APRT's present in bacteria, yeast, plants as well as mammals and are involved in adenine salvage. In many pathogenic bacteria that lack, so called *de novo pathway*, salvage pathway is the only way to produce AMP, an essential component of DNA synthesis and also a precursor for ATP. We are perusing structural and functional characterization of APRT's from few pathogenic bacteria, which are lacking the *de novo* synthesis and hence are expected to be potential drug targets.



**Ms. Swetha L.**  
**(Graduate Student)**

Ms Swetha is working on Ligand-receptor interactions between cells of the immune system have a vital role in its functioning. Any intervention in these interactions can have a considerable impact on the immune reactions. Modulating these ligand receptor interactions through modified co-stimulatory molecules for therapeutic use is the bottom line of my work.

## Sponsored Projects:

1. 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

### 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.

Previously we had completed and deposited the structure of apo APRT from *Y. pseudotuberculosis* in the PDB with an ID 4MB6. During the previous year we were able to crystallize apo APRT from *F. tularensis*, collect X-ray diffraction data from the crystals and refinement of the structure is completed. To understand the mode of protein-ligand interactions at the molecular level, co-crystallization of APRT from *Y. pseudotuberculosis* with its ligands, adenine, adenosine monophosphate (AMP) and phosphoribosyl pyrophosphate (PRPP) has been carried out. X-ray diffraction data was collected from crystals of protein complexed with all three ligands. We have also complexed APRT from *F. tularensis* with adenine and collected diffraction data for the complex. Refinement of the structures of all the complexes is completed.

### **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, for example, from atoms in the native protein molecules, like sulphur or surface bound metal ions like calcium, potassium etc that are picked up from crystallization conditions, to derive phases. 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 four of the nine cases used in this study, in which serendipitously acquired anomalous scatterers were observed, a draft manuscript has been prepared describing the methods used for phasing in each of the cases and discussing how use of weak serendipitous anomalous signals had led to phasing in each of these cases. The manuscript is currently under revision, and will be submitted soon. Through this manuscript 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.

In addition to this we have carried out an analysis of five cases using sulfur SAD, utilizing weak anomalous signals from native sulfurs for phasing. Manuscript preparation using the results of these analyses is in progress. This manuscript aims to highlight how weak anomalous signals from native sulfurs, from data collected well away from the absorption edge can still be exploited for phasing and structure solution.

## **Modification of TIGIT as potential immunotherapeutic agent against cancer and autoimmunity**

Primary Investigator: Dr. Ramagopal U. A.

Research Associate: Dr. Raghurama P. Hegde

T-cell immunoreceptor with Immunoglobulin and ITIM domains (TIGIT) is a recently identified co-stimulatory molecule expressed on T and NK cells that suppresses activation of T-cells and NK cells upon interaction with either of its two ligands, nectin-2 or PVR. Studies have shown that it could play a role in cancer and autoimmunity. The aim of this project is to modify some of the key residues that affect the interaction of TIGIT with nectin-2, to modulate the binding and use this as a potential immunotherapeutic agent against cancer and autoimmunity.

To tune the interaction of TIGIT with its partners we have planned some mutations and two surface mutations H111I and H111V were attempted. We were successfully able to obtain the H111V mutant. Work has been initiated for scaling up the expression to obtain more amounts of the protein which will be used for standardizing the refolding protocol and then for further crystallographic/biochemical/biophysical studies.

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

Primary Investigator: Dr. Ramagopal U. A.

Research Student: Ms. Swetha. L.

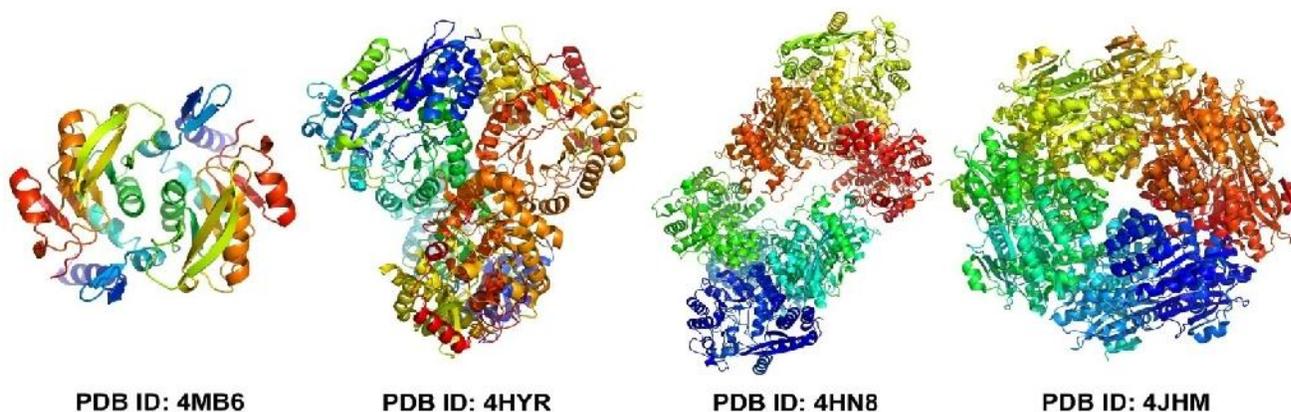
In this project we would like to modify the B7-1 and B7-2 ligands binding surfaces to fine-tune their recognition and avidity towards either CTLA-4 or towards CD28. Efficacy of the modified B7 molecules to bind to their cognate receptors will be assessed using biophysical methods including X-ray crystallography. The results are expected to provide lead molecules that are effective against auto-immune disorder or cancer. We have procured several reagents and chemicals for cloning and expression of these proteins.

In the last year (march 2014-march 2015), hB7.2V and hCTLA-4v with Cys genes were cloned into pNIC28-Bsa4 vector. The recombinant proteins were expressed in BL21(DE3)CodonPlus RIL cells and the proteins formed inclusion bodies. The inclusion bodies were purified and the proteins were refolded. Four hB7.2V mutants were designed after analysis of the complex structures with PDB ID: 1I85 and 1YJD. The mutants were created by site-directed mutagenesis and the expression was confirmed in BL21(DE3)CodonPlus RIL strain.

## **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 signaling 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 (Available in PROTEIN DATA BANK (PDB)):**

## Research Highlights

- More instruments were ordered from this year's instalment of the VGST grant: 1. A nanospectrophotometer with kinetics capabilities; 2. A liquid nitrogen storage dewar with racks to hold cryo boxes and upto 3000 samples; 3. A -20°C freezer; 4. A microbalance and 5. A minicentrifuge with rpm control.
- Dr. Ramagopal visited Department of Biochemistry, Albert Einstein College of Medicine, New York from April 24, 2014 to June 27, 2014 on a collaborative project with Prof. Steven C. Almo.
- We have successfully completed the structures of apo form and several complexes of APRTs from *Y. pseudotuberculosis* and *F. tularensis*.
- Dr. Udupi Ramagopal delivered an invited talk "X-ray Vision: Snapshots of Biological Machines at Atomic Resoltion" as part of the 'Program in Biology for students' under the auspices of the Science Outreach Programs held at the Jawaharlal Nehru Centre for Advanced Scientific Research on 16 Dec 2014.
- Dr. Udupi Ramagopal delivered an invited talk "Macromolecular crystallography and its impact on biology" at the VGST sponsored Two Day Lecture series on 'Celebrating the International year of Crystallography (IYCR-2014)'- looking to the future, learning from the Past, on 13th-14<sup>th</sup> at KLE Society's B. V. Bhoomaraddi college of Engineering and Technology, Hubballi on 13 March 2015.

## Theoretical Sciences Division



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 Division 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 an 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. Mr. G. N. Chandan and Mr. Nepal Banerjee has joined with Dr. Sujit Sarkar, are the four students with the Division.

### **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.

## Faculty Profiles

### Dr. SUJIT SARKAR A, Assistant Professor

#### Area of Research Interest

1. Quantum Many Body Physics and Quantum Field Theoretical Studies of Quantum Condensed Matter System.
2. Cavity Quantum Electrodynamics.
3. Non-equilibrium Statistical Physics.
4. Quantum Phase Transition and Topological Quantum Phase Transition.

#### Curriculum vitae

M. Sc (Kolkata University),

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

#### Postdoctoral Experience

1. IISc Physics Department
2. Bar-Ilan University
3. Max-Planck Institute, Germany as a Guest Scientist
4. The Weizmann Institute of Science.

#### Visiting Scientist Positions.

National Centre for Theoretical Science (NCTS, Taiwan),  
Karlsruhe Institute of Technology, Germany.

#### Ph.D Students

1. Mr. G. N. Chandan
2. Mr. Nepal Banerjee

#### Selected Publications

1. Quantum Criticality of Geometric Phase in Coupled Optical Cavity Under Linear Quenching, (2014), Sarkar S, Physica B, 447, 42 (2014).
2. Quantum Phase Transition of Light, Sarkar S, Journal of Advances in Theoretical Physics and Mathematical Physics, 18, 737, (2014). (The best journal of Mathematical Physics).
3. Quantum Correlation Function in Superconducting Quantum Dot Lattice, Sarkar S, Jour. Phys. Soc. Jpn 83, 104003 (2014).
4. Emergent Majorana Fermions in Cavity QED Lattice, Sarkar S, Journal of Mathematical and Theoretical Physics, (under review process, 2013-14). It has already appeared in Cond-Mat

Bulletin Board. arXiv reference number is 1309.7742.

5. Quantum Simulation of Dirac fermion mode, Majorana fermion mode and Majorana-Weyl fermion mode in cavity QED lattice. Sarkar S, Euro Physics Letters (under review process)It has already appeared in Cond-Mat Bulletin Board. arXiv reference number is 1409.3823.
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).

## Sponsored project: DST Project

### **Geometric Phase and Quantum Phase Transition in Quantum Many Body System**

Principal Investigator: Sujit Sarkar

Project in a Nutshell: Total Amount: 26 Lakhs 33 Thousands Rupees.

Time Duration of the Project: 3Years

Number of Students Involve in This Project: 2

Number of Paper published in this project: 4

## Scientific Collaborations

- 1) Prof. C. D. Hu and Dr. N. Kuo (The National Taiwan University).
- 2) Prof. R. K. Lee (National Centre for Theoretical Science, Taiwan).
- 3) Prof. Masaki Tesuzaka (Tokyo, Japan).
- 4) Prof. Igor Goryni (Karlshruhe, Germany).

## Seminar/Lectures given at

- 1) Harish Chandra Research Institute.
- 2) University of Delhi.
- 3) The National Taiwan Normal University.

## National Workshop/Conference/School/Meeting

- 1) "Quantum Measurements" at the Phys. Dept of IISc Bangalore, 22-24 October (2014).
- 2) "Light and Matter Physics" at the Phys. Dept of IACS, Kolkata, December 18-22nd (2014).
- 3) "Discussion Meeting on Condensed Matter Physics" at the Phys. Dept of IISc Bangalore, January 17-19th (2015).
- 4) "Topological Phases of Matter" at Harish Chandra Research Institute, Allahabad, 9th to 21st February (2015).

## Projects

**Quantum simulation of quantum criticality in 1-dimension:** Simulating a quantum system is a difficult problem specially when dealing with a large interacting system. We study the quantum criticality of a simulated one dimensional Heisenberg spin system with competing nearest-neighbor and next-nearest-neighbor interaction in cavity QED lattice. The effective coupling strengths are expressed in terms of the adjustable parameters of the cavity QED system. We present the different quantum phases in terms of the photon hopping, Rabi frequencies, laser frequencies and the atom-

photon coupling strengths. We predict two kinds of Luttinger liquid phases, one is originating from commensurate to incommensurate transition and the other from the XY criticality. We analyze the exact ground state of this simulated system with applied magnetic field, the quantum critical surface and the excitation spectrum by using the Bethe ansatz method results. We present the exactly solvable Majumder-Ghosh point, fermionization point and the Ising point through the deeply rooted analytical relation in terms of the cavity QED parameters. We also present a correspondence between the different quantum phases of simulated spin physics of this cavity QED model system to the polaritonic state of the cavity QED lattice. (With Mr. Nepal Banerjee)

**Quantum simulation of Dirac fermion mode, Majorana fermion mode and Majorana-Weyl fermion mode in Quantum simulation** aims to simulate a quantum system using a controllable laboratory system that underlines the same mathematical model. Cavity QED lattice system is that prescribes a system to simulate the relativistic quantum effect. We quantum simulate the Dirac fermion mode, Majorana fermion mode and Majorana-Weyl fermion mode and a crossover between them in cavity QED lattice. We also present the different analytical relations between the field operators for different mode excitations. (With Mr. G. N. Chandan)

**Solitons and spin transport in an antiferromagnetic spin chain.** We study the spin transport on a  $S=1/2$  antiferromagnetic chain with external fields which provides a phase angle. The equation of motion becomes the sine-Gordon equation after Jordan-Wigner transformation and bosonization. Soliton solutions of the sine-Gordon equations for a system of finite length are found and the quantum fluctuations are calculated. The spin is transported as the soliton solutions evolved with the adiabatical variation of the phase angle in the phase space. We observe that the spin is transported by  $\hbar = 1$ , as the phase angle changes by the period of  $2\pi$  when the quantum fluctuation enables the system to make a transition between two solutions. This quantum spin transport is not affected by disturbance of environment. (With Prof. Nan Hong Kuo and Prof. C. D. Hu)

## Dr. R. SRIKANTH, Assistant Professor

### Area of Research Interest

- 1) Open quantum system effects in quantum information processing.
- 2) Foundations of quantum mechanics.
- 3) Quantum cryptography.
- 4) Metamathematics and computation theory in physics

### Curriculum vitae

- B.E BITS, Pilani
- Ph. D "On the Solar chromospheric network in the Ca II K line" from Indian Institute of Science.

### Postdoctoral Experience

1. Indian Institute of Astrophysics, Bangalore
2. Center for Theoretical Studies, IISc, Bangalore
3. LAMP group, Raman Research Institute, Bangalore

### Students

- 1.Mr. S. Omkar (thesis submitted to Manipal University).
- 2.Mr. S. Aravinda.

### Selected Publications

1. Characterization of quantum dynamics using quantum error correction.S.Omkar, R. Srikanth, S. Banerjee. Phys. Rev. A 91, 012324 (2015).
2. The operator sum-difference representation for quantum maps: application to the two-qubit amplitude damping channel S. Omkar, R. Srikanth, Subhashish Banerjee. (Accepted in Quantum Information Processing).
3. Orthogonal-state-based cryptography in quantum mechanics and local post-quantum theories. S. Arvinda, Anindita Banerjee, Anirban Pathak, R. Srikanth. Int. J. Quantum Infor. (2015).
4. A Simplified Hierarchical Dynamic Quantum Secret Sharing Protocol with Added Features. Sandeep Mishra, Chitra Shukla, Anirban Pathak, R. Srikanth, Anu Venugopalan. Int. J. Theor. Phys. (2015)
5. Two-step orthogonal-state-based protocol of quantum secure direct communication with the help of order- rearrangement technique.Preeti Yadav, R. Srikanth, Anirban Pathak Quantum Inf Process 13:2731{2743 (2014).
6. Complementarity between signalling and local indeterminacy in quantum nonlocal correlations.S.Aravinda and R. Srikanth To appear in Quantum Information & Computation (2015).

7. Counterfactual quantum certificate authorization. Akshata Shenoy H., R. Srikanth, T. Srinivas Phys. Rev. A 89, 052307 (2014).
8. The quantum cryptographic switch. N. Srinatha, S. Omkar, R. Srikanth, S. Banerjee and A. Pathak. Quantum Information Processing 13, 59 (2014).

## National Workshop/Conference/School/Meeting

International Quantum Structures Association (IQSA) meeting 2014 attended by student Mr. S. Aravinda, who was selected to present a talk, and given full funding. 23-27 June 2014, Olomouc, Czech Republic

## Sponsored project

DST PROJECT: Entanglement, nonlocality and Superluminal Signaling in Deterministic and Indeterministic Extensions of Quantum Mechanics."

Principal Investigator: R. Srikanth

Project in a Nutshell: Total Amount: About 13 Lakhs.

Time Duration of the Project: 3 Years

Number of Students Involved in This Project: 1

Number of Paper published in this project: 4

## Scientific Collaboration

- 1) Prof. Dipankar Home (Bose Institute, Kolkata).
- 2) Prof. A. Pathak (JIIT, Noida).
- 3) Prof. Subhashish Banerjee (IIT-Rajasthan, Jodhpur).
- 4) Prof. Archan Majumdar (SNBNCBS, Kolkata).
- 5) Prof. Debajyoti Gangopadhyay, VBU, Hazaribag.

## Projects

- The essence of nonclassicality: more effect than cause. Nonclassical properties of correlations (like unpredictability, no-cloning and uncertainty) are known to follow from two assumptions: nonlocality and no-signaling. For two-input-two-output correlations, we derive these properties from a single, unified assumption: namely, the excess of the communication cost over the signaling in the correlation. This is relevant to quantum temporal correlations, resources to simulate quantum correlations and extensions of quantum mechanics. We generalize in the context of such correlations the nonclassicality result for nonlocal-nonsignaling correlations (Masanes, Acin and Gisin, 2006) and the uncertainty bound on nonlocality (Oppenheim and Wehner, 2010), when the no-signaling condition is relaxed. An analogy of nonclassicality with Gödel incompleteness is suggested, motivated by the expectation that quantum unpredictability is somehow comparable with metamathematical undecidability. This line of research could shed light on why randomness may be inevitable in Nature. (with Mr. S. Aravinda)
- Ambiguous stabilizer codes and quantum noise characterization. A quantum error correcting code is a subspace  $C$  such that allowed errors acting on any state in  $C$  can be corrected. A quantum code for which state recovery is only required up to a logical rotation within  $C$ , can be used for detection of errors, but not for quantum error correction. Such a code with stabilizer

structure, which we call an "ambiguous stabilizer code" (ASC), can nevertheless be useful for the characterization of quantum dynamics (CQD). The use of ASCs can help lower the size of CQD probe states used, but at the cost of increased number of operations. (With Mr. S. Omkar and Prof. Subhashish Banerjee)

- Orthogonal-state-based cryptography in quantum mechanics and local post-quantum theories. In contrast to the well-known quantum key distribution (QKD) protocols, which encode secret bits in non-orthogonal states, orthogonal-state-based protocols for QKD transmit secret bits deterministically. Even though secure, such a protocol cannot be used to transmit a secret message directly, because an eavesdropper is not prevented from learning something about the direct message before being detected. A quantum secure direct communication (QSDC) scheme satisfies this stronger security requirement. In this work, we study the relationship between security in QKD and QSDC. We show that replacing qubit streaming in a QKD scheme by block-encoding of qubits, we can construct a QSDC scheme. This forms the basis for reducing the security of a QSDC scheme to that of a QKD scheme, in the sense that if the latter is secure, then so is the QSDC scheme built on top of it. We refer to this as block reduction. Further, we show that the security of QKD reduces to that of QSDC, in the sense that if a QSDC protocol is secure, then by sending a random key as the direct message, the corresponding QKD protocol is also secure. This procedure we call as key reduction. Finally, we propose an orthogonal-state-based deterministic key distribution (KD) protocol which is secure in some local post-quantum theories. Its security arises neither from geographic splitting of a code state nor from Heisenberg uncertainty, but from post-measurement disturbance. (With Mr. S. Arvinda, Ms. Anindita Banerjee, Prof. Anirban Pathak)
- A Simplified Hierarchical Dynamic Quantum Secret Sharing Protocol with Added Features. Generalizing the notion of dynamic quantum secret sharing (DQSS), a simplified protocol for hierarchical dynamic quantum secret sharing (HDQSS) is proposed and it is shown that the protocol can be implemented using any existing protocol of quantum key distribution, quantum key agreement or secure direct quantum communication. The security of this proposed protocol against eavesdropping and collusion attacks is discussed with specific attention towards the issues related to the composability of the subprotocols that constitute the proposed protocol. The security and qubit efficiency of the proposed protocol is also compared with that of other existing protocols of DQSS. Further, it is shown that it is possible to design a semi-quantum protocol of HDQSS and in principle, the protocols of HDQSS can be implemented using any quantum state. It is also noted that the completely orthogonal-state-based realization of HDQSS protocol is possible and that HDQSS can be experimentally realized using a large number of alternative approaches. (With Mr. Sandeep Mishra, Ms. Chitra Shukla, Prof. Anirban Pathak, Prof. Anu Venugopalan).
- Characterization of quantum dynamics using quantum error correction. Characterizing noisy quantum processes is important to quantum computation and communication (QCC), since quantum systems are generally open. To date, all methods of characterization of quantum dynamics (CQD), typically implemented by quantum process tomography, are offline, i.e., QCC and CQD are not concurrent, as they require distinct state preparations. Here we introduce a method, "quantum error correction based characterization of dynamics", in which the initial state is any element from the code space of a quantum error correcting code that can protect the state from arbitrary errors acting on the subsystem subjected to the unknown dynamics. The statistics of stabilizer measurements, with possible unitary pre-processing operations, are used to

characterize the noise, while the observed syndrome can be used to correct the noisy state. Our method requires at most  $2(4n+1)$  configurations to characterize arbitrary noise acting on  $n$  qubits (With Mr. S. Omkar and Prof. S. Banerjee)

- Counterfactual quantum certificate authorization. We present a multi-partite protocol in a counterfactual paradigm. 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. (With Ms. Akshata Shenoy H. and Prof. T. Srinivas)

## Highlights of Research Activities

1. Dr. Ramagopal visited Albert Einstein College of Medicine, New York, USA for two months during April-June 2014 on a collaborative work.
2. Dr Halgeri delivered a lecture on the topic entitled Eco-friendly Catalysts and Process for Sustainable Chemistry” at Basaveshwar Science College, Bagalkot on September 13, 2014.
3. Dr. Halgeri presented a talk on the topic entitled “Role of Research Institute for Technology Development in Oil and Gas” at Durgapur IDFRD meeting in November 2014.
4. Dr. Halgeri gave a lecture on “Future Energy Challenges through Biofuel and Biorefinery Technologies” at Govt Science and Arts College in November 2014.
5. Dr. Halgeri delivered a lecture on the topic entitled “Development of Novel Catalysts of Industrial Importance at PPISR” at SABIC on December 19, 2014.
6. Dr. Halgeri gave a talk on the topic “Novel Catalytic Materials and its Applications to Chemical Manufacturing Processes” at MSRIT College in December 2014.
7. Dr. Ananda participated as Judge in EXPRO 2014 (Final year students Project exhibition and competition) held at NMAM Institute of Technology, NITTE, Udupi on 19/04/2014.
8. Dr. Ananda participated in the Seminar on Radiation and Radioisotopes: tools for scientific research on 28<sup>th</sup> April 2014 at CARRT, Mangalore University, Mangalagangothri.
9. The Research Advisory Committee meeting for the Theoretical Sciences group, with Prof. C. Sivaram of St. Joseph University and Prof. Hema Ramachandran of Raman Research Institute as the external advisors was held on May 8, 2014. Both appreciated the work done in the group, in particular appreciating the collaborative works initiated in it.
10. Mr. Suhas gave an oral presentation on “Graphene oxide based nanocomposite membranes for pervaporative dehydration of alcohols: An economic approach” at 6<sup>th</sup> National Conference on Advances in Polymeric Materials (POLYCON-2014) held at Sri Jayachamarajendra College of Engineering, Mysore, Karnataka, 25-26<sup>th</sup> April 2014.
11. Inspire student Ms. Gargi Sabaraya from Poornaprajna college Udupi working on endophytic fungi from two Casia species from May 30 –June 14, 2014.
12. Doctoral Advisory committee meeting held for Mr. Sathish and Ms. Pavithra GC on May 9<sup>th</sup>, 2014 and submitted 5<sup>th</sup> six month progress report.
13. Nine students from PPISR presented their pre-thesis colloquium in the last six months, and two of them submitted their thesis to Manipal University.
14. Ms. Swehta Lankinpalli got the best participant award at the workshop on Cell Culture and Molecular Techniques in Animal Biotechnology held at Bharathidasan University from 5-11 Nov 2014.
15. Dr. Sowmya Palimar and Mr. Pradeep Shanbogh INUP Familiarization Workshop Conducted by Indian Nano Users Program in CeNSE IISc from 21-05-2014 to 23-05-2014.
16. Dr. Nalini, Dr. Sowmya and Ms. Swetha. S. M gave talks in the summer school organized by PPISR for students of PP College Udupi. Mr. Pradeep Shanbogh helped in laboratory demonstrations.
17. Mr. Pradeep Delivered a lecture on “Nanoscience and Technology” at Widia Poornaprajna School
18. The fifth DAC meeting of Ms. Swetha. S.M. and Mr. Srinidhi Raghavan was successfully conducted in April 2014. The DAC members recommended both students to start writing their thesis.

19. Ms. Swetha S.M. presented her pre-synopsis Colloquium on 28<sup>th</sup> November 2014
20. Dr. Nalini visited and interacted with the Poornaprajna School teachers at Delhi on September 19<sup>th</sup> 2014.
21. Dr. Sowmya Palimar attended the Indian Nano Users Program (INUP) hands-on training Workshop conducted at CeNSE IISc from 18<sup>th</sup> -28<sup>th</sup> August 2014.
22. Mr. Pradeep presented a poster titled “Sunlight Driven Photocatalytic Degradation of Congo-Red by RE substituted Bi<sub>2</sub>WO<sub>6</sub> nanoparticles” at Advanced Oxidation Process conference held at Munnar, organized by M.G University, Kottayam, in August 2014.
23. Mr. Srinidhi Raghavan presented his pre-synopsis Colloquium on September 4, 2014 and submitted his thesis on November 2014
24. Ms. Swetha.S.M and Mr. Pradeep presented their research work to Prof. Krishnamurthy from IIT madras on 6<sup>th</sup> September 2014
25. Ms. Swetha .S. M. presented her research work and also the overall work of our group to the RAC chairman Dr Prahalada on 26<sup>th</sup> September 2014
26. Dr.Nalini’s research proposal titled “Design of Lanthanum based Perovskite Nanoparticles for The Development of Thick Film Gas Sensor” has been technically approved by DST, India for extramural research funding for three years from April 2015
27. Mr. Pradeep Shanbogh was awarded the **second prize** for the poster titled "Sunlight driven Photocatalytic Degradation of Congo-Red by RE substituted Bi<sub>2</sub>WO<sub>6</sub>" at the Two Day workshop on "Crystallography in The Sciences" organized by Bangalore University in lieu of the International Year of Crystallography 2014, on October 16th and 17th 2014.
28. Mr. Pradeep Shanbogh was selected to attend the Neutron School at BARC Bombay in January 2015.
29. Mr. Srinidhi Raghavan submitted his thesis to Manipal University in November 2014.
30. The poster titled “Development of lanthanum based perovskite nanoparticles for the detection of sulphur dioxide gas” Sowmya Palimar, Alison E. Viegas, Nalini G. Sundaram was presented in Nano India -2015, SASTRA University , Jan 29-30.
31. Dr. Sowmya has been selected to appear for an interview on January 15, 2015 to a select scientific committee for the post of CSIR-Research Associate.
32. M.Tech Student, Ms. Uma from Dayanand Sagar Engineering College is working on Rare earth based Bismuth oxides for Photocatalytic degradation of dyes” in the Functional Nanomaterials Group with Ph.D student Mr. Pradeep.P.Shanbogh as part of her M.Tech project for 8 months.
33. Dr. Nalini Sundaram and her students successfully conducted a 5 days hands on workshop on “X-ray Rietveld Refinement” using the program GSAS-EXPGui at MRC, IISc from February 25 – March 3 2015
34. Ms. Akshata Shenoy of ECE Dept, IISc, whose PhD work was co-guided by Dr. R. Srikanth, successfully defended her thesis work on Jan 7, 2015, her research being on the topic of quantum nonlocality, counterfactuality and quantum cryptography.
35. Dr. Udipi Ramagopal delivered an invited talk “X-ray Vision: Snapshots of Biological Machines at Atomic Resoltion” as part of the ‘Program in Biology for students’ under the auspices of the Science Outreach Programs held at the Jawaharlal Nehru Centre for Advanced Scientific Research on 16 Dec 2014.
36. Dr. Sujit made academic visits elsewhere in the country (HRI, Allahabad during June 2014) and abroad, at the National Center for Theoretical Science, in Taiwan (September 2014).
37. Dr.Ananda K, was one of the member of the Life Science Judging panel for “The Amateur Scientist 2014” held at PES University on August 23rd, 2014 and judged 35 science projects Presented by the 8-12th Class students from all over India.

38. Mr. Chandan's thesis synopsis has been approved by the doctoral advisory committee, and will be shortly registered at Manipal University. He is being joined by Mr. Nepal Bannerjee as a student working for PhD with Dr. Sujit Sarkar.
39. M.Tech Student, Ms. Uma from Dayanand Sagar Engineering College is working on "Rare earth based Bismuth oxides for Photocatalytic degradation of dyes" in our group with Ph.D student Mr. Pradeep.P.Shanbogh as part of her M.Tech project for 8 months.
40. Mr. Manish Kumar, M.Tech Student, Chemical Engineering Department, Manipal University, Manipal is working on "*Mesoporous polymers as catalyst for etherification of glycerol with t-butyl alcohol to t-butyl ethers of glycerol, a potential fuel additive*" for his M.Tech project for 10 months under the guidance of Dr. Sanjeev P. Maradur.
41. Mrs. Pavithra G C and Ms. Swetha Lankipalli participated in the National Seminar cum Workshop on Cell Culture and Molecular Techniques in Animal Biotechnology held at Bharathidasan University from 5-11 Nov 2014.
42. Dr.Ananda K., delivered a talk on "Blood and Blood substitutes" to the students of Poornaprajna Pre University College Udupi and delivered another talk on "The Blood, can we synthesize artificially?" to the High School students of Poornaprajna Education Centre, Yelahanka, Bangalore.
43. Dr. Ananda K was a Chief Guest and inaugurated the "Exhibition – EDU-VISION" held at Poornaprajna Education Centre (Primary section), Yelahanka, Bangalore on November 21<sup>st</sup>, 2014.
44. Dr. Ananda attended Conference on "Ecosystem: Emerging issues" organized by Poornaprajna College udupi along with Karnataka Science and Technology Academy held during January 9-10, 2015 at PPC, Udupi. Presented a poster on Titled "Endophytic fungi as an alternative source of medicine to save medicinal plants in the ecosystem" awarded 3<sup>rd</sup> best poster presentation.
45. Two MSc students Ms. Ayshwarya and Ms. Anjusha joined for MSc project for six months from January 2015.
46. Dr. Ananda as a PhD co-ordinator visited Manipal University Registrar evaluation and Registrar academics on January 8, 2015 for discussing about the protocols to be followed for the PhD thesis submission and examination process.

## Patent/Publications during 2014-15

Since the inception of PPISR research activity more than 130 research articles have been published with PPISR affiliation.

### Patent

- Catalyst composition for converting light naphtha to aromatic compounds and a process thereof R. Ravishankar, P. V. Rao, N. V. Choudary, G. V. Shanbhag, H. L. Janardhan, A. B. Halgeri and S. Gandham, Indian patent Application No: 1235/MUM/2014, PCT patent Application no. PCT/IB2014/064041, filed by HPCL, R & D Centre, Bangalore.

### Publications

1. 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.
2. A composition-dependent “re-entrant” crystallographic phase transition in the substitutional metal acetyl acetonate complex(Cr<sub>1-x</sub>Gax)(acac)<sub>3</sub>, M. Srinidhi Raghavan, Piyush Jaiswal, Nalini.G. Sundaram and S. A. Shivashankar. *Polyhedron* 70C (2014), pp. 188-193.
3. Synthesis and characterization of novel polyurethanes based 4,4'-{oxy-1,4-diphenyl bis(nitromethylidene)} diphenol Schiff base hard segment” D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu\*, “, *Polymer Engineering and Science*, (2014), 54, 24-32.
4. Targeting Mycobacterium tuberculosis nucleoid-associated protein HU with structure-based inhibitors Bhowmick T, Ghosh S, Dixit K, Ganesan V, Ramagopal UA, Dey D, Sarma SP, Ramakumar S, Nagaraja V, *Nature Communications*, (2014), 5:4124.
5. Evaluation of antimicrobial activity of secondary metabolites and enzyme production from endophytic fungi isolated from *Eucalyptus citriodora*. L. Sathish, N. Pavithra and K. Ananda, *Journal of Pharmacy Research*, 8(3),269-276.
6. *The quantum cryptographic switch*. N. Srinatha, S. Omkar, R. Srikanth, S. Banerjee and A. Pathak. *Quantum Information Processing* 13, 59 (2014).
7. Characterization of quantum dynamics using quantum error correction. S. Omkar, R. Srikanth and Subhashish Banerjee. *Phys. Rev. A* ,91, 012324 (2015)
8. Quantum Criticality of Geometric Phase in Coupled Optical Cavity Under Linear Quenching, (2014), Sarkar S, *Physica B*, 447, 42 (2014).
9. Quantum phase transition of light in coupled optical cavity arrays: A renormalization group study, Sarkar S, *ADV. THEOR. MATH. PHYS.* Volume 8, Number 3, 737–756, 2014.
10. Counterfactual quantum certificate authorization. Akshata Shenoy H., R. Srikanth, T. Srinivas. *Phys. Rev. A* 89, 052307 (2014).
11. Quantum Correlations of Two Superconducting Charge Qubits in a Magnetic Field, Sarkar S, *Journal of the Physical Society of Japan* 83, 104003 (2014).
12. The Essence of nonclassicality— more effect than cause. S. Aravinda and R. Srikanth (submitted to Proceedings of International Quantum Structures Association 2014).

13. "Metal ion-exchanged zeolites as solid acid catalysts for the green synthesis of nopol from Prins reaction" V. S. Marakatti, A.B. Halgeri and G. V. Shanbhag, *Catalysis Science and Technology*. 2014, DOI: 10.1039/C4CY00596A.
14. Phosphate modified ZSM-5 for the shape-selective synthesis of para-diethylbenzene: Role of crystal size and acidity, Janardhan L. Hodala, Anand B. Halgeri, Ganapati V. Shanbhag\*, *Applied Catalysis A: General*, Volume 484 , 2014, 8-16.
15. "Room temperature synthesis of solketal from acetalization of glycerol with acetone: Effect of crystallite size and the role of acidity of beta zeolite" P. Manjunathan, S. P. Maradur, A. B. Halgeri and G. V. Shanbhag, *J. Mal. Catal. A: Chem.* DOI: 10.1016/j.molcata.2014.09.028.
16. Swetha S M Bhat, Ashfia Huq, Diptikant Swain, Chandrabhas Narayana and Nalini G Sundaram "Photoluminescence Tuning of Na<sub>1-x</sub> K<sub>x</sub>NdW<sub>2</sub>O<sub>8</sub> (0.0d" x d"0.7) Nanoparticles; Synthesis, Crystal Structure and Raman Study" just accepted in *Physical Chemistry Chemical Physics*, RSC publications.
17. "Graphene loaded Sodium alginate Nanocomposite Membranes with Enhanced Isopropanol dehydration performance via Pervaporation" D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghunath, "RSC Advances" online DOI: 10.1039/C3RA42062K.
18. Targeting Mycobacterium tuberculosis nucleoid-associated protein HU with structure-based inhibitors," Bhowmick T, Ghosh S, Dixit K, Ganesan V, Ramagopal UA, Dey D. Sarma SP, Ramakumar S and Nagaraja V. *Nature Communications*, (2014)5:4124.
19. **Invited** article titled Fullerenes Revisited: Materials Chemistry and Applications of C60 Molecules Pradeep P. Shanbogh Nalini G. Sundaram, *Resonance*, February 2015, 20 (02), (p.123)
20. Photocatalysis of Bi<sub>4</sub>NbO<sub>8</sub>Cl hierarchical nanostructure for degradation of dye under Solar/UV irradiation, Swetha S M Bhat and Nalini Sundaram *New J. Chem.*, 2015, DOI: 10.1039/C4NJ01814A.
21. Controlled inversion and surface disorder in zinc ferrite nanocrystallites and their effects on magnetic properties, Ranajit Sai, Suresh D. Kulkarni, Swetha S. M. Bhat, Nalini G. Sundaram, Navakanta Bhat and S. A. Shivashankar, *RSC Adv.*, 2015, 5, 10267-10274
22. L. Sathish, N. Pavithra and K. Ananda (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.
23. Garudachari B, Isloor AM, Satyanarayana MN, Ananda K, Fun H-K. (2014) Synthesis, characterization and antimicrobial studies of some new trifluoromethyl quinoline-3-carbohydrazide and 1,3,4-oxadiazoles. *RSC Advances*. 2014;4(58):30864-30875.
24. Pavithra N., Sathish L., Suneel Kumar A., Venkatarathanamma, V., Pushpalatha H., Bhanuprakash Reddy, G., Ananda K. (2014): In-vitro Studies on  $\pm$ -Amylase,  $\pm$ -Glucosidase and Aldose Reductase Inhibitors found in Endophytic Fungi Isolated from *Ocimum sanctum*, *Current Enzyme Inhibition*, 10(2)129-136.
25. N. Pavithra, L. Sathish, Nagasai, Babu, V. Venkatarathanamma, H. Pushpalatha, G. Bhanuprakash Reddy, K. Ananda (2014) Evaluation of  $\pm$ -Amylase,  $\pm$ -Glucosidase and Aldose Reductase inhibitors in ethyl acetate extracts of endophytic fungi isolated from anti-diabetic medicinal plants. *Int J Pharm Sci Res*, 5 (12) 5334-5341.

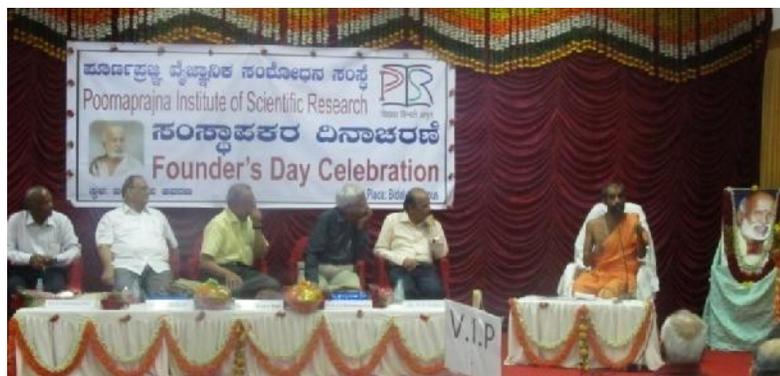
## Events and meetings

### 1. Founder's Day Celebration

PPISR celebrates its founder's day during the first week of July every year, with scientific sessions followed by a valedictory function. Prof. S Asokan, Department of Instrumentation and applied physics and chairman Rober Bosch Centre for Cyber Physical System, IISc, Bengaluru, inaugurated the scientific sessions on 2 -July-2014 and Dr. AB Halgeri, Director PPISR gave a welcome address. Prof. Anantharaj, Vision Group on Science and Technology, Govt. of Karnataka, chaired the first scientific session. This year's talks were different in that all the students who are in the verge of finishing their PhD gave talks related to their thesis work. Scientific sessions were chaired by eminent scientists Prof. N. Nagaraj, HOD, Saint Joseph's College, Bangalore; Dr. Manjunath, Senior Scientific Officer, NIMHANS, Bengaluru and Prof. Shiv Sethi, Raman Research Institute, Bengaluru respectively for Materials, Biological and Theoretical Sciences.



A valedictory function in recognition of Founder's Day Celebration was organized at Bidalur Campus on July 03, 2014. Prof. P Rama Rao, a renowned scientist, Chairman, Governing Council, International Advanced Research Centre for Powder Metallurgy and New Materials, Hyderabad and the first Director of PPISR was the guest of honour, while Prof. V S Ramamurthy, Director NIAS, Bengaluru presided over the valedictory function. Paramapoojya Sri Vishwapriya Teertha Swamiji, chairman, AMEF and PPISR graced the occasion. A welcome address and brief note on AMEC and AMEF was delivered by the Hon. Secretary Dr. K Srihari followed by lighting of a lamp by the dignitaries. Dr. Anand B Halgeri gave a brief introduction on the research activities at the institution. "AMEF gave best research scholar award to Mr. Omkar, Mr. Suhas and Ms. Pavithra and also appreciation certificate to Mr. Manjunathan and Mr. Satish Burla for successfully completing GTC Project". During his Address, Prof Rama Rao spoke about his cordial relationship with the founder Paramapoojya Sri Vibudhesha Teertha Swamiji and his



interactions with him. Prof. Rao has also served PPISR as the first Director in 2003. During the function, the students those who were recognised for their meritorious works, were honoured by Prof. Rama Rao and Paramapoojya Sri Swamiji blessed them with awards.

## 2. Foundation stone laid for new hostel building



Scientific activities at PPISR have shown an upward trend. We are accepting more students for Ph.D programme in all the three divisions. Considering the future growth of PPISR, the management has decided to construct a new hostel building to accommodate forthcoming students on the campus. In this regard, the Chairman of the institution Paramapoojya Sri Vishwapriya Teertha Swamiji laid the foundation stone for the new hostel building at the Bidalur Campus on July 03, 2014, on the auspicious occasion of Founder's Day Celebrations. The construction activities for the 10 roomshostel building with 2 guest rooms are going on in full swing.

## 3. Visitors' to the Institute: Vice Chancellor, Central University, Karnataka

Prof. M.N Sudhindra Rao, Vice Chancellor of Central University of Karnataka, Gulburga along with Prof Chandra Sekhar, Chairman, School of Chemical Sciences visited PPISR on 24<sup>th</sup> January, 2015. They were taken



around materials science and biological science laboratories and a meeting was held with the delegates later on. The Director addressed the gathering with opening remarks along with presentation on overall activities of PPISR. Faculties of all the three departments made presentations about their ongoing research activities in their respective group. An academic discussion with the Vice Chancellor of CUK to identify the common areas of research interest which will mutually benefit CUK and PPISR in near future in the form of collaborative research and/or student exchange programs were discussed in detail in the second half of the session. The delegates expressed their happiness about PPISR's progress at research campus in a short span of five years since 2010.

## 4. Release of eighth volume of biannual issue of PPISR news letter



The eighth volume of biannual issue of PPISR newsletter was released by the chairman of PPISR Paramapoojya Sri Vishwapriya Teertha Swamiji on February 13, 2015 (Friday) at the Bidalur Campus. The newsletter features the events took place from July to December, 2014 highlighting the

Research Works, Papers published and the celebration of Founder's Day, Outreach Programmes etc.,

During this time, it was also brought to the notice of the chairman of PPISR that, first batch of nine doctoral students had submitted their PhD thesis to Manipal University, Manipal, which is a very proud moment for budding institute, PPISR by seeing the dream come true of our beloved Paramapoojya Sri Vibudhesha Teertha Swamiji. The research work carried out and the hardship they underwent during the initial years of start of the institute and ultimately achieving this goal was expressed by all the nine students in brief to Paramapoojya Sri Vishwapriya Teertha Swamiji.

## 5. Outreach Program for high school students of Poornaprajna schools, Bangalore



In addition to research, faculties and students of PPISR are also involved in outreach activities for high school students with the aim of “**Today's Science for Tomorrow's Scientists**” in order to develop innovative and imaginative platform for research in young minds. The objective was to motivate and inspire young students to take science as a career in the future.

The second year, Open Day session started at Bidalur Campus from 19<sup>th</sup> to 23<sup>rd</sup> January, 2015. About 90 students each from all the five PPEC schools in Bengaluru participated in the programme. Experiments were conducted in Physics, Chemistry and Biology.

Few interesting experiments like *Chemical Snow* Faltwherein benzoic acid which goes from solid to gaseous phase by sublimation upon heating above its melting point and re-solidify upon cooling, Also the role of *Photo catalysis* in waste water treatment, Conversion of  $CuSO_4 \cdot 5H_2O$  to anhydrous  $CuSO_4$ , Wave nature of light in materials science, *Polarization of light*, Diffraction of light. 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. Bacteria, Preparation and observation of different stages of mitosis, growing and observation of small and macro molecular crystals.

Students were also taken around Central Instrument Facility to have the glimpses of the instruments. The feedback got from the teachers and students on the outreach program were very favorable and they appreciated the Director, faculty and students of PPISR for this initiative. In addition they also invited our faculty and students to give a talk/demonstration at their schools.

## 6. Agreement signed for the new project between PPISR and GTC, USA



**Dr. Ding ZhongYi** Technology Process Manager, GTC USA visited PPISR on 2-11-2014 to review the completed project and to discuss the start of the new project for 2014-2015. There were discussions on the technical requirement and literature on the new project related to the catalyst development for natural gas conversion to value-added chemicals. Natural gas rich in methane is a fossil fuel obtained from the earth's crust which can be a cheap and abundant raw material for synthesis of valuable chemicals. Since methane is highly inert gas for

chemical reaction, it is challenging to develop catalyst for methane activation reactions. Such processes are popularly known as Gas to Liquid (GTL) processes.

Dr. Halgeri, Director, PPISR signed an agreement with GTC for the new collaborative project on “design and development of a catalyst and process for natural gas conversion to value added products”. Dr. Ganapati Shanbhag is the Principal Investigator and Dr. Sanjeev Maradur is co-investigator of the project. During this period, two new project assistants were recruited for this project and a new quartz reactor was set up for this process. The technical aspects of the work and timeline for this project was discussed and finalized during the visit of Dr. Ding ZhongYi, November 2014. Previous 3 years project on toluene methylation to produce xylenes was successfully licensed by GTC to a company in China. To finalize remaining technical requirements of this process, few more toluene methylation time on stream experiments were carried out during this period. Dr. ZhongYi expressed happiness over the progress of the concluded project in which PPISR successfully developed a 2<sup>nd</sup> generation catalyst for aromatics conversion.

## 7. Successful completion of HPCL sponsored project

The two-year collaborative project with R & D Centre, Hindustan Petroleum Corporation Ltd, Bangalore on “*development of modified catalysts for hydrocarbon conversions*” was successfully completed. The project term of two years was completed on October 29, 2014. During October, optimization of reaction parameters with standardized catalyst recipe was conducted for both light naphtha aromatization and toluene side chain alkylation reactions. Final project report was prepared and submitted to HPCL. A final review meeting was conducted in November and presentations were made on the yearly progress of the project. During last two years 2 patents were filed by HPCL in which PPISR members are co-inventors and 2 joint publications in international journals are finalized. The 3<sup>rd</sup> patent on side chain alkylation work is in the final stage of preparation. From HPCL R & D, Dr. N V Choudhary, General Manager, Dr. P.V.C. Rao, Dy General Manager, Dr. Ravishankar, Senior Manager ((Principal Investigator of the project for HPCL) participated in the meeting. Dr. A.B. Halgeri, Dr. G. V. Shanbhag (Principal Investigator, PPISR) and Dr. Sanjeev Maradur were present from PPISR. HPCL team appreciated the overall progress made during the span of two years. Based on the excellent progress made during last two years, HPCL has shown interest in working a collaborative project with PPISR in near future and invited to submit a new project proposal. A proposal will be finalized soon.

## 8. Summer School in Physics, Chemistry and Biology for undergraduate Students

The five day research orientation programme Physics, Chemistry and Biology was inaugurated by our Chairman, H H Sri Vishwapriya Theertha Swamiji in the presence of Dr. K. Srihari (Hon. Secretary, AMEC and AMEF) and Dr. A.B. Halgeri, Director, PPISR. 16 undergraduate students and 2 Faculty from the Poornaprajna College Udupi attended this programme. After lighting of the lamp, a brief introduction to



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the summer school by our director, followed by a motivational speech by Dr. Sri Hari where he requested the students to use this opportunity to fulfil their research career and aspirations. Later, the session ended with a benediction by Swamiji. The technical programme for the Chemistry session was inaugurated with a lecture by Dr. Ganapathi V Shanbhag, on introduction to catalysis science and its application in industry. The second lecture was delivered by Mrs. B.V. Swetha on Material Characterization. On the second day Mr. Vijay M gave a talk on Introduction to Materials Science, followed by Ms. Swetha's talk on Photocatalysis and its applications. The last talk of the day was by Mr. Janardhan on the mechanism of chemical reactions. Third day Dr. Sowmya Palimar presented a lecture on Thin Film Technology, followed by Dr. Nalini Sundaram on Nanomaterials. Finally last lecture from Materials science division was delivered by Mr. Suhas D.P. on Polymers and Plastics. Laboratory Sessions were handled by Mr. Pradeep, Mr. Manjunathan and Ms. Sowmya provided a glimpse into the working style of research laboratories, handling laboratory equipments and analyzing results with sophisticated instruments.



The technical session in Biology on day 4 started with a talk by Dr. Ananda on Research Methodology.

The second lecture of the day was on Diabetes and Nutraceuticals by Ms. Pavithra N. This was followed by a talk introducing Endophytic fungal research and Instruments of Biological Sciences by Dr. Ananada. In the evening there was a special lecture about the various research opportunities in Indian institutions by Mr. Aravinda S who covered most of the Institutes of India and the opportunities available for the students with inputs from Dr. Shanbhag, Ms. Swetha L and Mr. Pradeep Shanbhog.

Dr. Raghurama Hegde delivered a lecture providing an overview of protein crystallography which was followed by a lecture on Drug Discovery from Fungi by Mr. Sathish L. The laboratory sessions in biology was guided by Ms. Swetha L and Mrs. Pavithra G C. The students were provided a glimpse of what happens in a molecular biology laboratory and had hands on opportunity to carry out recombinant expression. Simultaneously the concepts behind each step were explained. They had also setup protein crystallization and were provided hands on experience in handling protein crystals. On day 5, in the Physics Session, Mr. Omkar, emphasis was placed on mathematical

problem solving skills, with topics covered being classical electromagnetism, with a view to helping students take up entrance exams successfully for higher studies. Other topics covered were introductions to thermodynamics and quantum mechanics, by Mr. Aravinda, basic computer programming for physics, by Chandan; Einstein's theory of lasers, by Dr. Sujith; and the Deutsch algorithm in quantum computation, by Dr. R. Srikanth.

## New members

1. Mr. Sathyapal Churipard. R. has joined for PhD in Materials Science Division under Dr. Sanjeev Maradur. He has done M.Sc in Organic Chemistry from Bangalore University 2014.
2. Mr. Saikiran. M has joined as Project Engineer in industry sponsored Project in Materials Science Division under Dr. G. V. Shanbhag. He has done M.Tech in Chemical Engineering from Siddaganga Institute of Technology, Tumkur.
3. Mr. Kempanna S. Kanakikodi has joined as Research Fellow in industry sponsored Project in Materials Science Division under Dr. G. V. Shanbhag. He has done M.Sc General Chemistry from Rani Channamma University Belagavi.
4. Ms. Kavitha KN joined as JRF with Dr. Ananda's group in the Biological Sciences under BRNS project. She has completed M.Sc in Biotechnology from Department of Biosciences, Mangalore University. She had prior research experience on endophytic fungi in a project in the Department of Microbiology, University of Mysore.
5. Archana K M has joined as a JRF with Dr. Nalini in the Materials Science Division, PPISR. She completed M.Sc in Inorganic Chemistry from Central College Bangalore University, Bangalore. Following that she has worked as an Assistant Professor in the department of Engineering Chemistry at C. Byre Gowda Institute of Technology, Kolar.

## Invited Talks

- **Dr. Digamber. G.Porob**, Lead Scientist, GE Global Research, Bangalore, gave a lecture on "Preparative Solid State Chemistry Techniques" on 13th May, 2014.
- **Dr. B. M. Nagaraja.**, Asst. Professor, Center for Nano and Materials Science, Jain University Bangalore gave a talk on 29th April 2014. on the topic "*Dehydrogenation of alkane to light olefin over PtSn/Al<sub>2</sub>O<sub>3</sub> catalyst: Effect of Sn loading*".
- **Prof. B.S. Jai Prakash**, Director, Institute of Environment and Hazardous Materials Management (IEHMM), Bangalore and Honorary Professor, PPISR, gave a talk on "Laboratory Safety" as a part of Research Methodology Course on 23th May, 2014.
- **Prof. D.S Viswanath**, Emeritus Professor of Chemical Engineering Department, University of Missouri, USA, delivered a lecture on "Random Thoughts" on 24th July 2014.

- **Dr. Chaitanya Hiremath**, Founder President & CEO, APODvision, Inc. USA delivered a lecture titled "1. Abbreviated th Profile of Drugs (APOD): A Novel Integrated Approach for Drug Discovery and 2. The World Flag" on 7 August 2014.
- **Ms.Manju Sivasankaran**, Principal Investigator, Women Young scientist scheme, IISc gave talk titled "Genome scale network modelling of Fungus" on 9 September 2014.
- **Dr. Angushman Roy Choudhary**, Department of Chemistry, IISER Mohali, **gave a talk on** "Polymorphs, Salts and Cocrystals of Drugs and Pharmaceuticals: Enhancement of Physicochemical Properties for Better Formulations" on 27<sup>th</sup> Feburary 2015.

## In-house Seminars

1. Mr. Manjunathan: Mesoporous carbon materials: Synthesis and applications, 16/05/2014.
2. Dr. Raghuram Hedge: TIGIT- a possible immunotherapeutic agent against autoimmune and cancer, 27/07/2014.
3. Mr. Aravinda: Theoretical study of weak magnetic field effects on the radical ion pair reaction & understanding a model for photoreceptor based magnetoreception in birds, 14/08/2014.
4. Mr. Pradeep Shanbhogh: Semiconductor heterostructure next generation photocatalyst, 26/08/2014.
5. Dr. Nalini G. Sundaram: Rechargeable Lithium ion batteries: from cell phones to electric vehicles, 10/10/2014.
6. Ms. Swetha Lankipalli: It's not just genetics its epigenetics, 29/10/2014.
7. Mr. Janardhan H.L.: Catalysis lab from within walls to a computer, 28/11/2014.

## Campus life

### 1. Independence day celebration at Bidalur campus

Independence Day for the fourth year in row was celebrated on August 15, 2014 at the Bidalur Campus. The Directorhoisted the National Flag and delivered a speech to the gathering of students, faculty and staff members. Sri. PSreenivasa Rao, Financial Advisor of PPISR was also present during occasion and addressed the gathering andadvised about internal discipline of each departments and its role in building up the institution. All faculty members,their families and other members were present during the small get-together celebration.For last three years PPISR had the tradition of planting trees on the occasion of Independence Daywith a concern to love & care for the nature as nature alone is our future sustenance, which was continued this year too. One hundred saplings were planted by the members of the institution successfully addingmore greenery to the existing green campus.



## 2. Saraswathi/Ayudha Pooja At Bidalur Campus



Ayudha pooja and Saraswathi puja were performed at the Campus on October 1, 2014. The Director, all the staffs, faculties, students and other PPISR members participated enthusiastically and paid respect to the Goddess of knowledge.

## 3. Free Medical Checkup Camp at Bidalur Campus

A medical checkup camp was organised on March 01<sup>st</sup>, 2015 at the Bidalur Campus for the nearby villagers as a social outreach for the mankind. This camp was organised under the banners of Rural Service Trust, Sadashivanagar in jointly with Poornaprajna Institute of Scientific Research with the blessings of Udupi Sri Admar Math Peethadhipati Paramapoojya Sri Vishwapriya Teertha Swamiji. Specialized Doctors in Gynaecology, Dental, Diabetic and General Physician alongwith Rotary Eye Centre ventured voluntarily to make this social outreach programme a grand success. Also some of the students of PPEC, Sadashivanagar and students, staff and faculty members of PPISR extended their support for this social cause alongwith the Director 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 internet service provider.

## Poornaprajna Analytical Centre

PPISR has procured several analytical instruments that are vital for the faculty and students to pursue advanced research in basic and applied sciences. The Analytical Facility has several sophisticated instruments namely Powder X-ray Diffractometer, Fourier Transform Infrared Spectroscopy (FTIR) Ultra Violet-Visible Spectroscopy (UV-VIS), Atomic Absorption Spectroscopy (AAS), Fluorescence Spectrophotometer, etc., that are necessary for general analysis. The instruments are available for use mainly by the Scientists and the Research students at PPISR and our collaborators. This facility is also extended to all researchers from academic institutions and industries, to characterize their samples at nominal charges. Poornaprajna Analytical Center has been very helpful for academic institutions in and around Karnataka and would like to continue to offer this facility in the years to come. Any interested individuals can analyze their samples under the guidance of a PPISR staff or submit their samples for analysis. In case if you want to download sample registration form or need any further information, you are requested to visit our website [http://www.ppISR.res.in/analytical\\_center.html](http://www.ppISR.res.in/analytical_center.html)

## Research facilities added during 2014-15



**Sonicator from  
Ultrasonics Solutions**



**Eppendorf  
Biospectrometer**



**Photocatalytic  
Reactor (Huber)**



**Autoclave Unit  
50&100 mL Capacity  
(Make: Amar)**

## Contact Us



**UV-Vis Microplate  
Reader**

Dr. Nalini G. Sundaram  
[nalini@poornaprajna.org](mailto:nalini@poornaprajna.org)

Mrs. Latha Srinivasan  
[latha@poornaprajna.org](mailto:latha@poornaprajna.org)

**City Campus** : # 4, 16<sup>th</sup> Cross, Sadashivanagar, Bangalore – 560 080. Ph:  
080 - 2361 1836

**Main Campus** : # 167, Poornaprajnapura, Bidalar Post, Devanahalli,  
Bengaluru - 562 110. Ph:080 - 2760 7242

Web Site: [www.ppISR.res.in](http://www.ppISR.res.in) Email: [admin@poornaprajna.org](mailto:admin@poornaprajna.org)

## Visitors' view

- ❖ **Bipin V Vora**, Consultant R&D Advisor, UOP LLC, A Honeywell Company, U.S.A “The Institute has done excellent ground work to become a world class research institution. A very professional highly qualified staff and enthusiastic young students,”
- ❖ **Prof. Gundu Rao**, Emeritus Professor, University of Minnesota,U.S.A “I was very much impressed with the way research activity has been developed in such a short time. There is a great window of opportunity for developing research that can be used for providing new molecules of interest.”
- ❖ **Prof. Anil C Banerjee**, Columbus State University, U.S.A “We were very impressed with the knowledge and devotion of faculty and research students. This is a small institution made of very dedicated group. We are thankful to Dr. Halgeri and his team for providing us hospitality”.
- ❖ **Dr. Subhangi Umbarkar**, Scientist, CSIR-NCL, Pune, India “I am really impressed with the setup with so few faculty and students. I wish all the best for bright future of this institute and congratulate the entire team for successful beginning”
- ❖ **Dr. Venkata Ramanujam**, GTC technology, U.S.A “PPISR is impressively located with serenity and peace. Environment is stimulating to mind which of primary importance to produce quality research and results. We wish PPISR to grow many folds and expand to different areas of R&D. We sincerely pray that the vision of founders become true as quickly as possible and surpass world leading R&D institution.
- ❖ **Prof. S ASOKAN**: Chairman, Robert Bosch Centre for Cyber Physical Systems, IISc, Bengaluru.Highly impressed by the quality of research and enormous progress made by the centre in the last four years
- ❖ **Prof. Dabir S. Vishwanathan**: Emeritus Prof. in Chemical Engineering, University of Missouri, California. “Dr. Halgeri and his colleagues are doing excellent scientific work and I wish them all the success and my pranamas to Swamiji”.
- ❖ **Dr. CHAITANYA HIREMATH**, Founder President, APODvision, USA, Founder president SEALOEarth, USA It was a pleasure to visit the institute. It is great to see excellent infrastructure which has been put to good use. People are outstanding and producing good publications. Keep up the good work.