

## Poornaprajna Institute of Scientific Research Bangalore, India Annual Report: 2012–2013



Recognized by the Dept. of Scientific and Industrial Research (DSIR) and Manipal University Promoted and Managed by Udupi Sri Admar Mutt Education Foundation. ©PPISR (2013)

## Founder's Message



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

> HH Sri Vibudhesha Theertha Swamiji, Founder President, PPISR

## Chairman's message



My beloved Guruji and illustrious predecessor, HH Sri Vibudhesha Theertha Swamiji, considered the Poornaprajna Institute of Scientific Research (PPISR) the crest jewel among the Poornaprajna family of schools and institutes founded by him. He envisioned for fundamental scientific research to be undertaken here in the same free spirit of curiosity, that marked the investigations of the ancient Upanishadic sages.

The progress that I have witnessed in the past three years, in terms of the quality of research and infrastructural improvement at PPISR, give me ample reason to hope that the institute is quite well on track to fulfil Swamiji's vision for it, thereby benefiting Indian science and the community of Indian students.

The past year, I had number of informal and fruitful interactions with scientists and

students of PPISR, thanks to for a facilitated by the Director, Prof. A. B. Halgeri and the Secretary, Prof. K. Srihari. The interaction between basic science and spiritual philosophy, which was one of the visions that motivated Swamiji to found PPISR, finally took on a concrete form with the creation of the Center for Foundational Study (CFS).

Although science and philosophy have traditionally had different foci and priorities, there are a number of topics where they can meet and benefit each other through a process of dialog, which was prevalent in ancient India. I think that the topics chosen for research in CFS, such as identity, individuation and free will are quite apt in this regard. Scientists may wish to consult the works of Sri Madhwacharya and other sages in this regard.

May Lord Sri Krishna bless and guide the members of PPISR!

HH Sri Vishwapriya Theertha Swamiji Chairman, AMEF

## Contents

1	Message from the Secretary	6
<b>2</b>	Foreword from the Director	8
3	Board of Trustees	9
4	Research Advisory Committee	10
5	Administration 5.1 Director and Financial Advisor	<b>11</b> 11
	<ul> <li>5.2 Administrative Staff</li></ul>	11 11
6	Adjunct and Honorary Faculty	12
	<ul> <li>6.1 Adjunct faculty</li></ul>	$\begin{array}{c} 12\\ 12\end{array}$
7	Doctoral Advisory Committee	13
8	About the Institute	<b>14</b>
	8.1 History and Mission	14
	8.2 Contact details	15
9	Division Structure, Faculty and Students	16
	9.1 Materials Science	16
	9.2 Biological Sciences	16
	9.3 Theoretical Sciences	17
10	Materials science	18
	10.1 Introduction	18
	10.2 Academic and Research Highlights	18
	10.3 Faculty Profiles	20
	10.3.1 Dr. A. B. Halgeri	20
	10.3.2 Dr. A. V. Raghu	22
	10.3.3 Dr. Ganapati V. Shanbhag	25
	10.3.4 Dr. Nalini Sundaram	33
	10.3.5 Dr. Sanjeev Maradur	38

11 Biological sciences	40			
11.1 Introduction	40			
11.2 Academic and Research Highlights	41			
11.3 Faculty Profiles	43			
11.3.1 Dr. Ananda K	43			
11.3.2 Dr. Udupi Ramagopal	47			
11.3.3 Prof. Prasad Koka	51			
12 Theoretical Sciences	52			
12.1 Introduction $\ldots$	52			
12.2 Research Highlights	53			
12.3 Faculty Profiles	54			
12.3.1 Dr. Sujit Sarkar	54			
12.3.2 Dr. R. Srikanth $\ldots$	56			
12.3.3 Dr. S. G. Bhargavi	59			
13 Events and achievements	60			
13.1 Representative Publications	61			
13.2 Achievements	62			
13.3 Conferences and workshops	64			
13.4 New Appointments	67			
$13.4.1$ Faculty $\ldots$	67			
13.4.2 RA and postdocs	67			
14 Acadomic activities	68			
14.1 Collaborative vigita	68			
14.1 Collaborative visits $\dots \dots \dots$	60			
14.2 In-House seminars	60			
14.5 Invited Tarks $\dots \dots \dots$	70			
14.4 RAC meetings	70			
14.5 Academic Outreach Activities	70			
15 Research Facilities	72			
15.1 Sophisticated Instruments	72			
15.2 Library	76			
15.2 Computers and internet	77			
15.4 Other Facilities	77			
16 Campus life				
17 Visitors' Views	80			

## 1. Message from the Secretary

His Holiness Sri Vibudhesha Theertha Swamiji, even as chief pontiff of Sri Admar Mutt, Udupi, remained a science enthusiast who enjoyed discussing physics with scientists and drawing comparisons with scriptural lore, until he attained the Lotus Feet of Lord Sri Krishna. As the tangible symbol of his love for science and its integration with the spiritual sciences, PPISR stands as a wonderful place where scientists pursue uninterrupted research and provide training to younger minds. It is a matter of pride that, in addition to the existing facilities, construction of a new biological wing is under progress.



Udupi Sri Admar Mutt Education Council (AMEC), founded by Poojya Swamiji, oversees 30 Poornaprajna Schools and also the Udupi Sri Admar Mutt Education Foundation (AMEF), which manages the Poorna Prajna Institute of Scientific Research (PPISR), considered by Poojya Swamiji as the Crest Jewel (*chUDAmaNi*) of all Poornaprajna Institutions founded by Him. The sacred responsibility now rests upon AMEC and AMEF to further the physical, biological and materials sciences, while also trying to brigde the gap between the ancient spiritual traditions of the country with modern science and education.

PPISR is now previleged to be placed under the able and wise guidance of His Holiness

Sri Vishwapriya Theertha Swamiji, the presiding pontiff of Sri Admar Mutt, Udupi, the president of AMEC and Chairman of AMEF.

The past year has seen a number of milestones passed by PPISR: a number of industrysponsored and Govt.-sponsored have been taken up, while the number of publications has crossed the 100 mark. I believe that taken per capita of faculty, PPISR's count of publications in the same period of time exceeds that of many better known institutes. A heartening development over the past year has been the frequent encouragement researchers have received from HH Sri Swamiji's visits and interactions with scientists.

In our attempt pursue and achieve the lofty vision set forth by H H Sri Vibudesha Theertha Swamiji, and continued under the dynamic leadership and guidance of H H Sri Vishwapriya Theertha Swamiji, PPISR, which is funded mainly through AMEC, has received help from many corporate well-wishers. We fondly hope that more members from the corporate world and the general public would join us. Dr. K. Srihari (Hon. Secretary, AMEC and AMEF, Professor (Rtd), UAS, Bengaluru

## 2. Foreword from the Director

I am happy to present the third Annual Progress Report describing various research and academic activities of Poornaprajna Institute of Scientific Research (PPISR). It has now become an academy of innovative science and applied research.



We have been able to consolidate many of our academic activities in terms of completion of course work for Ph.D. students who got registered with Manipal University. As per the guidelines of DSIR, we have constituted a Research Advisory Committee at PPISR under the Chairmanship of Dr. Prahlada, Vice Chancellor, Defence Institute of Advanced Technology, Pune and other eminent scientists as distinguished members.

The Institute has made a significant progress in terms of getting sponsored research projects from Industry. Based on our successful completion of the project, M/s. GTC Technology, USA has extended the project for one more year on catalyst development for aromatics production. Under the collaborative programme between GTC and PPISR, we have been able to develop zeolite based catalyst from lab scale to scaled up level and also testing of scaled up catalyst using Catalyst Testing Unit for the Toluene Methylation processes technology. We look forward for commercial exploitation of this catalyst and process technology in the near future by M/s. GTC Technology, USA. Similarly, M/s. Shell Technology India and Hindustan Petroleum Corporation Ltd Corporate R&D Centre have also sponsored research projects on the development of catalyst for hydrocarbon conversions.

In addition, our faculty members have received sponsored projects from DST, VGST, DBT and BRNS. Our Institute has published more than 15 research papers in internationally reputed journals. Based on our ongoing research projects, our faculty members and research scholars have all attended various National and International conferences and have won best presentation awards. Several distinguished Professors and scientists from both India and abroad visited our Institute and have given lectures.

We have also taken several collaborative research porgrammes with renowned institutes like Indian Institute of Science, National Center for Catalysis Research - Indian Institute of Technology, Madras, The National Institute of Technology, Surathkal and also many engineering colleges and Universities in Karnataka.

The science outreach programmes like Summer School for undergraduate students have been successful. Several young INSPIRE Fellow students from various colleges have spent their vacation to carry out short term projects with our faculty members.

We are confident with the enthusiastic support of Admar Mutt Education Foundation and Trustee members, ands also unstinted support and blessings from our President H. H. Vishwarpriya Theertha swamiji, PPISR will be poised for growth from strength to strength.

Dr. A. B. Halgeri, Director, PPISR

## 3. Board of Trustees

- 1. H. H. Sri Vishwapriya Theertha Swamiji, Chief Pontiff of Admar Mutt
- 2. Sri Rajendra J. Hinduja, Industrialist, Bengaluru
- 3. Prof. K. J. Rao FASc, FNA, FNASc Professor, SSCU, IISc, Bengaluru
- 4. Sri. B. R. Prabhakara, (Rtd.) Former Chief Secretary Govt of Karnataka
- 5. Sri. Laxmisha G. Acharya, Industrialist
- Prof. P. Rama Rao FASc, FNA, FNASc, Ex. Secretary, Ministry of Science and Technology, GOI
- 7. Sri. K. R. Prasad, Advocate, Bangaluru
- 8. Dr. U. Shankar Rao, Medical Director, National Medical Hospital, Chennai.
- 9. Dr. Gautham Nadig, Director, Metahelix Life Sciences Pvt Ltd
- 10. Dr. V. R. Prahalada, Vice Chancellor, Defence Institute of Advanced Technology, Pune.
- 11. Dr. K. Srihari (Hon. Secretary, AMEC and AMEF) Professor (Rtd), UAS, Bengaluru
- 12. Sri. M. Ashok Kumar (Hon. Treasurer) Chartered Accountant, Bengaluru.

## 4. Research Advisory Committee

A Research Advisory Committee (RAC), consisting of eminent scientists in their respective fields, was constituted in Aug 2012 in order to provide technical guidance to the faculty members on the general direction of research being pursued. We are gratified that Prof. Prahlada has kindly consented to chair the RAC.

The following are the present RAC members:

- 1. Dr. Prahlada, Chaiman, Vice Chancellor, Defence Institute of Advanced Tecnology, (Deemed University)
- 2. Prof. G.U.Kulkarni, Member, Professor, Chemistry and Physics Materials Unit, Jawaharlal Nehru Center for Advanced Scientific Research,
- 3. Prof.T.N. Guru Row, Member, Professor, Solid State an Structural Chemistry Unit Indian Institute of Science
- 4. Prof. N.Kumar, Member, Emeritus Professor, Raman Research Institute
- 5. Prof. T.M. Aminabhavi, Member, CSIR Emeritus Scientist, Cavendish Lab, Cambridge University, U.K. AICTE, Emeritus Fellow
- 6. Prof. A Jagannadha Rao, Member, Professor, Rajaramanna Fellow;DST, Department of Biochemistry, Indian Institute of Science
- 7. Prof. K.R.Krishnamurthy, Member, Chair Professor in Catalysis, National Centre for Catalysis Research
- 8. Prof. S. Ramakumar, Member, Professor, Bio Informatics Centre, Indian Institute of Science
- 9. Prof. C. Sivaram, Member, Indian institute of Astrophysics
- 10. Prof. A.B. Halgeri, Member Secretary, Director, Poornaprajna Institute of Scientific Research

The first general RAC meeting, presided by the Chair, was held on Nov 6, 2012, following which RAC meetings were separately held for the institute's three divisions.

## 5. Administration

#### 5.1 Director and Financial Advisor

- Director: Prof. Anand B. Halgeri e-mail: abhalgeri@gmail.com Phone: 080-2361 1836
- Financial Advisor: Sri P.Sreenivasa Rao, Former Sr. Dy. General Manager, Finance and Vigilance, Bharat Electronics Ltd. Bengaluru.

#### 5.2 Administrative Staff

- 1. Administrative Officer: Mr. Kishore L. Gaikwad E-mail: admin@poornaprajna.org
- 2. Accountant: Mr. Nagarajan E-mail: finance@poornaprajna.org
- 3. Administrative Secretary: Mrs. Latha Srinivasan E-mail: latha@poornaprajna.org

#### 5.3 Support staff

- 1. Mr. Subrahmanya A. (Electricals)
- 2. Mr. Praveen Kadam (Transport)
- 3. Mrs. Nagamma (Office)
- 4. Mr. Shashidhara (Canteen)
- 5. Mr. S. Jagadeesha (Canteen)

## 6. Adjunct and Honorary Faculty

#### 6.1 Adjunct faculty

- 1. Prof. S Asokan, IISc (Glasses & Sensors)
- 2. Prof. Y S Bhat, BIT (Catalysis)
- 3. Prof. Dipshikha Chakravortti, IISc (Biology)
- 4. Prof. T N Guru Row, IISc (Crystallography)
- 5. Prof. S A Shivashankar, IISc (Thin films)
- 6. Prof. B. S. Ramchandra, CFRCE, Bangalore (General relativity)
- 7. Prof. R. Srivatsa, Brainstars, Bangalore (Liquid crystals)
- 8. Prof. Suryaprakash, IISc (NMR Studies)

#### 6.2 Honorary faculty

- 1. Prof. T. M. Aminabhavi, UGC Emts Scientist (Polymers)
- 2. Prof. B.S. Jaiprakash, BIT/IEHMM (Catalysis)
- 3. Prof. K.J. Rao, IISc (Glasses & Ceramics)
- 4. Prof. K. Sadashiva, (Rtd.) RRI (Soft condensed matter)
- 5. Prof. K.G. Satyanarayana, Ex.Director, RRL (Polymers)
- 6. Prof. N.J. Shetty, Bangalore University (Biology)

## 7. Doctoral Advisory Committee

Per the rules of Manipal University, with whom PPISR has an MOU for award of PhD degrees, each student is guided by a panel of two or more eminent scientists, who constitute a Doctoral Advisory Committee (DAC) for the student. Here we list together our esteemed DAC members (in alphabetical order).

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

## 8. About the Institute

#### 8.1 History and Mission

PPISR was conceptualized and founded by late HH Sri Vibudesha 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 27 Poornaprajna Education Institutions which have earned a name for themselves in providing quality education at school and college levels. A board of trustees consisting of eminent personalities was constituted to oversee

the growth of PPISR. Since March 2010, 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.

During March 2010, Dr. Halgeri, an eminent scientist from Reliance Petrochemicals, one of Indias top industries, took charge as Director of PPISR. He along with the support of Prof. K. J. Rao, Emeritus Scientist at IISc, pioneered the expansion of PPISR into Materials Science and Biological Sciences departments. The research campus at Bidalur went through phenomenal changes in terms of infrastructure and procurement of equipment in the last two years. A Laboratory dedicated to Materials Science has been built and inaugurated by the present Chairman, Sri Vishwapriya Theertha Swamiji. The Biological Sciences division has been growing with the induction of two faculty members and procurement of instruments, chemicals etc., for pursuing molecular biology, mycology and protein crystallography research.

Initially in order to initiate research programmes in Materials and Biological sciences at the centre about 14 distinguished professors from other renowned institutes IISc, RRI, BIT, Bangalore University etc, graciously agreed to be associated with PPISR as adjunct and honorary professors. New faculty appointments have been made and new research directions identified. A number of young student researchers have been selected to pursue their doctoral studies at PPISR.

Currently in PPISR, there are three divisions, (A) Theoretical Sciences, (B) Materials Sciences, and (C) Biological Sciences where research programmes of advanced nature are in progress. The research laboratories are now equipped with state of the art instruments to give every advantage to the students and faculty pursuing research here. In addition to research, PPISR has ambitious plans for outreach activities to develop innovative and imaginative platform for pedagogy aimed at school and college students and teachers.

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

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

#### 8.2 Contact details

The institute's city office, which is suitable for correspondence, can be reached at:

Poornaprajna Institute of Scientific Research No 4,16th Cross, Sadashivnagar, Bangalore- 560 080 Karnataka, India. Phone: 080-2361 1836

The main campus contact details are:

Poornaprajna Institute of Scientific Research Poornaprajnapura, Bidalur(post), Near Woodrich, Devanahalli, Bangalore - 562 110 Karnataka, India. Telephone: 080-2760 7242

Website: http://ppisr.res.in The Administrative Officer, Mr. Kishore, may be reached at admin@poornaprajna.org

# 9. Division Structure, Faculty and Students

#### 9.1 Materials Science

<b>Dr. A B Halgeri</b> (Catalysis) Professor and Director	
<b>Dr. A V Raghu</b> (Polymers), Asst. Professor	Mr D P Suhas (Research Scholar)
<b>Dr. G V Shanbhag</b> (Catalysis), Asst. Professor	Dr S Ramesh, Postdoc Mrs. Swetha Sandesh (Research Scholar, SRF) Mr Vijay S Marakatti (Research Scholar) Mr Janardhan H L (Research Scholar) Mr Satish Burla (Project Assistant) Mr. Prashant (Project Assistant)
<b>Dr. Nalini G Sundaram</b> (Nanomaterials), Asst. Professor	Ms S. M. Swetha (Research Scholar, JRF) Mr R Srinidhi, Research Scholar
<b>Dr. Sanjeev Maradur</b> (Catalysis), Asst. Professor	Mr. Manjunathan P. (Project Assistant)

### 9.2 Biological Sciences

<b>Dr. K Ananda</b> (Mycology), Asst. Professor	Mr L Sathish (Research Scholar), Ms N. Pavithra (Research Scholar)
<b>Dr. U A Ramagopal</b> (Structural Biology), Asst Professor, Ramalingaswami Fellow	Dr Raghurama P Hegde (Research Associate) Ms. G C Pavithra (Research Scholar)
<b>Dr. Prasad Koka</b> (HIV/AIDS research), Assoc. Professor, Ramalingaswami Fellow	Dr R. Bharati (Research Associate)

#### 9.3 Theoretical Sciences

**Dr. Sujit Sarkar** (Quantum Many body physics), Asst. Professor

**Dr. R Srikanth** (Quantum Information and Foundations of Quantum Mechancs), Asst. Professor

**Dr. S G Bhargavi** (Astronomy & Astrophysics), (Hon) Asst. professor

Mr Omkar Srikrishna (Research Scholar), Mr Aravinda Srinivasamurthy (Research Scholar, JRF)

## 10. Materials science



#### 10.1 Introduction

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

- 1. To forge a fruitful academia-industry partnership by innovating, designing and developing novel multifunctional materials that have wide-ranging applications, in catalysis, nanotechnology, etc.
- 2. To develop a strong doctoral program to train students by fostering excellence and original thinking.

The department engages with other national academic institutions through collaborations, education training and outreach activities. The broad areas of the department include: (1) Novel functional materials; (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.

#### 10.2 Academic and Research Highlights

Other work completed in the last two years includes: Synthesis and characterization of novel polyurethanes having practical applications; studies on properties of graphene/waterborne

polyurethane nanocomposites; development of graphite oxides as effective fire retardants of epoxy resin.

The Catalysis group at PPISR has expertise in pore engineering of zeolites and other microporous materials for shape-selective organic transformations and hydrothermal synthesis of zeolites and mesoporous Materials and their applications in green chemistry. The group is also working on designing eco-friendly solid catalysts for glycerol transformations to value-added products such as glycerol carbonate, acrolein, solketal, acetins etc. and biodiesel synthesis from transesterification of vagitable oils. The group especially working on designing new heterogeneous acid and base solid catalysts and their utilization in organic transformations such as Prins cyclization, Baeyer-Villiger reaction and photo catalysis. Preparation of inorganic nanomaterials, mostly oxides, tungstates, oxychlorides, phosphates, organometallic precursors etc., under optimum, easier conditions Characterization of these nanomaterials using tools like PXRD, TEM, DSC etc. Measurement of photoluminescence, photocatalytic activity etc. Expertise in studying the detailed crystal structure of the phase using powder X-ray and powder Neutron diffraction techniques Finally correlating the structure with the property to generate materials with improved properties.

Development of method of low-cost carbon fiber technology; synthesis of highly waterselective sodium alginate-based inorganic-organic hybrid membranes for pervaporation dehydration of ethanol.

#### **10.3** Faculty Profiles

#### 10.3.1 Dr. A. B. Halgeri



Professor Director, PPISR.

#### **Educational Qualifications**

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

#### Broad areas of research

He has extensively worked on Alkylation of Aromatics using modified Zeolites as Eco-friendly catalysts. He has developed Zeolite based catalyst for Alkylation of Toluene to produce selectively para-Xylene which is raw material for polyester industry and transferred for the first time to advanced country to M/s. GTC Technology Inc. USA. Subsequently, super selective pore size engineered modified Zeolite catalyst has been successfully developed and commercialized for the manufacture of speciality 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, Kolkatta.
- 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.
- Awarded as "Pride citizen of Baroda" in recognition of significant contribution for Science & Technology from Community Science Centre/Rotary Club of Baroda - 2008.
- 7. He has been advisory member of several professional bodies, Department of Science & Technology, CSIR, IOCL (R&D) and Reliance Industry. He has traveled widely and presented several invited lectures in both National and International symposia.

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

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

#### Students

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

#### Projects

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

#### 10.3.2 Dr. A. V. Raghu



#### Assistant Professor

#### Education and work experience

- 1. Ph. D. in polymer science, Karnatak University, Dharwad
- 2. Lecturer, centre of Excellence in polymer science, Karnatak University, Dharwad.
- 3. Postdoctoral Scientist, Department of Chemistry, University of Ulsan, South Korea.
- 4. Manager, Reliance Industries Limited, Mumbai, India

#### Areas of interest

- 1. Synthesis and characterization of various types of polymeric nanocomposite for PEMFC and Pervaporation separation applications;
- 2. Synthesis of nanographene / GO based waterborne polyure thanes for electrostatic charge applications.
- 3. Synthesis and characterization of Novel Polymers for various applications.
- 4. Synthesis and antibacterial study of some novel Indole derivaties.

Total no of publications in international journals: 27 + 1 review article and two communicated. Participation in workshops, conferences and symposiums: 17

#### Awards and recognitions:

- Member of Intl. Scholarly Research Network (ISRN) Nanomaterials Editorial Board
- Editorial Board, Elsevier journal Drug Invention Today (www.ditonline.org/edboard)
- International Scholarly Research Network (ISRN) Polymer Science Editorial Board
- Scientific reviewer for international journals like ACS Nano, Journal of Polymer Science Polymer Chemistry Part A, Journal of Applied Polymer Science, Journal of Membrane Science, Carbohydrate Polymers, Polymer International, European Polymer Journal, Desalination, etc.,
- Award from SEED MONEY FOR YOUNG SCIENTIST 2011-12 From VGST, Government of Karnataka.

#### Students

Mr. Suhas D. P. (Research scholar)

#### **Current Projects**

 Poly(vinyl alcohol)/H-ZSM5 Zeolite-based Mixed Matrix Composite Membranes for Pervaporation Dehydration of Alcohols: Effect of Silica Alumina Ratio (Project Completed) Principal Investigator: Dr. A.V. Raghu Student: Mr. D.P. Suhas

Zeolites are micoporous alumina silicates and their water interaction can be changed by varying the Si/Al ratio of their composition, higher silica in the frame work are hydrophobic and lower ones are hydrophilic. In this work mixed matrix membranes (MMMs) of poly(vinyl alcohol) (PVA) loaded with H-ZSM5 particles having different silica alumina ratio (SAR) were prepared and used in the perevaporation (PV) dehydration of ethanol and isopropanol for their aqueous mixtures. The membranes were characterized by XRD, FTIR, FE-SEM, DSC and contact angle measurements, which reviled good physico-chemical interactions between PVA and H-ZSM5. The membrane selectivity to water increased along with a slight increase in the total flux by decreasing the SAR of H-ZSM5. Selectivity for isopropanol-water mixture was found to be higher than ethanol-water mixture. Such a gradual improvement in membrane performance with decreasing SAR of the zeolite is attributed to favourable interaction between the zeolite particles and the polymer matrix. Selectivity for isopropanol-water mixture was found to be higher than ethanol-water mixture.

Current status: Paper communicated to a peer reviewed international journal

 Graphene-loaded sodium alginate nanocomposite membranes with enhanced isopropanol dehydration performance via pervaporation technique. (Project completed) Principal Investigator: Dr. A.V. Raghu Student: Mr. D.P. Suhas

In this work the versatility of graphene is extended to perevaporation applications. Graphene oxide-loaded sodium alginate (NaAlg) nanocomposite membranes have been prepared to enhance the pervaporation (PV) dehydration of isopropanol. The effect of graphene loading on physico-chemical properties, micro-morphology and barrier performance of the derived nanocomposite membranes was investigated as a function of temperature and feed water composition of isopropanol mixture. Interaction of graphene with NaAlg matrix as well as water and isopropanol seem to influence the thermal, kinetic and Arrhenius activation energy parameters. At the lowest concentration of grapheme, the membrane performance was optimum, which is the most desirable factor in mixed matrix preparation. The sorption interaction between membrane and polymer were calculated by Flory-Huggins and kinetic parameters by Ficks law.

Current status: Paper communicated to a peer reviewed journal

3. Activated clay loaded sodium alginate based mixed matrix membranes for dehydration of isopropyl alcohol via perevaporation: Insights of thermodynamic and kinetic interaction parameters (near completion) Principal Investigator: Dr. A.V. Raghu Student: Mr. D.P. Suhas

Clays are important class of layered silicates. Their crystal structure consists of an alumina octahedra sandwiched between two sheets of silica tetrahedra interconnected by sharing of O2- atoms at polyhedral corners and edges. Mountmorillonite is important smectic type

clay widely used in mixed matrix preparation. In the present work the clays are activated by treating with para toluene sulfonic acid (p-TSA), which increased both surface area and hydrophilicity of the material. After incorporating, the activated clay into sodium alginate matrix the resulting membranes has shown enhanced permeance and selectivity as compared to unmodified clay. Membrane characterizations using FTIR, XRD, FE-SEM, TGA revel good physico-chemical interaction between filler and polymer.

Current status: Calculation of thermodynamic and kinetic interaction parameters based on the results, along with writing the manuscript concludes the work.

#### 10.3.3 Dr. Ganapati V. Shanbhag



#### Assistant Professor

#### Academic Qualifications

- 2010–Present: Asst. Professor, PPISR, Bangalore, India
- 2008–2010: Research Scientist, Dept. of Chemistry, National Taiwan University and National Center for Theoretical Sciences, Taiwan.
- 2002–2008: Ph.D. National Chemical Laboratory, Pune India (Degree by University of Pune).
- 2000–2001: Research Associate in ICI India Ltd, Mumbai, India
- 1999–2000: Lecturer, M.M Arts and Science College, Sirsi, Karnataka, India
- 1999: M.Sc. Organic Chemistry, Karnatak University, Dharwad

#### **Broad Areas of Research:**

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

Total no of publications in international journals: 19 Participation in workshops, conferences and symposiums: 12

#### **Representative Publications**

- "Sulfated zirconia; an efficient and reusable acid catalyst for the selective synthesis of 4phenyl-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
- "Mesoporous sodalite: A novel stable solid catalyst for base catalyzed organic transformations", Ganapati V. Shanbhag, M. Choi, J. Kim and Ryong Ryoo, Journal of Catalysis, Volume 264, 2009, 88-92.
- "Chemoselective synthesis of -amino acid derivatives by hydroamination of activated olefins using AlSBA-15 catalyst", G. V. Shanbhag, S.M. Kumbar and S.B. Halligudi, Journal of Molecular Catalysis A: Chemical, Volume 284(1-2), 2008, 16-23.

- "Copper(II) ion exchanged AlSBA-15: a versatile catalyst for intermolecular hydroamination of terminal alkynes with aromatic amines", Ganapati V. Shanbhag, Trissa Joseph and S. B. Halligudi, Journal of Catalysis, Volume 250 (2), 2007, 274-282.
- "Heterogeneous intermolecular hydroamination of terminal alkynes with aromatic amines", Ganapati V. Shanbhag, S.M. Kumbar, T. Joseph and S.B. Halligudi, Tetrahedron Letters, Volume 47 (2), 2006, 141-143.

#### Students

Research Associate:

1. Dr. Ramesh S.

**Research Scholars:** 

- 2. Mrs. Swetha Sandesh
- 3. Mr. Vijaykumar S. M.
- 4. Mr. Janardhan H. L

**Project Assistants:** 

5. Mr. Satish Burla

M.Tech Project student:

6. Mr. Prashant Kumar

#### **Review meetings**

- 1. Review meeting of GTC project: Dr. Ding ZhongYi, Project manager, GTC, USA visited PPISR on 03-06, November 2013. The project work was reviewed with the meetings between Dr. ZhongYi and catalysis group of PPISR. The progress in the project so far was found to be satisfactory.
- 2. Quarterly review meeting of Shell sponsored project: PPISR team of Dr. Halgeri, Dr. Shanbhag, Dr. Sanjeev and Dr. Ramesh went to Shell Technology Centre, Bangalore on 12-1-2013 for a project review meeting with Shell team. The research work conducted so far was presented before the Shell team. Shell expressed their satisfaction over the progress achieved so far and also gave useful suggestions to further improve the work.
- 3. Quarterly review meeting of HPCL sponsored project: A quarterly review meeting was held between the PPISR and HPCL in Feb-2013. The students, Mr. Janardhan and Mr. Vijaykumar presented the literature survey and preliminary results on the project. HPCL team consisted of Dr. N.V. Choudhary (GM, R&D), Dr. P.V.C. Rao (DGM, R&D), Dr. R. Ravishankar (Sr. Manager) and Dr. Ramesh (Dy. Manager). HPCL team, gave several suggestions on further research work and expressed their happiness on research capabilities of PPISR.

#### **Current Projects**

Industrial projects:

 Design and development of a catalyst and process for selective alkylation of aromatics (Industrial Project sponsored by: GTC Technology, USA Principal Investigator: Dr. Ganapati V. Shanbhag Co-investigator: Dr. Sanjeev Maradur Project Assistants: Mr. Satish Burla, Mr. Manjunathan P.

The second phase of the project focused on the development of a novel catalyst for vapor phase alkylation of aromatics to produce alkylated aromatics with high conversion, selectivity and longer catalytic lifetime. The work mainly concentrated on industrial requirement of catalyst and process like mechanical strength of the catalyst in terms of attrition loss and crush strength and impurities present in reaction products such as oxygenates, ketones, chloride and acidity of effluent water.

The scale up studies of catalyst preparation was carried out in Shenyang, China by Dr. Shanbhag during 16-23, Aug 2012 where many different catalyst formulations were made in KG level. Their crush strength and attrition loss were found to be satisfactory. Catalyst evaluation of those catalysts was done later at PPISR. In the meantime, about 400 h time on stream was demonstrated with PPISR made silica bound catalyst with one regeneration after 200 hours. The catalyst showed marginal deactivation under high performance conditions.

Catalyst scale-up work for GTC project was started in October 2012. The GTC USA donated few instruments to PPISR namely, Keading machine, Electric extruder, Crush strength instrument and Attrition measurement unit. All these instruments are useful to make the catalyst extrudates in a kg level and their testing for crush strength and attrition loss. On November 3-6, 2012, Dr. Ding ZhongYi from GTC, USA visited PPISR and reviewed the project activities. After receiving the raw materials and equipments, catalyst scale-up preparation work was started. As many as 60 batches with different compositions have been prepared and tested for physical and chemical properties. Selected catalyst were short listed and evaluated for their performance in catalyst testing unit. Hydrothermal ageing test set-up was established and few catalysts were evaluated for hydrothermal stability.

After optimization of catalyst recipe, good crush strength of 8 Kg and low attrition loss of i 2% was achieved. The catalyst showed very good hydrothermal stability at 600 C for 100 hours without loss of mechanical strength and catalytic activity. Then a long time on stream run for 300 hours was carried out with a selected catalyst. Catalyst showed a long life of 300 hours. Subsequently, one more catalyst with different composition was tested for 250 hours and 200 hours run under different reaction parameter. This catalyst also showed a high stability and performance. One catalyst recipe is finally selected for next scale-up work. Teleconference between GTC, USA and PPISR is held weekly thrice to review the project work. GTC expressed their happiness with the research work and results generated at PPISR so far.

2. Post-synthesis modification and surface treatment of some solid catalysts (Sponsored by: Shell Techonology Center, Bangalore Principal Investigator: Dr. Ganapati V. Shanbhag Co-investigator: Dr. Sanjeev Maradur Research Associate: Dr. Ramesh S.

A flow reactor was set up to execute this project. Shell Technology Centre provided materials which were to be modified and pore engineered. Catalyst modification work started by modification of catalysts and evaluation of its performance by probe reaction, disproportionation. A high selectivity for required products is achieved and selectivity ratio was measured to estimate the extent of modification.

Reports have been sent to Shell Technology Centre every month and a Teleconference is held between Shell and PPISR every month to review the project work. On 12-1-2013, PPISR team of Dr. Halgeri, Dr. Shanbhag, Dr. Sanjeev and Dr. Ramesh went to Shell Technology Centre, Bangalore for a project review meeting with Shell team. The research work conducted so far was presented before the Shell team. Shell expressed their satisfaction over the progress achieved so far and also gave useful suggestions to further improve the work. The Shell team has expressed their satisfaction on the progress made so far in this project. The shell also insisted to follow the safety procedures while doing the project work. Accordingly the safety equipments such as personal gas detector, eye wash and shower, fire extinguishers, smoke alarm and gas leakage alarm etc have been installed at PPISR.

3. Development of Zeolite Modified Catalysts for the Hydrocarbon Conversions such as light naphtha aromatization and side chain alkylation of toluene. (Sponsored by: HPCL R&D Centre, Bangalore Principal Investigator: Dr. Ganapati V. Shanbhag Co-investigator: Dr. Sanjeev Maradur Senior Research Fellow: Mr. Vijaykumar, Mr. Janardhan

Project work started from 1st of November 2012 by the recruitment of project assistants Mr. Vijaykumar and Mr. Janardhan to execute the project work. Initially, required chemicals, glasswares and small equipments have been purchased. A flow reactor has been set up by procuring components such as syringe pump, tube furnace, quartz reactor, temperature controller etc. and assembled on a scaffold. Hexane is used as model compound to study aromatization of light naphtha for HPCL sponsored project. Catalyst evaluation and quantification method for this reaction were standardized. ZSM-5 zeolite was found to be better than H-Y due to its intersecting pore system, where cracked products oligomerize and cyclize. These intersecting channels are absent in H-Y hence cracking products can only be observed in HY. Hexane and pentane were taken as model compounds for light naphtha and compared for performance. Hexane and pentane showed similar aromatic yield. Hence for further studies were carried out with n-hexane as feed.

Toluene side chain alkylation to styrene project was started as a part of HPCL industrial sponsored project. The project main objective is to produce selectively styrene from toluene and methanol as feed using basic catalyst in vapor phase reaction. Styrene is an industrially important chemical that is used for the production of plastics and rubbers. The project started with extensive literature survey based on research publications and patents. Preliminary experiments were carried out to reproduce old literature methods as benchmark. Further on the screening of novel catalyst for the following reaction is under progress. A quarterly review meeting was held between the PPISR and HPCL in Feb-2013. The students, Mr. Janardhan and Mr. Vijaykumar presented the literature survey and preliminary results on the project. HPCL team, gave several suggestions on

further research work and expressed their happiness on research capabilities of PPISR.

Research projects:

- 1. Sulfated zirconia- an efficient and reusable solid acid catalyst for selective synthesis of 4-phenyl-1, 3-dioxane by Prins reaction of styrene (project completed)
  - Principal Investigator: Dr. Ganapati V. Shanbhag

Student: Mr. Vijaykumar SM

Prins cyclization of styrene with paraformaldehyde was carried out over sulfated zirconia (SZ) catalyst in liquid phase. The 4-phenyl-1,3-dioxane obtained from Prins cyclization of styrene is applied in industry as high boiling solvent, plasticizer, curing agent and pigment dispersant. The SZ catalysts were synthesized by precipitation method with different sulfur impregnation and characterized by XRD, FT-IR, Nitrogen sorption, NH3-TPD. The SZ showed best performance among different types of acid catalysts. The acidity of SZ optimized by different concentrations of H2SO4 treatment influences the selectivity for dioxane. The sulfur loading, nature of solvent, temperature, catalyst amount, mole ratio and reusability of catalyst were investigated. The SZ catalyst synthesized by impregnating 2N sulfuric acid was found to be highly selective for the synthesis of 4-phenyl-1,3-dioxane (93%) with almost complete conversion of styrene (100%). The catalyst was recycled thrice with negligible decrease in the yield of 4-phenyl-1,3-dioxane.

Published in Applied Catalysis A journal (2012) (Publisher: Elsevier, Impact factor: 3.9)

2. Tin(II)hydroxychloride : A novel heterogeneous solid acid catalyst for the condensation reactions (completed)

Principal Investigator: Dr. Ganapati V. Shanbhag

Student: Mr. Vijaykumar SM

The Prins reaction of -pinene with paraformaldehyde results in the formation of nopol, an unsaturated primary alcohol.Nopol finds wide applications in agrochemical industry as a pesicide and as a fragrance in soap/detergent industries. The condensation of ethyl acetoacetate with ethylene glycol to produce the fructone is an example of ketalization. Fructone is used as a flavouring agent with apple scent. Claisen-Schmidt condensation of 2-hydroxy acetophenone with benzaldehyde is another condensation reaction results in the formation of flavanone.

The flavanoids find their wide application in the pharmaceutical industry as anti cancer, antiin-flammatory, anti-bacterial and anti-AIDS pharmacological activities. In the present study we describe the synthesis, characterization and application of Sn(OH)Cl as a heterogeneous catalyst. The characterization by FT-IR pyridine adsorption and 1H MAS NMR showed the presence of Brnsted acidity in the catalyst.



Brönsted acidity in Sn(OH)Cl is attributed to a strong hydrogen bonding between -OH and Cl groups. The Sn(OH)Cl is a novel and highly efficient acid catalyst for the selective synthesis of nopol, flavanone and fructone by respective condensation reactions. The higher activity of Sn(OH)Cl compared with Sn2(OH)2O, SnO and SnO2 is due to the presence of Brnsted acidity. The catalyst is truly heterogeneous and can be used up to 3 recycles with minimal decrease in activity.

Publication: RSC Advances (2013, Under revision).

3. Utilization of chemicals from biorefinery: Conversion of bioglycerol to glycerol carbonate by carbonylation and transesterification reactions (project completed) Principal Investigator: Dr. Ganapati V. Shanbhag

Student: Mrs. Swetha Sandesh

Glycerol carbonate is an important derivative which has a high potential application in polymer and cosmetic industries. It has been synthesized using glycerol and dimethylcarbonate by transesterification reaction using KF supported catalyst. All the synthesized catalysts were characterized by XRD, AAS, N2 adsorption and CO2-TPD measurements. The physicochemical properties of the catalyst were correlated with the activity and selectivity. KF was impregnated on various oxides and non-oxide supports like Al2O3, SiO2, ZnO, ZrO2, H-beta, and carbon to study the influence of the support on the catalytic performance. The generation of basic sites by KF depends upon the extent of KF interaction with the support. The KF/Al2O3 catalyst with optimized amount of 3.8 mmol KF, gave the highest activity with 95.8 % glycerol conversion and almost 100 % selectivity for glycerol carbonate. The catalyst showed better performance when compared to conventional solid base catalysts such as MgO, CaO and hydrotalcite.

Paper communicated to a peer reviewed journal

4. Pore engineering of ZSM-5 zeolite by phosphorous oxide modification for the shape selective synthesis of p-diethylbenzene (PDEB) by alkylation of ethylbenzene with ethanol Principal Investigator: Dr. Ganapati V. Shanbhag

Student: Mr. Janardhan HL

PDEB is an important chemical used in the separation of p-xylene by PAREX process. ZSM-5 is a medium pore zeolite with pore size similar to the molecular size of PDEB. A novel modification of ZSM-5 is going on using phosphorous compounds to achieve high selectivity for PDEB. Catalysts with different P content were prepared and characterized with XRD, FTIR and 31P MAS NMR and TPD of ammonia measurements. The reaction was carried out in fixed bed, down-flow, tubular, quartz reactor in continuous vapor phase conditions. Preliminary studies indicated that shape selectivity improved with phosphorous modification and about 95% PDEB selectivity was achieved. Selectivity for PDEB improved further to 98% after doing silvation on P-modified ZSM-5 catalyst.

5. Pore engineering of ZSM-5 zeolite by phosphorous oxide modification for the shape selective transformation of 2-Methoxy naphthalene acetylation with acetic anhydride Principal Investigator: Dr. Ganapati V. Shanbhag Student: Mr. Janardhan HL

Acetylation of 2-methoxy naphthalene yields kinetically preferred major product 1-acetyl-2-methoxynaphthalene whereas 2-acetyl-6-methoxynaphthalene is a pharmaceutically important intermediate used in the manufacture drug named naproxen. One step selective acylation to produce 2-acetyl 6-methoxynaphthalene is an important transformation.

Reaction was carried out with structured and non-structured catalyst such as zeolite beta, clay etc. Catalyst selectivity towards the desired product decreases with decrease in acid site strength and availability of external acid sites. Phosphate modification of zeolite beta with different concentrations showed decrease in selectivity for 2-acetyl-6methoxynaphthalene and the conversion decreased with increase in phosphate concentration. External surface dealumination of zeolite beta with EDTA and silanation to understand the conditions to achieve maximum selectivity is under study.



Glycerol transformations to value added products



Product analysis by GC.

6. Gas-phase dehydration of glycerol over molybdenum trioxide supported on silica catalyst for sustainable synthesis of acrolein

Principal Investigator: Dr. Ganapati V. Shanbhag

Students: Mr. Satish B (1 year M.Tech Project)

Glycerol is a waste byproduct of biodiesel synthesis by transesterification of vegetable oils. The project aims at converting glycerol into value added products. Glycerol dehydration reaction yields acrolein which is used in the production of acrylic acid esters, superabsorber polymers and detergents. After screening different solid acid catalyst is is found that MoO3/Silica is a best catalyst in terms of activity and lifetime. Effect of reaction parameters such as temperature, mole ratio and WHSV is being investigated,

The thesis prepared based on the above work by Satish B was accepted as a part of M.Tech. (Chemical Engineering) degree in Gayathri Vidya Parishad College of Engineering (GVPCE), Vizag, Andra Pradesh.

7. Zinc-tin mixed hydroxide a novel promising catalyst for the synthesis of glycerol carbonate using glycerol and urea

Principal Investigator: Dr. Ganapati V. Shanbhag Student: Mrs. Swetha Sandesh

A novel solid bifunctional catalyst called zinc-tin mixed hydroxide was designed for glycerol carbonate (GC) synthesis by transcarbonylation of glycerol with urea. Glycerol carbonate has potential application in various fields like pharmaceutical, polymer and paint industries. Urea is a cheap and abundant raw material as a carbonylating agent. In this project, Zinc-tin mixed hydroxide has been designed and proposed as a solid bi-functional catalyst for the synthesis of glycerol carbonate by glycerol and urea. The catalyst was synthesized and characterized by various techniques such as XRD, N2 sorption, TGDTA, FTIR, SEM etc. We achieved excellent glycerol conversion (98%) with 97% glycerol carbonate selectivity. It also showed good reusability. The acidity and basicity measurements of this catalyst to show its bifunctional active sites are under progress.

8. Novel organic substituted heteropoly acid catalyst for condensation of glycerol with acetone to form solketal at room temperature

Principal Investigator: Dr. Ganapati V. Shanbhag

Student: Mrs. Swetha Sandesh

Synthesis of Solketal (2,2-dimethyl-4-hydroximethyl-1,3-dioxolane) has been performed using acetone by condensation reaction using organic-inorganic hybrid catalyst. This catalyst, tetra propyl ammonium exchanged heteropoly acid has been synthesized for the first time and reported as a solid acid catalyst. The condensation reaction of glycerol with acetone was carried out under room temperature liquid phase batch reactor. The catalyst was prepared and characterised by using various techniques like XRD, FTIR, TGA/DTA, C, H, N analyzer and morphological properties by SEM and BET measurements. Preliminary results with this catalyst showed high glycerol conversion (94%) and also 99.6% of solketal selectivity higher than other well-known acid catalysts like amberlyset-15, montmorillonite K-10, H-beta and Cs/PWA. Further studies on this reaction is under progress.

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

Principal Investigator: Dr. Ganapati V. Shanbhag

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

The aim of the project is to design a novel eco-friendly catalyst for biodiesel synthesis from non-edible oil source. For this purpose waste cooking oil, honge oil and simauruba oil were taken for the study. Initially the reaction was carried out with NaOH, a conventional homogeneous catalyst and optimized reaction conditions and work-up procedure. Several factors such as free acid content of oil, esterification of oil to remove free acids were carried out. Further, several solid basic catalysts such as hydrotalcite, KF/ alumina, KF/ CaO etc were tested for transesterification of waste cooking oil. Further work is under progress.

#### 10.3.4 Dr. Nalini Sundaram



#### Assistant Professor

#### Education and work experience

- 1. Ph.D in Solid State Chemistry ,Indian Institute of Science, Bangalore, India,2003
- Post Doctoral Researcher, Los Alamos National Laboratory, New Mexico and Stanford Synchrotron Laboratory, Stanford, U.S.A 2004-2005
- Post Doctoral Scholar, University of California Santa Cruz, California, U.S.A 2005-2008
- 4. Lecturer at the Materials Science Division, Poornaprajna Institute of Scientific Research, Bangalore 2010-2011
- 5. Assistant Professor, PPISR 2011-
- 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)

#### **Broad Areas of Research**

Our research deals with the study of functional nanomaterials as applied in the energy sector. We study a broad range of materials systems such as:

1. Photoluminescent Materials for Solid state lighting Devices

2. Photocatalytic Materials active under visible light for degradation of dyes and other contaminants

3. Metal Organic Precursors for Optoelectronic devices

#### **Representative Publications:**

- 1. Jiang, F. Bridges, N. Sundaram, D.P. Belanger, I.E. Anderson, J.F. Mitchell, and H. Zheng Study of the local distortions of the perovskite system La1-xSrxCoO3 using the extended x-ray absorption fine structure technique Phys. Rev. B80,144423 2009
- N. Sundaram, Y. Jiang, I. E. Anderson, D. P. Belanger, C. H. Booth, F. Bridges, J. F. Mitchell, Th. Proffen and H. Zheng, Local Structure of La1-xSrxCoO3 determined from EXAFS and neutron PDF studies, Physical Review Letters, 2009, 102, 026401

Awards and Scholarship

- 3. Ombretta Masala; Darin Hoffman; Nalini Sundaram; Katharine Page; Thomas Proffen; Gavin Lawes; Ram Seshadri, Preparation of magnetic spinel ferrite core/shell nanoparticles: Soft ferrites on hard ferrites and vice versa, Solid State Sciences v.8, No.9, 1015-1022,2005
- 4. G. Nalini and T. N. Guru Row, Phase transitions in rubidium hydrogen sulfate: crystal structures at 293K and 200K, Phase Transitions, 2003, 76, 923
- 5. 5. G. Nalini and T. N. Guru Row, Variable temperature X-ray crystal structure analysis of a type I Langbeinite : Rb2Cd2(SO4), Chemistry of Materials, 2002, 14, 4729

#### Students

- 1. Ms. Swetha M. Bhat
- 2. Mr. Srinidhi. R (Joint Student with Prof. Shivashankar, IISc).

#### **Current projects**

1. Design and Development of Nanocrystalline Layered Bismuth compounds for Photocatalytic Degradation of Dyes and Organic Pollutants in the Visible Region: Aurivillius-sillen phases are reported to exhibit photocatalytic activity in the visible region due to their unique layered structure and high chemical stability. Our objectives are to synthesize nanoparticles of these materials and investigate crystal structure and electronic structure analysis for these phases. This would provide insights into the structure- particlephotocatalytic activity and thus help us design different combinations of nanocrystalline A-S phases that show high photocatalytic activity in the visible light region.



2. Synthesis, Crystal Structure and Photoluminescence of Rare Earth Tungstates for Application in Solid State Lighting Devices

(2a) Correlation of crystal structure and PL activity of  $KNdW_20_8$  polymorph-nanoparticles. Solid state lighting devices have received much attention in recent years because of their wide applications and advantages over the conventional light sources. Rare earth doping into a host materials has been exploited intensively since it produces new defects and improves the persistent luminescence. Rare earth phosphors can be separated into two types of emissions; broad band emissions owing to the 4d-5f transition and narrow band emissions owing to the transition between the 4f levels. They are important activators since 4f levels are not influenced by any external crystal field. AR(XO4)2 (A=K,Na; R=Nd; X=W) are multifunctional, disordered materials and their luminescent properties could be designed for solid state lighting devices. Synthesis of bulk and nano alkali metal rare earth doped tungstate nanoparticles is a hot area due to the applications of these nanopowders in solid state lighting (SSL) devices, LEDs etc. For example doping of Eu or Gd in rare earth tungstates would give either enhanced red or green light which is very useful for producing high coloring index necessary for SSL devices.



Tetragonal KNdW<sub>2</sub>O<sub>8</sub>

(2b) Influence of the Alkali metal ion on the Crystal Structure and Photoluminescence of Na(1-x)KxW2O8 (0.2ixi0.8).

Powder sample of NaKNdW was prepared by glycothermal method. Rietveld refinements confirmed the occupancy of Na and K according to stoichiometry. TEM analysis reveal that the average particle size is 145nm. PL measurements shows two peaks of high intensity in the wavelength range of 590-700nm which correspond to the reddish orange region in the visible region. From the PL spectra it can be observed that the 60% K doped composition has the maximum PL. Further doping of K results in decrease in the luminescence indicating that the threshold composition for obtaining maximum PL is Na0.4K0.6NdW2O8. A careful analysis b of bond lengths reveal that the W-O bond is largest for the 60%

Potassium doped composition. Further analysis of the local structure at the K/Na-O stretching frequencies using Raman is in progress to understand the role of the K doping on the PL of these materials. b. Correlation of Crystal Structure and PL Activity of Polymorphs of KNdW2O8 Nanoparticles KNdW2O8 exhibits polymorphism and crystallizes in the tetragonal and monoclinic phases. Our interest is to synthesize nanoparticles of these polymorphs by combustion methods and correlate their crystal structure with their PL activity. Stoichiometric amount of oxidizer and fuel were dissolved in water and heated at desired temperature to in a preheated furnace to get Polymorph A. Phase purity was analyzed by PXRD. It crystallizes in tetragonal phase. Efforts are being made to prepare polymorph B by same method and to compare their PL properties.

## 3. Crystal Structure of Substituted Complexes, $\{Ga_xCr_{1-x}\}\ (acac)_3$ using Single crystal X-ray diffraction Techniques

Metal coordination compounds (containing carbon but no direct metal-carbon bond) e.g., metal -diketonates, metal -diketoiminates, metal alkoxides, metal amides and metal carboxylates have been used as precursors in the CVD process for metal oxides, etc. Among these, metal -diketonates are an often-used class. They have several advantages, viz., low vaporization and decomposition temperatures, non-pyrophoric/non- toxic nature, stable oxidation, hydrolytic and photo-thermal reactions, relative ease of synthesis, and environment-friendly benign by-products. The present project is aimed at developing single-source precursors for the deposition of thin films and nanoparticles of  $(Cr_xGa_{1-x})_2O_3$  (x = 0.10.9).

Single crystals of  $Cr_xGa_{1-x}(acac)_3$ , have been grown, with x varying from 0.1 to 0.9, in steps of 0.1. in 1:1 solution of analytical-grade methanol and acetone. The solution was maintained at 4C for 7 days, whereupon dark brown, needle- shaped crystals resulted. Diffraction data collection was performed on a Bruker-AXS- SMART (CCD 1000) diffractometer, equipped with a cryogenic nitrogen cold stream to prevent loss of solvent and using Mo-Kalpha radiation (0.71073).. The data were collected at 108 (2) K. At present single crystal structure solution and refinement is being carried out using WinGX software. Upto x=30% all the crystals crystallize in the monoclinic system with the centrosymmetric P21/c space group. Preliminary analysis of the x=0.4 composition indicates that this crystallizes in the noncentrosymmetric space group. Further analyses on these samples are in progress. This project is being carried out in collaboration with Professor. Shivashankar, MRC, IISc. Most of the experimental work has been done at IISc.

#### 4. Influence of a Novel Rapid Microwave Assisted Synthesis Method on the Magnetic

Properties Of  $ZnFe_2O_4$  Nano particles- a Combined X-ray and Neutron Diffraction Study Zinc Ferrite,  $ZnFe_2O_4$  (ZFO) is a technologically important multi-functional ceramic that has been studied for its interesting humidity-sensing, oxygen-sensing, photoelectrical and super-paramagnetic properties. As such, at room temperature ZFO, a normal spinel, is antiferromagnetic (AF) below 10 K. The most remarkable observation in these ferrites is the strong dependence of magnetic properties on the cation site occupancy of the material. A novel, rapid microwave irradiation-assisted chemical route has been used by Prof. Shivashankars group at IISc, to prepare ZnFe2O4 nanoparticles, lasting a few minutes, using an ethanolic solution metal  $\beta$ -diketonates as the precursor As magnetic properties of ZFO are determined by site occupancy, even within the same composition, we have employed two different post-synthesis annealing protocols, thereby to alter the degree of inversion and thus the magnetic properties: one, conventional annealing in air (CA), lasting two
hours; two, rapid annealing in air (RA), lasting two minutes. We at PPISR collected high resolution X-ray data on all the samples and carried out occupancy refinements in order to find the inversion parameter that influences the magnetic properties. Neutron data at the Oakridge National Laboratory was also collected and work is in progress to refine the Neutron data and ascertain the inversion parameter unequivocally. This project is being carried out in collaboration with Professor. Shivashankar, MRC, IISc.

### **Future Projects**

1. Influence of Electron Beam Irradiation on the Crystal Structure and Photoluminescence of Rare Earth doped Tungstate Nanophosphors

This project, funded by Board of Research in Nuclear Studies Under the scheme PPA: Application for Research Grants will be initiated in May 2013 The objective of the project is to determine the stability of photoluminescent rare earth doped oxide nanoparticles that could be potentially used as solid state lighting devices in many industries including the nuclear industry. The primary interactions between energetic radiation and inorganic materials result in ionization, where an electron hole pair is produced. Here highly mobile electrons in the valence band are excited to the conduction band. So the production of holes trapped in these materials have been known to cause changes in the device performance[6]. The interaction of the electron with the crystalline lattice depends on the energy and dose rate of the electrons. If the imparted energy is higher than the binding energy of the nucleus in the lattice, the atom is permanently removed from its site, resulting in the appearance of new energy levels in the crystal due to irradiation. In this context, electron beam irradiation of these nanoparticles could change the crystal structure parameters, increase the efficiency of the PL lines, result in the emission of new lines and also thermoluminescent glow depending on the dose rate of the electrons.

2. Synthesis of Nanostructured p-type doped La-based Perovskites for Design of Selective Gas Sensors

Funding agency considered: DRDO, India, for an extramural research grant.

Recently La-based perovskite have been studied for gas sensing applications due their micro structural and morphological stability which helps improve reliability and long-term sensor performance. The focus of our work is to synthesize nano crystalline doped p-type Lanthanum based perovskites using various simple synthetic techniques and check their response to various toxic gases like CO,CO2, NH3, Hydrocarbons. Depending on the response we intend modify and develop the nanostructured perovskite gas sensors by systematically doping at the A and B site and bring about selective sensitivity to one particular gaseous species. We also intend to investigate the effect of doping and particle size on the subtle crystal structural changes and on the sensitivity of the sensor. The inputs obtained from the crystal structure analysis would be extremely valuable to design gas sensors of perovskite materials with similar crystal structure that can show high sensitivity and selectivity.

# 10.3.5 Dr. Sanjeev Maradur



#### Assistant Professor

#### **Education and Work Experience**

- 1. 2012-Present: Asst. Professor, PPISR, Bangalore, India.
- 2. 2011-2012: Postdoctoral Research Associate, Dept. of Chemistry, University of Oklahoma, USA.
- 3. 2010-2011: Postdoctoral Student, Alan MacDiarmid Energy Research Institute (AMERI), Chonnam National University, Gwangju, South Korea.ese
- 4. 2009-2010: Postdoctoral Scientist, Dept. of Chemistry, Korea Advanced Institute of Science and technology (KAIST), Daejeon, South Korea.
- 5. 2007-2009: Research Scientist, Jubilant Life Sciences Ltd, Noida, India.
- 6. 2006-2007: Senior Research Fellow, Dept. of chemistry, IIT-Bombay, Mumbai, India.
- 2003-2006: Ph.D. Dept. of Chemistry, Shivaji University Kolhapur, India.

## **Broad areas of Interest:**

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

#### **Representative publications**

- 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 Metals162 (2012) 453-459.
- 2. Sanjeev P. Maradur, Changbum Jo, Dae-Heung Choi, Kyeongyeon Kim and RyongRyoo; Mesoporous Polymeric Support Retaining High Catalytic Activity of Polyoxotungstate for Liquid-Phase Olefin Epoxidation Using H2O2.ChemCatChem3(2011)1435-1438.
- V. T. Magalad, A. R. Supale, S. P. Maradur, G. S. Gokavi, T. M. Aminabhavi Preyssler type heteropolyacid-incorporated highly water-selective sodium alginate-based inorganicorganic hybrid membranes for pervaporation dehydration of ethanol. Chemical Engineering Journal, 159 (2010) 75-83.

- 4. S. P. Maradur.and G. S. Gokavi; "Heteropoly acid catalyzed synthesis of 3,4-Dihydropyrimidin-2(1H)-ones". Catalysis Communications 8 (2007) 279284.
- S. P. Maradur. S. B. Halligudi and G. S. Gokavi; "Oxidation of aliphatic and benzylic alcohols by Oxone, calalyzed by aliphatic and benzylic alcohols by 12-tungstocobaltate (II)". Catalysis Letters. 96 (2004) 165-167.

### 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. Application number: KR 2010-0072055, Dated 2010/07/26.
- 2. Inventors: Yang, KapSeung. MaradurSanjeev P .Kim, YeongCheol. "Method for preparation of carbon fibers using lignin copolymer and the carbon fibers thereby". Patent Application Number: KR10-2011-0027663, Dated 2011/03/28.

## Students

Mr. Manjunathan P. (Project assistant)

## **Current projects**

1. Development of solid acid catalysis for production of fuel additives from biomass derived chemicals

Principle Investigator: Dr. Sanjeev Maradur

Project Assistant: Mr. Manjunathan P. (jointly with Dr. Ganapati V. Shanbhag)

The rapid growth of the automobile industry and improved technology lead to greater consumption of fuel which initiated the development of different kinds of additives to improve fuel quality. The most prominent of these are octane enhancers (anti-knocking agents). Even though an additive is often added in less than 1 % to the base fuel, it provides an advantage to the chemical industry to produce it in hundreds of tons with respect to fuel consumption. By definition a fuel additive can be any compound that is added to the fuel in a less than 1 % concentration to attain certain properties and to improve the quality of the base fuel.

An important element in the formulation of gasoline is the addition of oxygenates, replacing other fuel components, which were required to be substituted by different laws. The oxygenate market was dominated by methyl tert-butyl ether (MTBE), due to its octane blending value, relatively low volatility, complete miscibility with gasoline, low susceptibility to phase separation in the storage and distribution system and low tendency to undergo peroxidation. MTBE became the fastest growing chemical of the 1980s. The widespread use of gasoline containing MTBE has resulted in significant air quality improvements. However, an issue concerning the presence of MTBE in groundwater supplies, as a component of gasoline that has entered the environment through incorrect storage or handling has forced to look for an alternative oxygenates.

Based on the ongoing work at PPISR on conversion of glycerol to more value added products and our expertise on solid acid catalysis, We are planning to develop a solid acid catalysis for the synthesis of oxygenates from biomass derived chemicals which may find applications as fuel additives.

# 11. Biological sciences



# 11.1 Introduction

Driven by curiosity to understand Natures ingenuity in creation, starting from simple atoms to the generation of molecules, assemblies and their controlled interaction culminating at continuously evolving creatures appears to be a never ending endeavour. We at the biological sciences division are striving to play our part towards this journey and our mission is to advance knowledge of basic biological sciences and apply research discoveries in ways that 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.

Biological Sciences division currently has core faculty working in frontier areas in mycology, protein chemistry and structural-biology. The biological science division has research facility with more than 3000 sq. ft. of lab space, 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.

### **Broad Areas of Research**

- 1. Endophytic fungi from medicinal plants and their secondary metabolites, bioactive compounds, enzymes from endophytic fungi.
- 2. Bioconjugation and PEGylation technology: Chemical modification of therapeutic proteins and drugs using linker chemistry and polyethylene glycol to enhance their activity and half-life.

3. Structure based functional characterization of key molecules of biological and medicinal importance.



4. De novo design of self-assembling proteinaceous materials exploiting intrinsically symmetric and stable protein motifs.

The faculty members are recognized guides with Manipal University (MU) and the doctoral research students currently working at the biological sciences division are registered with MU. The Doctoral advisory committee (DAC) for each student have met every six months to assess the progress and the quality of the research has been well appreciated by the distinguished members of the DAC.

Overall, the department has made considerable progress in two years since its inception. More than 100 endophytic fungi are isolated and secondary metabolite extractions were tested for their anti-microbial, anti-oxidant and anti-diabetic properties. Several promising endophytic fungi were identified by their genetic signatures. Adenine phosphoribosyltransferase from Yersinia pseudotuberculosis has been crystallized in its apo and complex forms together with Adenine and Adenosine Monophosphate. Data extending to 2.0 have been collected for both crystals of apo and complexed forms.

# 11.2 Academic and Research Highlights

One focus of research is on bioactive compounds of endophytic fungi isolated from medicinal plants. Endophytic fungi which are producing antimicrobial, anti-oxidant and anti-diabetic compounds were collected and optimization of their production is made. Antibacterial compounds were tested against multidrug resistant pathogenic bacterial and fungal isolates. The other interest is on antioxidant compounds which are very much essential to scavenge free radicals in the system and stops many cell damaging chain of reactions. These compounds are known to produced by many fungi, so we are searching in endophytic fungi isolated from medicinal plants. The other aspect of our research is also to find out some anti-diabetic compound/s from the endophytic fungi. There are advantages of fungi over plants due to their fast growth and easy to harvest compounds of interest. The one more wing of our research interests is on chemical modification of therapeutic proteins to improve their half life and pharmacokinetics. Another focus is on the structure-function studies of molecules of biological and medicinal importance using techniques like crystallography, bioinformatics and various biochemical, biophysical techniques. These studies play an important role in understanding key biological processes at the molecular level that could lead to the development of novel therapeutics. We are also interested



in de novo design of self-assembling proteinaceous materials exploiting intrinsically symmetric and stable protein motifs.

# 11.3 Faculty Profiles

# 11.3.1 Dr. Ananda K.



# Educational and Professional Qualifications

- 1. 2011- : Assistant Professor, PPISR, Bangalore, India
- 2. 2010-2011 : Faculty Fellow, PPISR, Bangalore, India
- 3. 2004-2010 : Post Doctoral Fellow, Albert Einstein College of Medicine, NY, USA
- 4. 2004-2004 : Lecturer, P A College of Engineering, Mangalore, India
- 5. 2003-2004 : Project Associate, IWST, Bangalore, India
- 6. 1999-2003 : Administrative Supervisor, KSRTC, Govt. of Karnataka, India
- 7. 1996-2001 : PhD, Mangalore University, Mangalore, India.
- 8. 1995-1996 : Project Assistant, College of Fisheries, Mangalore, India
- 9. 1993-1995 :MSc, Biosciences, Mangalore University, Mangalore, India

## Broad areas of interest

- 1. Endophytic fungi from medicinal plants and bioactive compounds such as antimicrobial, anti-oxidants, anti-diabetic compounds from endophytic fungi.
- 2. Bioconjugation of therapeutic proteins and PEGylation technology
- 3. Studies on Mangrove and Marine filamentous fungi.

## Membership of Professional bodies

Life Member of Mycological Society of India, India



## Recent Publications from the list of 23:

- 1. Garudachari, B., Isloor, A.M., Satyanarayana, M.N., Fun, H-K., Sathish, L., and Ananda, K., Design and regioselective synthesis of rifluoromethylquinolone derivatives as potent antimicrobial agents. European Journal of Medicinal Chemistry (Under Review)
- Chethan PD, Vishalakshi B, Sathish L, Ananda K, and Poojary B. (2013) Preparation of substituted quaternized arylfuran chitosan derivatives and their antimicrobial activity. Int J Biol Macromol. 2013 Apr 19. pii: S0141-8130(13)00228-6. [Epub ahead of print]
- Sathish L., Pavithra N and Ananda K. (2012) Antimicrobial Activity and Biodegrading Enzymes of Endophytic Fungi from Eucalyptus. Int J Pharm Sci Res; Vol. 3(8): 2574-2584.
- 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
- Remadevi, O.K., Rao,K.S., Ananda, K., Veeranna,R., Tarakanadha, B., (2011) Status of insects and fungi intercepted from wood imported into India. J Indian Acad Wood Sci. 8(2):139142
- Ananda, K., Manjula, B. N., Meng, F., Acharya, V. N., Intaglietta, M., and Acharya, S. A. (2012) Packing Density of the PEG-Shell in PEG-Albumins: PEGylation Induced Viscosity and COP are Inverse Correlate of Packing Density. Artif Cells Blood Substit Immobil Biotechnol. 40(1-2):14-27.
- 7. Acharya, S. A., Intaglietta, M., Tsai, A. G., Ananda, K. and Meng, F. (2011) Engineering the Molecular Shape of PEG-Hemoglobin Adducts for Supraperfusion, in Chemistry and Biochemistry of Oxygen Therapeutics: From Transfusion to Artificial Blood (eds A. Mozzarelli and S. Bettati), John Wiley & Sons, Ltd, Chichester, UK. doi:10.1002/9781119975427.ch25

## Other activities

- 1. Dr. Ananda compiled and edited PPISR news letter for the period from July-Dec 2012.
- 2. Dr. Ananda co-ordinated DAC meetings for the PhD students and progress report for six months submitted.

#### Research grants Submitted

- 1. ICMR detailed project submitted in January 2013 after getting approval of concept proposal on Title: Alpha amylase inhibitors from endophytic fungi isolated from Tulsi for the treatment of diabetes
- 2. DST proposal called for presentation at Indore on 18/03/2013: Anti-microbial compounds and enzymes of endophytic fungi isolated from medicinal plants
- 3. BRNS: DAE submitted and called for presentation on 19/03/2013: Effect of electron beam radiation on endophytic fungi producing ligninase enzyme, antimicrobial and anti-diabetic compounds.
- 4. ICMR preproposal in collaboration: Clinical and biochemical studies on association of chronic Periodontitis and type 2 Diabetes in rural and urban Karnataka, India

### Students

- 1. Ms. Pavithra N.
- 2. Mr. Sathish L.

### **Current Projects**

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

The project is focusing on isolation of endophytic fungi from plants which are already been proven for medicinal values for the treatment of various diseases. We are isolating endophytic fungi from these plant and screen for anti microbial activity against various pathogenic microorganisms and also we study their anti oxidant properties. The active endophytic fungi which are showing preliminary activity will be further grown in large scale and extraction of secondary metabolites will be done. The secondary metabolites are further tested for the activity. Those fungi which posses good anti-microbial activity and anti-oxidant properties will be identified based on molecular DNA technology. Secondary metabolites are further separated using various techniques by solvents and chromatography to get a pure compound. Finally, we check for the activity and characterize the compound for biophysical and biochemical parameters.

In this project we have isolated more than 100 endophytic fungi from Eucalyptus and Simarouba plants and screened for their antimicrobial and antioxidant properties. Out of which about eight endophytic fungi were selected for the detailed studies. We have grown them in large flasks (250 ml and 500 ml) for the extraction of secondary metabolites. Using ethyl acetate as solvent secondary metabolites were extracted. These extracts were dried in rotary vacuum evaporator and collected in vials. The solid extracts were further dissolved using standard solvents and used for the test. The purification of crude extract using TLC is under progress. These compounds will be separated using column chromatography for the further characterisation. All the active fungi were identified using molecular method. One publication is made from this project and two more manuscripts are getting ready and to be submitted to the journal.

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

Principal Investigator: Dr.Ananda Research Fellow: Pavithra N

Many herbal plants used for the treatment of diabetes. Recent studies shows that the compounds responsible for the medicinal values of plants were also produced by the endophytic fungi isolated from these plants. The present project is focusing on the antidiabetic compounds from the endophytic fungi living inside the medicinal plants. We have isolated about 60 endophytic fungi from various antidiabetic plants and screened them for their activity against various inhibitors such as alpha amylase inhibitor.

Those fungi which are showing positive for these inhibitors were grown in 250 or 500 ml flasks in a broth for 21 days. The mycelia and broth were used for the secondary metabolite extraction using ethyl acetate. The solvent was evaporated to dryness using the rotary vacuum evaporator and remaining solid was weighed and used for test. Many of the fungi showed positive for the alpha amylase inhibitor, aldose reductase inhibitor and glucosidase inhibitors. The purification of these compounds is under process now. A manuscript is prepared from this work for the publication in reputed journal. The preliminary data was published in a journal.

# 3. Anticancer metabolites from endophytes of medicinal plants

Pricipal Investigator: Dr. Ananda

Endophytic fungi isolated from plants used for the cancer treatment. Grow them in fungal broth media and extract secondary metabolites. Concentrated crude extracts screened against cancer cell lines in collaboration with G7 synergon, Bangalore. 10 endophytic fungal extracts from Eucalyptus tested against 3 cell lines and 3 isolates inhibited upt to 75% of Colon cancer cell lines (Colo 205) Isolated 20 endophytic fungi from Turmeric rhizome and growing them for secondary metabolite extraction.

# **Research** Collaboration

- 1. Dr. Arun M Isloor, NITK, Surathkal collaboration for the antimicrobial assay of synthetic compounds
- 2. Dr. Sooryanarayanan, Vivekananda Institute of Tropical Mycology, Chennai for the joint project on anticancer compounds from the endophytic fungi isolated from plants.
- 3. Dr. Boja Poojari and Dr. Vishalaxi B, Department of Chemistry, Mangalore University, in collaboration for the testing of synthetic compounds for anti-microbial activity.

# 11.3.2 Dr. Udupi Ramagopal

Ramalingaswami fellow (DBT)



Assistant Professor Ramalingaswami fellow (DBT)

## Educational and Professional Qualifications

- 1. Ph. D. in Biocrystallography, Indian Institute of Science, Bangalore, India
- 2. Visiting Fellow, National Institute of Health, USA
- 3. Senior Research Associate, Dept. of Biochem., AECM, USA
- 4. Associate of Biochemistry (Faculty), AECM, USA
- 5. Instructor, Albert Einstein College Of Medicine (AECM), USA
- 6. Visiting Faculty, Albert Einstein College Of Medicine (AECM), USA

## **Broad Areas of Research**

- 1. Costimulatory molecules: Biology and therapeutic intervention.
- 2. Structural study of proteins from enolases superfamily.
- 3. Structural Studies of Adenine Phosphoribosyltransferases from Pathogenic Bacteria
- 4. Testing the limits of phasing methodologies using weak anomalous signal
- 5. Designing soft-smart materials with protein supramolecular assemblies

#### Awards and achievements

- 1. Ramalingswami fellow, DBT (2011 current).
- 2. Visiting Fellow (2001 2003, NIH, USA).
- 3. Best thesis Kumari L. A. Meera Award and Gold Medal, 2001, Indian Institute of Science, India.
- 4. Invited Instructor (from 2003-2010) at RapiData, a comprehensive course offered at Brookhaven National Laboratory for budding crystallographers around the world (http://www.bnl.gov/rapidata/).
- 5. Proposal reviewer: Macromolecular Crystallography, APS, Argonne National Laboratory.

- 6. Served in the "User Executive Committee 2002-2003" of National Synchrotron Light Source, Brookhaven National Laboratory, USA.
- 7. Acknowledged in prestigious publications by various groups for initial phasing and structure solution of difficult structures.
- 8. Jeffery Award (poster award IUCr 2002, co-author).
- 9. Contributed ¿200 protein structures to World Wide Protein Data Bank (wwPDB).
- 10. Served as referee for International journals.
- 11. Invited Chief-Guest-Editor Journal of Amino Acids .

#### **Representative Publications**

- Rubinstein, R., Ramagopal, U. A., Nathenson, S. G., Almo, S. C., Fiser, A. 2013, Functional Classification of Immune Regulatory Proteins, Structure (cell press), 21(5), 707-717.
- Vigdorovich, V., Ramagopal, U. A., Eszter Lzr-Molnr1, Eliezer Sylvestre1, Jun Sik Lee1, Kimberly A. Hofmeyer1, Xingxing Zang1, Nathenson, S. G., Almo, S. C. 2013, Structure and T-cell inhibition properties of B7 family member, B7-H3, Structure (cell press), 21(5), 766-776.
- Samanta, D., Ramagopal, U. A., Nathenson, S. G., 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). 108(33), 13682-13687
- Samanta, D., Mukherjee, G., Ramagopal, U. A., Chaparro, R. J., Nathenson, S. G., DiLorenzo, T. P., Almo, S. C. 2011, Structural and functional characterization of singlechain peptide-MHC that modulate both nave and activated CD8+ T cells. Proc. Nat. Acad. Sci. (USA). 109(37), 14836-14840.
- Chattopadyay, K., Ramagopal, U. A., Brenowitz, M., Nathenson, S. G., 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. News:http://stke.sciencemag.org/cgi/content/abstract/sigtrans;1/3/ec30
- Ramagopal, U. A., Thirumuruhan, RA., Fedorov, L., Dauter, Z., Almo, S.C. 2005. Radiation-induced site-specific damage of mercury derivatives: phasing and implications. Acta Cryst. D61, 1289-1298.
- 7. Ramagopal, U. A., Dauter, M., Dauter, Z. 2003. Phasing on anomalous sulfurs: What is the limit? Acta Cryst. D59, 1020-1027. NSLS Newsletter: http://www.nsls.bnl.gov/newsroom/publications/newsletters/2003/03-nov.pdf
- Ramagopal, U. A., Ramakumar, S., Saha, 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.

## **Review meetings**

1. Mrs. Pavithra G C presented her synopsis in the presence of Doctoral Advisory Committee (DAC) on 14-02-2013 and at Manipal University on 30-03-2013. Manipal University has approved her synopsis and we have received her provisional registration letter from Manipal University.

#### **Students and Associates**

Research Associate:

1. Dr. Raghurama Hegde

**Research Scholars:** 

1. Ms. Pavithra G. C.

# **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. pneumoniae and F. tularensis that are known to cause pseudotuberculosis, atypical pneumonia and tularemia respectively depend solely on the salvage pathway for their survival. Blocking this key enzyme of salvage pathway in the absence of other means of AMP production, is an attractive strategy. 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.

 Structural Study of proteins from the enolase superfamily: Primary Investigator: Dr. Ramagopal U. A. Research Associate: Dr. Raghurama P. Hegde

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

3. The structure based functional characterization of an unusual restriction endonuclease KpnI.

Primary Investigator: Dr. Ramagopal U. A.

KpnI is a type-II Restriction-Modification (R-M) system originally isolated from the organism Klebsiella pneumoniae strain OK8. It recognizes the hexameric sequence GGTACC and catalyzes the hydrolysis of the phosphodiester bond between the two cytosines. The cognate methyltransferase methylates the N6 position of the adenine in both strands using Adenosyl methionine as the cofactor. Both the enzymes function as dimers. R.KpnI has been widely used in molecular biology experiments. However, its structure, mode of DNA binding and the key interaction responsible for its mechanism of action are not well understood. We believe that the structure characterization of R.KpnI will help us to understand the mechanism of action and aid in the generation of mutants with altered specificity.

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

Primary Investigator: Dr. Ramagopal U. A.

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.

# 11.3.3 Prof. Prasad Koka



#### Education and work experience

- 1. PhD at Texas Tech University.
- 2. Postdoc at University of Georgia
- 3. Postdoc at Brookhaven National Laboratory
- 4. Postdoc at Cold Spring Harbor Lab, MIT
- 5. Postdoc at Harvard Medical School

## Awards and Recognitions

- 1. Paediatric AIDS Foundation scholar, California HIV/AIDS Program, NIH (R0-1).
- 2. Editor-in-chief of Journal of Stem Cell Research
- 3. Editor-in-chief of Journal of Sexually Transmitted Diseases
- 4. Editor-in-chief of World Journal of Virology

During the past 20 years, he has been working on HIV/AIDS and generation of cancer stem cells using the immune difficient mouse model. He has edited a number of books on stem cells.

At PPISR, his group's first and most important objective was to establish a HIV lab to carry out the Ramalingaswami project of Prof. Koka at Poornaprajna Institute of Scientific Research at Bidalur campus. Hence we got quotations from four to five different vendors for 25 important equipments which are required to establish the lab.

To this end, literature survey at Indian institute of Science was conducted, which led to the writing three review articles on Cancer biology, submitted to two different Journals. They are as follows: -

- 1. Cancer Stem Cells as Targets for Prevention of Recurring Disease Etiology: Role in Relapse or Metastasis of Human Cervical Carcinoma– *Biomed Research International*.
- 2. Hematological Malignancies: Disease Etiology, Mechanisms and Therapeutic Intervention-Journal of Stem Cell.
- 3. Functional role of Cancer Stem cells in Disease Etiology and Susceptibility to Therapeutic Interventions- *Journal of Stem Cells*.

All the above three review articles are still under review.

# 12. Theoretical Sciences



# 12.1 Introduction

The Division was established in 2005 with the induction of Dr. Sujit Sarkar in 2005, and formally recognized as such during the renewal of PPISR's recognition by Manipal University (MU) in 2010, along with the Materials Science and Biological Sciences Divisions. Per the suggestion of Prof. K. J. Rao of AMEF and the Director, Prof. A. B. Halgeri, the scope of the Divison was enlarged to include philosophical studies, apart from mainstream physics research being pursued by the existing faculty members, Drs. Sujit Sarkar and R. Srikanth. Mr. Omkar, who registered for his PhD in Sep 2011 with MU, and Mr. Aravinda, who registered for his in Feb 2012 are the two students with the Division. In early January 2012, Dr. S. G. Bhargavi joined as a honorary faculty member.

Broad areas of research:

- 1. Quantum physics of many-body systems and condensed matter physics
- 2. Quantum information processing and foundations of quantum mechancis
- 3. Gamma ray burst and UV astronomy

Specific problems pursued by members include: (1) Quantum correlations of spin chain systems; (2) Quantum spin pumping and superconducting quantum dots; (3) Quantum cryptography: counterfactual and device-independent protocols; (4) Non-classicality from a signaling perspective; (5) the science of free will; (6) Multi-wavelength studies of gamma-ray bursts, UV astronomy, optical spectroscopy of hard X-ray sources.

Researchers in the Division have over 75 papers in prestigious, peer-reviewed international journals over the last 7 years, presented various invited talks, and have served as referees for various journals of repute.

# 12.2 Research Highlights

Derivation of perfect entanglement transport in quantum spin chain system and Josephson Relations in Superconducting Charge Qubit Lattice have been obtain in recent work by Dr. Sujit Sarkar.

Some recent results include: (a) An analytical method to obtain a generalized Kraus representation for the open system dynamics of systems of dimension four and higher; (b) quantum secret sharing with security check performed directly on the encoded quantum secret using Bell tests on degenerate graph states; Counterfactual approach to secret sharing and bit commitment; proposal of a device-independent intra-particle based quantum key distribution protocol (c) Studies on the implications of relaxing the no-signaling condition for certain bipartite systems in post-quantum correlations.

# 12.3 Faculty Profiles

# 12.3.1 Dr. Sujit Sarkar



# Assistant Professor

### Education and work experience

- 1. M. Sc (Kolkata University),
- 2. Ph. D in Quantum Many Body Physics in Strongly Correlated System from Saha Institute of Nuclear Physics.
- 3. Postdoc at IISc Physics Department,
- 4. Postdoc at Bar-Ialn University,
- 5. Postdoc at Max-Planck Institute, Germany as a Guest Scientist,
- 6. Postdoc at The Weizmann Institute of Science.

#### Areas of interest

- 1. Superconducting quantum dots
- 2. Quantum information processing in condensed matter systems
- 3. Many-body system physics
- 4. Quantum correlations in different one-dimensional quantum systems.

## **Recent** publications

- 1. "Collapse and Revival of Entanglement in Superconducting Quantum Dot Lattice with Magnetic Flux", Sujit Sarkar, Physica B 414, 26 (2013).
- 2. "Non-universal Tunneling Resistance at Quantum Critical Point of a Mesoscopic SQUID Array", Sujit Sarkar, Journal: International Journal of Mod. Phys. B 26, 1250099, (2012).
- 3. "Josephson Decoupling Phase in Superconducting Qubit Lattice", Sujit Sarkar, Octoberissue of International Journal of Modern Physics B.
- 4. "Dynamics of Geometric Phase in a Quantum Spin Chain System in the Adiabatic Limit of Quenching", Sujit Sarkar and B. Basu, Euro. Phys. Jour. B 85, 403 (2012)
- 5. "Quantum Correlation of Two Superconducting Charge Qubit in Presence of Magnetic Flux", Sujit Sarkar, Annals of Physics (submitted/process).
- 6. "Quantum Criticality of Geometric Phase in Coupled Cavity Arrays Under Linear Quench", Sujit Sarkar , Annals of Physics (submitted/process)
- 7. "Quantum Phase Transition of Light: A Renormalization Group Study", Sujit Sarkar, Nuclear Physics B ( submitted/process).

## Participation in workshop, Conference and Sysmosism

- 1. Top Higgs Meeting and Dirac Materials Chandrashekar Discussions Meeting at ICTS.
- 2. Lectures given: Saha Institute of Nuclear Physics, JNCASR (Bangalore) titled "Quantum Phase Transition of Light".

# **Current Projects**

- Quantum Phase Transition of Light: Cavity Quantum Electrodynamics. Principal investigator: Dr. Sujit We have used quantum field theoretic renormalization group theory to study the quantum phase transition of light. We have predicted different kinds of RG flowing process in this system. The physics of Berezenski-Kosterlitz-Thouless transition is the most important and interesting one.
- 2. Quantum correlation function (quantum entanglement and quantum discord physics) in different quantum condensed matter system.

Principal investigator: Dr. Sujit

We have studied the superconductiong quantum dots, mesoscopic SQUIDs and quantum spin chain system from a quantum information perspective, in particular studying the physics of quantum entanglement and quantum discord.

- 3. Quantum Phase Transition on a Spin Chain with a Double Quantum Dot Principal investigator: Sujit Sarkar (independent project) Quantum phase transition in qubit systems are known to produce singularities in the entanglement which could in turn be used to probe the quantum phase transition. Current proposals to measures the entanglement are challenging however, because of their nonlocal nature. We propose some experimental and theoretical projection methods to measure the quantum entanglement.
- 4. Josephson relations in charge qubit lattice Principal investigator: Dr. Sujit Sarkar In this study, Dr. Sujit found several Josephson relations for the superconducting charge qubit lattice. These relations are not the universal. He also consider the presence of magnetic flux for tuning the charge qubit lattice.

DST Project (on coming): "Geometric Phase and Quantum Phase Transition in Quantum Many Body System" has granted/approved. Ph.D student and Post-Doctoral Fellow will work in this project.

Publications (published + accepted + submitted): Five in internationally reputed journals.

# 12.3.2 Dr. R. Srikanth



## Education and work experience

- 2006– : PPISR, Bangalore, India.
- 2003–2006: Postdoc, RRI, Bangalore
- 2001– 2003: Postdoc, CTS, IISc, Bangalore
- 1999–2001: Postdoc, IIA, Bangalore.
- 1999: PhD, IISc, Bangalore, India.

#### Areas of interest

- 1. Foundations of quantum mechanics
- 2. Quantum information processing
- 3. Quantum cryptography
- 4. Philsophical issues in physics (individuation, identity and free will) from

#### Selected recent publications

- 1. "The quantum cryptographic switch", Srinatha Narayanaswamy, Omkar Srikrishna, R. Srikanth, Subhashish Banerjee, Anirban Pathak, accepted in Quantum Information Processing (2012).
- "Beyond the Goldenberg-Vaidman protocol: Secure and efficient quantum communication using arbitrary, orthogonal, multi-particle quantum states", Chitra Shukla, Anirban Pathak, R. Srikanth, Accepted for publication in Int. Jl. for Quantum Information (2012).
- 3. "Quantumness of noisy quantum walks: A comparison between measurement-induced disturbance and quantum discord", Balaji Rao, R. Srikanth, C. M. Chandrashekar and Subhashish Banerjee.

Phys. Rev. A 83, 064302 (2011)

- "Quantumness in decoherent quantum walk using measurement-induced disturbance", R. Srikanth, Subhashish Banerjee, C. M. Chandrashekar, Physical Review A 81, 062123 (2010). arXiv:1005.0183.
- "Complementarity in atomic and oscillator systems"
  R. Srikanth and Subhashish Banerjee
  Physics Letters A 374, 3147 (2010).
- 6. "Relationship Between Quantum Walk and Relativistic Quantum Mechanics", C. M. Chandrashekar, Subhashish Banerjee, R. Srikanth Physical Review A 81, 062340 (2010); arXiv:1003.4656
- 7. "Entanglement, Intractability and No-signaling", R. Srikanth Physica Scripta 81 (2010) 065002; arXiv:1005.3449.

Other activity

- 1. Designed an earlier version of PPISR's webpage, and currently responsible for upkeep.
- 2. Founded the Center for Foundational Study, with encouragement from Swamiji, the Director Prof. A. B. Halgeri, and Prof. K. Srihari.

#### Students

- 1. Mr. Omkar Srikrishna
- 2. Mr. Aravinda Srinivasamurthy
- 3. Ms. Akshata Shenoy (ECE, IISc)

#### **Current projects**

1. The operator sum-difference representation for quantum maps: application to the twoqubit amplitude damping channel

Principal investigator: R. Srikanth Collaborator: Prof. Subhashish Banerjee (IITR) Student: Mr. S. Omkar

On account of the Abel-Galois no-go theorem for the algebraic solution to quintic and higher order polynomials, the eigenvalue problem and the associated characteristic equation for a general noise dynamics in dimension d via the Choi-Jamiolkowski approach cannot be solved in general via radicals. We provide a way around this impasse by decomposing the Choi matrix into simpler, not necessarily positive, Hermitian operators that are diagonalizable via radicals, which yield a set of 'positive' and 'negative' Kraus operators. The price to pay is that the sufficient number of Kraus operators is  $d^4$  instead of  $d^2$ , sufficient in the Kraus representation. We consider various applications of the formalism: the Kraus representation of the 2-qubit amplitude damping channel, the noise resulting from a 2-qubit system interacting dissipatively with a vacuum bath; defining the maximally dephasing and purely dephasing components of the channel in the new representation, and studying their entanglement breaking and broadcast properties.

- $2. \ {\rm Dual} \ {\rm quantum} \ {\rm information} \ {\rm splitting} \ {\rm with} \ {\rm degenerate} \ {\rm graph} \ {\rm state}$ 
  - Principal investigator: R. Srikanth

Collaborators: Ms. Akshata Shenoy (IISc) and Prof. T. Srinivas (IISc)

We propose a protocol for secret sharing, called dual quantum information splitting (DQIS), that reverses the roles of state and channel in standard quantum information splitting. In this method, a secret is shared via teleportation of a fiducial input state over an entangled state that encodes the secret in a graph state basis. By performing a test of violation of a Bell inequality on the encoded state, the legitimate parties determine if the violation is sufficiently high to permit distilling secret bits. Thus, the code space must be maximally and exclusively nonlocal. To this end, we propose two ways to obtain code words that are degenerate with respect to a Bell operator. The security of DQIS comes from monogamy of nonlocal correlations, which we illustrate by means of a simple single-qubit attack model. The nonlocal basis of security of our protocol makes it suitable for security in general monogamous theories and in the more stringent, device-independent cryptographic scenario.

3. On a general criterion for nonclassicality from a signaling perspective Principal investigator: R. Srikanth Student: Mr. S. Aravinda

We argue that the essence of nonclassicality of a bipartite correlation is a positive signal deficit– the communication cost excess over the available signaling. By this criterion, while violations of Bell-type and contextuality inequalities are necessarily non-classical, some violations of the Leggett-Garg inequality are classical. Further, signaling tends to diminish nonclassical properties, such as intrinsic randomness, no-cloning, complementarity, etc. Signal deficit is shown to have its ultimate origin in intrinsic randomness. A possible analogy of nonclassicality to the metamathematical concept of Gödel incompleteness is noted.

4. Beyond the Goldenberg-Vaidman protocol: Secure and efficient quantum communication using arbitrary, orthogonal, multi-particle quantum states Principal investigators: Anirban Pathak (JIIT) and R. Srikanth

Student: Ms. Chitra Shukla

It is shown that maximally efficient protocols for secure direct quantum communications can be constructed using any arbitrary orthogonal basis. This establishes that no set of quantum states (e.g. GHZ states, W states, Brown states or Cluster states) has an advantage over the others, barring the relative difficulty in physical implementation. The work provides a wide choice of states for experimental realization of direct secure quantum communication protocols. We have also shown that this protocol can be generalized to a completely orthogonal state based protocol of Goldenberg-Vaidman (GV) type. The security of these protocols essentially arises from duality and monogamy of entanglement. This stands in contrast to protocols that employ non-orthogonal states, like Bennett-Brassard 1984 (BB84), where the security essentially comes from non-commutativity in the observable algebra.

5. Google In A Photonic Lattice

Principal investigator: Prof. T. Srinivas

Collaborators: Mr. Kallol Roy, Mr. Ji Liu, Mr. Le Luo, Prof. Bhanu Das.

The quantum version of Google PageRank has recently been investigated by various groups and shown to be quadratically faster in time than the classical PageRank algorithm. In this paper we propose the implementation of Quantum PageRank by a stochastic quantum walk of correlated photons in a photonic waveguide lattice, where we allow the density matrix to evolve according to the Lindblad-Kossakowski master equation. This yields a stationary state, the diagonal of whose density matrix gives the page ranking.

# 12.3.3 Dr. S. G. Bhargavi

# Projects

1. Luminosity functions of Gamma Ray Bursts:

This project was supported under 'one-time special grant from ISRO/DOS through letter # RES/C-S/2012-13 dated 10, May 2012. Gamma Ray Bursts (GRBs) are the brightest explosions in the universe. To date, they are the farthest known astronomical event detected upto redshifts of z 9. Therefore GRBs play an important role in the study of cosmology. Objective of this project is to study the potential role of instruments aboard Astrosat in the detection of GRBs and attempt to compute: (i) the expected number of GRBs observable by Astrosat, given the sensitivites of the Astrosat instruments. This requires the knowledge of luminosity function of GRBs. (ii) Following Sethi & Bhargavi (2001) luminosity function of GRBs are computed for the larger redshift data from current and previous GRB satellites viz. Swift, BATSE and so on.

Project Report: "Luminosity Function of Gamma Ray Bursts with Astrosat", Bhargavi, SG (2012) is attached.

2. Study of hard X-ray sources through Optical Spectroscopy

This project is in collaboration with Masetti et al. (INAF/Bologna, Italy). We proposed to perform optical spectroscopy using the 'Hanle Faint Object Spectrograph (HFOSC)' at the two-meter Himalayan Chandra telescope (HCT) to study the un-identied hard Xray sources detected by Integral and Fermi missions. It is an on-going project which uses 13 telescopes around the globe. Over 200 hard xray sources have been successfully identied by the authors using the data from elsewhere. Hanle telescope is useful particularly to explore the objects from northern hemisphere.

We were allotted 3 nights at HCT in May and June 2012. Sky conditions were not very good. We observed selected dozen sources on these nights. At PPISR, the required astronomical packages have been installed on the desk-top for the analysis of the data.

## Lectures & Teaching program

- 1. Introductory Astronomy lectures for the PPISR summer school in 2012
- 2. 'Optical spectroscopy of hard X-ray sources', presentation during the Founder's day, 2012.
- 3. Series of lectures in 'The Galaxy and Galactic structure' for the REAP program of JN Planatarium, Bangalore in Feb-mar 2012.
- 4. 'Astronomical facilities in India across the electro-magnetic spectrum', Lecture given at the summer school at JN Planatarium, Bangalore.
- Two lectures including 'High energy astronomy' were presented at the Science Academies' lecture workshop in introductory astronomy held at SDM College, Ujire from 20-22 Dec, 2012

# **13.** Events and achievements

1. Nov 26, 2012 AMEF Board of Trustees Meetings held at Bidlur campus. The meeting of the board of trustees of AMEF was held at Bidalur campus on Nov 26, 2012, presided by HH Sri Swamiji. Dr. Srihari, Hon. Secretary, AMEF/PPISR welcomed the Chairman and board members, while the Director presented the Quarterly Progress Report.



- 2. Nov 26, 2012 Launch of new web page. On Nov 26, 2012, HH Swamiji launched PPISR's new webpage www.ppisr.res.in, with hosting and webdesign provided by KGL Technologies, Bangalore. The previous webpage, maintained inhouse by PPISR, remains available as poornaprajna.org
- 3. Nov 15 Visit by Reliance Industries Team from Jamnagar. A team from Reliance Indistries Ltd, Jamnagar, a leading refinery and petrochemicals company in India, headed by Dr. D. Rajeshwar Dongra, Asst. Vice President, visited PPISR, and expressed to set up a sponsored research program at PPISR making use of the institute's facilities and expertises in catalyst preparation, characterization and testing.
- 4. July 5, 2012: **PPISR Founder's Day celebration at the Bidlur campus.** The scientific program was inaugurated by Prof. G. U. Kulkarni, Chemistry and Physics Materials Unit, JNCASR, Bangalore. Following this, presentations were made by all faculty members and students of PPISR, showcasing their work. The Materials science, Biological sciences and Theoretical Sciences sessions were chaired, respectively, by Prof. K. K. Nanda, MRC, IISc, Prof. P. K. Rajagopal, (Rtd) Botany Dept., MGM College, Udupi and Prof. Jagdev Singh, IIA, Bangalore.



During the valedictory function on the evening of July 26, 2012, presided over by HH Vishwapriya Theertha Swamiji, Dr. Prahlada, VC, DIAT, Pune was the chief guest. The meeting was also attended by Dr. K. S. Rangappa, VC Open University Mysore and Dr. Raj Mohan, Deputy Director, ICMR, Bangalore as guests of honor. HH Sri Swamiji expressed the hope that PPISR should provide the forum where scientists would use the modern scientific approach to interpret the teachings of ancient Indian saints. AMEF felicitated Dr. G. V. Shanbhag and his team for their successful completion of the GTC project.

# 13.1 Representative Publications

- V.S. Marakatti, G.V. Shanbhag and A.B. Halgeri, Sulfated zirconia; an efficient and reusable acid catalyst for the selective synthesis of 4phenyl-1,3-dioxane by Prins cyclization of styrene, Applied Catalysis A: General 451 (2013) 71 78.
- 2. Sathish, L., Pavithra, N., Ananda, K. (2012)Antimicrobial Activity and Biodegrading Enzymes of Endophytic Fungi from Eucalyptus. International Journal of Pharmaceutical sciences and Research. 3 (8), 2574-2583
- 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
- 4. Srinatha Narayanaswamy, Omkar Srikrishna, R. Srikanth, Subhashish Banerjee, Anirban Pathak, "The quantum cryptographic switch", accepted in Quantum Information Processing (2012).
- 5. "Beyond the Goldenberg-Vaidman protocol: Secure and efficient quantum communication using arbitrary, orthogonal, multi-particle quantum states",
- Remadevi, O.K., Rao,K.S., Ananda, K., Veeranna,R., Tarakanadha, B., (2011) Status of insects and fungi intercepted from wood imported into India. J Indian Acad Wood Sci. 8(2):139, 142
- D.P. Suhas, H.M. Jeong, T.M. Aminabhavi, A.V. Raghu, Synthesis and characterization of novel polyurethanes based 4,4-oxy-1,4-diphenyl bis(nitromethylidine) diphenol Schiff base hard segment, Polymer Engineering and Science, (2013) Accepted, online.

- A.V. Raghu, H.M. Jeong, Y.R. Lee, C.M. Shin, Preparation and Physical Properties of Waterborne Polyurethane/Functionalized Graphene Sheet Nanocomposites Macromol. Chem. Phys, 209, 2008, 2487-2493.
- A.V. Raghu, G.S. Gadaginamath, H.M. Jeong, N.T. Mathew, S.B. Halligudi, T.M. Aminabhavi, Synthesis and Characterization of Novel Schiff Base Polyurethanes. J. Appl. Polym. Sci., 113, 2009, 27472754.
- K.R. Reddy, H. M. Jeong, Y. Lee, A.V. Raghu, Synthesis and Structural properties of MWCNTs-Core/Thiophene polymer-Sheath Composite Nanocables by a Cationic surfactant-Assisted Chemical Oxidative Polymerization J. Polym. Sci. Polym. Chem., 48, 2010, 1477-1484.
- P.V. Kulkarni, C.A. Roney, P. Antich. F. J. Bonte, A.V. Raghu, T. M. Aminabhavi, Quinoline-n-Butylcyanoacrylate-based Nanoparticles for Brain Targeting for Diagnosis of Alzheimers Disease, Wiley Interdisciplinary Reviews: Nanomedicin and Nanotechnology, 2, 2010, 35-47.

# 13.2 Achievements

1. GTC Technology, USA continues its association with PPISR. GTC sanctioned another project for 1 year on "Catalyst development for alkylation of aromatics" which commenced from 1st of July 2012. In appreciation of the successful completion of the first phase of the project, Dr. Ding Zhong Yi, GTC Technology, USA awarded a plaque to the achievers during his visit to PPISR on July 15, 2012. The plaque bears the citation: Presented to Dr. Ganapati Shanbhaq and his students Mr. Vijay Marakaii and Mr. H. Laxminarayan Janardhan in recognition of their dedicated research in developing a modified zeolite catalyst enabling continued commercial exploration of this important aromatics technology. GTC Technology is grateful for the full support to the PPISR management, and looks forward to our long term relationship.



- 2. Shell technology Center, Bangalore has approved a one year project on Post synthesis modification of solid acid catalysts". The agreement was signed and the project was initiated in September 2012.
- 3. HPCL, Corporate R & D Centre, Bangalore approved a two year project to catalysis group on Development of Zeolite modified catalysts for the Hydrocarbon Conversions. The project was initiated in November 2012.
- 4. Dr. A.V. Raghu was selected for Editor in IRNS Nanomaterial international Journal.

- 5. Dr. A.V. Raghu was invited to present a lecture at Adichunchanagiri Mutt, Nagamangala Taluk, Mandya District for Refresher Course for PUC Science Lecturers on 14th April 2012, organized by VGST.
- 6. Dr. Nalini Sundaram was invited for a technical program discussion meeting at NIIST, Trivandrum by the Advanced Technology Committee, BRNS-DAE to present a project proposal titled Influence of Electron Beam Irradiation on the Crystal Structure and Photoluminescence of Rare Earth doped Tungstate Nanophosphors on January 7th 2013. This project has been approved for funding of Rs. 20,76000/- for a period of three years.
- 7. Swetha. S. M. was awarded the best oral presentation for her paper titled Crystal Structure of Nanocrystalline Layered Bismuth Xoychlorides and their Photocatalytic Activity 41st National Seminar on Crystallography (NSC) held from Oct 8th-10th2012 at Chennai
- 8. Ms. Swetha S.M. was selected to attend AsCA 12/CRYSTAL 28 2012 Conference and BRAGG Symposium which is to be held in Adelaide, Australia from Dec 2nd to Dec 6th 2012 for presenting her work. She has been awarded US \$ 760.00 to assist with her accommodation and/or travel arrangements to attend this conference.
- 9. MSRIT students Mr. Ameya and Mr. Rahul presented the project work "Synthesis of acetins from glycerol and acetic acid using Hbeta zeolite catalyst" in the Inter-College Project presentation organized by IIChE which won second prize award on 11th May 2012.
- 10. Dr. Shanbhag and his group received a Meritorious Award for Excellence in Research from AMEF during Founders day July 6, 2012.
- Mr. Aravinda S. won the First prize in the sciences category in the Researchers Scholars Meeting 2012 organized during Dec 17–19, 2012 at IIST, Trivandrum.
- 12. Dr. R. Srikanth was invited to join the Editorial team of the international journal Quanta devoted to the Foundations of Physics.
- 13. Pavithra G. C. from biological sciences division has registered for PhD at Manipal university under the guidence of Dr.U. Ramagopal
- 14. A research proposal for Neutron beam time at the Oakridge National Laboratory, USA was accepted. We were allotted two days of beam time to carry out neutron diffraction experiments on Photoluminescent polymorphs
- 15. Dr. Ramagopal has been awarded a grant from the Vision Group on Science and Technology, Department of Information Technology, Biotechnology & Science and Technology, Government of Karnataka for Establishment of Centre of Innovative Science & Engineering Education, for the project Design of modified B7-1 (CD-80) and B7-2(CD86) molecules to create potential reagents for cancer and auto-immune disorders.
- 16. Dr. Ramgopal's group have successfully completed the structure solution and refinement for three proteins from the Enolase superfamily: (i) a D-glucarate dehydratase from Pseudomonas mendociana and (ii) a putative glucarate dehydratase from Acidaminococcus and (iii) a mandalate racemase/ muconate lactonising enzyme from Pseudovibrio sp. All the three structure have been deposited in the Protein Data Bank (PDB) with ids 4HN8, 4HYR and 4JHM respectively.

# 13.3 Conferences and workshops

- 1. Swetha .S.M. and Dr. Nalini Sundaram Participated in Indo-US Workshop on Next Generation of Materials Using Neutrons held on 6-7 September 2012 at JNCASR, Jakkur
- 2. Mr . Srinidhi participated in The International Conference on Raman Spectroscopy from 12th 17th August, 2012 at the IISc JNT auditorium.
- 3. Mr. Srinidhi also participated in The Strength of Materials from Metallurgy department from IISc August 23rd- 25th, 2012
- 4. Swetha S.M. and Dr. Nalini Sundaram were selected to participate in the INUP Training Workshop on Nanofabrication Technologies held at the Centre of Nanoscience and Electronics, IISc, Bangalore from 16th to 18th April, 2012.
- 5. Swetha .S.M participated in Hands on training on nanoelectronic fabrication of the materials held on 18th-28th July at CeNSE, IISc and also presented our research proposal for the use of the CeNSE facility to make an optical device
- 6. Ms.Swetha S M presented a poster titled Photocatalytic activity and Crystal structure of Nanocrystalline layered Bismuth oxychlorides. At the second international conference on Advanced Oxidation Process held at the Mahatma Gandhi University, Kottayam, Kerala, India from October 5-8, 2012.
- Dr. Nalini G Sundaram was invited to participate in a two days seminar on Processing, Materials Characterization, Surface Science and Cryogenic Environments on20-21November, 2012 at IISc Bangalore.
- 8. Mr . Srinidhi participated in The International Conference on Raman Spectroscopy from 12th 17th August, 2012 at the IISc JNT auditorium.
- 9. Mr. Srinidhi also participated in The Strength of Materials from Metallurgy department from IISc August 23rd- 25th, 2012
- 10. Dr. Nalini G Sundaram was invited to deliver a talk on Nano/Micro Structure of KNd(WO4)2Polymorphs: Crystal Structure and Tunable Photoluminescence in the Visible Region at the conference on Condensed Matter Physics and Applications held at the Physics Department, MIT, Manipal on 27-28 December, 2012.
- 11. Dr. Raghu given a talk on Polymeric Membranes for Separation Applications for Student-Scientist interaction programme organized by Karnataka Rajya Vijnana Parishat in association with Vision Group on Science and technology. 15th December, 2012 at Shri Bhramarambha Kalyana Mantapa, Bapu nagara Mysore road, Kollegala & 26th December 2012 at Eshwari Vishwavidyalaya, Yellapura, Sirsi District
- 12. Dr. A.V. Raghu and Mr. Suhas D.P. [received invitation letter] attended the 5th Bangalore Nano Conference to be held at Lalit Ashok, Bangalore from December 5–7, 2012, sponsored by VGST, Govt. of Karnataka.
- 13. Dr. Sujit attended the Dirac Materials and Chandrashekar Discussion Meeting at the Physics Department of IISc Bangalore from December 16 to December 21, 2012.

- 14. Dr. Bhargavi SG presented two lectures including High energy astronomy at the Science Academies lecture workshop in introductory astronomy held at SDM College, Ujire from 20-22 Dec, 2012
- 15. Mr. Vijay Attended the 5 day orientation program on "Photochemistry and photo electrochemistry" held in December -2012 at NCCR, IIT Madras.
- 16. Mr. Suhas presented a poster titled "Poly (vinyl alcohol)/H-ZSM-5 Based Mixed Matrix Membranes for Pervaporation Dehydration of Alcohols : Effect of Silica-Alumina Ratio." at National Symposium on Polymers and Coatings (NSPC)-2012 held at IICT (Indian Institute of Chemical Technology)-Hyderabad from 7-8th September, 2012.
- Dr. Ananda, participated as Rapporteur for the plant biotechnology session in International conference on exploration of biotechnology by students and researchers (ICEBSR 2012) conducted by Sridevi Institute of Engineering and Technology, Tumkur on June 8-9, 2012.
- 18. Dr. Ananda attended and made oral presentation on Medically important compounds of endophytic fungi isolated from medicinal plants in International conference on Recent advances and challenges in Biotechnology on 27-29, December 2012 held at NITTE Mahalinga Advanthaya Memorial Institute of Technology, Nitte, Udupi.
- 19. Ms. Pavithra N Presented oral presentation in National seminar on Current Perspectives of Fungi in Health Care and Environment (KAVAASTHA) and 39th Annual Meeting of Mycological Society of India held on 13-14 March, 2013 at Bangalore University on title Aldose reductase inhibitors and extracellular enzymes of endophytic fungi isolated from Ocimum sanctum
- 20. Mr. Sathish L presented oral presentation in National seminar on Current Perspectives of Fungi in Health Care and Environment (KAVAASTHA) and 39th Annual Meeting of Mycological Society of India held on 13-14 March, 2013 at Bangalore University on title Endophytic fungi from Eucalyptus citriodora: Enzymes, antimicrobial activity and phylogeny
- 21. Dr. Ganapati Shanbhag delivered an invited lecture on "Introduction to catalysis" for PU College teachers under Refresher Course Programme sponsored by VGST, Govt of Karnataka, held in BGSIT, Bellur on 19th May 2012.
- 22. Dr. Shanbhag delivered a lecture on "Basics of Catalysis" during for 6 days Summer School- 2012 from May 21-26 2012 for undergraduate students.
- 23. "Prins cyclization of styrene with paraformaldehyde using sulfated zirconia as a catalyst for the selective synthesis of dioxane derivative" by V. S. Marakatti, G.V. Shanbhag and A.B. Halgeri, Poster presentation at 2nd International Indo-German Symposium 2012 on Green Chemistry and Catalysis for Sustainable Development at ICT, Mumbai from 29-31 October 2012
- 24. "Gas-phase dehydration of glycerol over molybdenum trioxide supported on silica catalyst for sustainable synthesis of acrolein" by Satish. B, G.V. Shanbhag and A.B. Halgeri, Poster presentation at 2nd International Indo-German Symposium 2012 on Green Chemistry and Catalysis for Sustainable Development at ICT, Mumbai from 29- 31 October 2012.

- 25. "Novel Tin based Photocatalyst for the Degradation of Azo Dyes", V. S. Marakatti, G.V. Shanbhag and A.B. Halgeri, Poster presentation at "Second International Conference on Advanced Oxidation Processes", Mahatma Gandhi University, Kottayam, Kerala, India from 5-8, October, 2012.
- 26. "Designing eco-friendly heterogeneous base catalyst for the conversion of waste bioglycerol to glycerol carbonate by two different routes" by Swetha Sandesh, G.V. Shanbhag, A. B. Halgeri, Poster presentation at 5th Annual KSTA conference on Science and Technology for Social Transformation organized by DST, Govt of Karnataka at Dayanand Sagar Institution, Bangalore on 19-20, December, 2012.
- 27. "Transesterification of glycerol with dimethyl carbonate using KF/Al2O3 as a solid base catalyst", Swetha Sandesh, G.V. Shanbhag, A.B. Halgeri Oral presentation by Swetha Sandesh 21st National Symposium on Catalysis at IICT, Hyderabad, 10-13, Feb, 2013
- 28. "The role of Bronsted and Lewis acid sites in the selective synthesis of dioxane from Prins reaction of styrene using sulfated zirconia", Vijaykumar S. Marakatti, G.V. Shanbhag, A.B. Halgeri. Poster presentation by V.S. Marakatti 21st National Symposium on Catalysis at IICT, Hyderabad, 10-13, Feb, 2013
- "Pore-size engineered ZSM-5 zeolite by phosphate modification for the shape-selective synthesis of para-diethylbenzene", Janardhan H. L., G.V. Shanbhag, A.B. Halgeri. Poster presentation by Janardhan H. L, 21st National Symposium on Catalysis at IICT, Hyderabad, 10-13, Feb, 2013
- 30. Dr. A.B. Halgeri and Dr. G. V. Shanbhag attended a 3 day Technology Conference organized by GTC Technology, USA at Radisson Blu Plaza, New Delhi from 3-5, Dec 2012.
- 31. Mr. Janardhan HL attended an 18 day National Orientation Program on Catalysis held at IIT-Madras, Chennai, from 26 Nov to 13 Dec, 2012 organized by National Centre for Catalysis Research (NCCR) IIT-Madras, Chennai.
- 32. Dr. G. V. Shanbhag, Dr. Sanjeev Maradur, Mr. Satish Burla and Mr. Prashant Kumar attended two days National Seminar and Workshop on Oil and Gas in MSRIT, Bangalore on 7-8, March, 2013.
- Dr. Ramesh and Mr. Manjunathan P. attended 21st National Symposium on Catalysis at IICT, Hyderabad, 10-13, Feb, 2013.
- 34. Dr. Ramagopal delivered an invited lecture titled CTLA-4 blockade by therapeutic mAB: Structural basis for anti-cancer activity at National Seminars on Crystallography, CLRI, Chennai on 09/10/2012.
- 35. Dr. Ramagopal was invited to give demonstration sessions on various phasing methods at Protein Crystallography Meeting, held at RajaRamanna Centre for Advanced Technology(RRCAT), Indore. India.
- 36. Dr. Ramagopal delivered (in Kannada language) an invited lecture titled How our immune system works? at Arasikere in a meeting organized by Karnataka Rajya Vijnana Parishat for college lecturers and students (Date: 12-01-2013).

- 37. Dr. Ramagopal, Dr. Raghurama Hegde and Mrs. Pavithra attended the International Conference on Biomolecular Forms and Function held at the Indian Institute of Science to commemorate 50 years of the Ramachandran map.
- 38. Dr. Ramagopal attended the Ramalingaswami Fellows conclave from 20-23rd, January 2013, held at Thiruvananthapuram, Kerala organized by Ragiv Gandhi Center for Biotechnology.

# 13.4 New Appointments

## 13.4.1 Faculty

1. The appointment of **Dr. Sanjeev Maradur** as Asst. Professor, who has considerable postdoctoral experience, strengthens the catalysis group in PPISR's Materials Science Division, as we seek ever more interaction with industry while also retaining our foothold in academia.

# 13.4.2 RA and postdocs

- 1. Dr. Raghurama P. Hegde: appointed as RA (Biological Sciences) with Dr. Ramagopal. Education and work experience
  - (a) PhD, IISc on crystallograhic characterization of de-novo designed pseudo-peptides and molecular modeling of a G-protein coupled receptor.
  - (b) RA at Dept. of Biological Sciences, NUS, Singapore.

No. of publications: 5 (including a book chapter)

- 2. Dr. Ramesh: appointed as postdoc (Materials Sciences) with Dr. G. V. Shanbhag.
  - (a) Phd from BIT, Bangalore associated with Vishwesharaiah Technological University, under the guidance of Dr. Y. S. Bhat and Dr. B. S. Jai Prakash.
  - (b) Doctoral work involved synthesizing novel clay based solid acid catalysts for solvent free microwave induced organic transformations.
  - (c) Publications: 4.





# 14. Academic activities

# 14.1 Collaborative visits

- Dr. R. Srikanth visited Dr. Subhashish Banerjee at IIT Jodhpur, Rajasthan during Jan 27, 28, 2013.
- 2. Visit to IIT, Jodhpur. Omkar S from Theoretical Sciences Division visited Prof. Subhasish Banerjee, Physics department, IIT-Jodhpur during 26/9/2012 8/10/2012 and 5/12/2012 24/12/2012 to carry out our collaborative research works towards his Ph.D degree. Visiting him has been very fruitful as we published a paper titled "The quantum cryptographic switch" and another paper titled "Dissipative and Non-dissipative Single-Qubit Channels: Dynamics and Geometry" and "The operator sum-difference representation for quantum maps: application to the two-qubit amplitude damping channel" are in communication with journal.
- 3. Dr. Ding ZhongYi, Project manager, GTC, USA visited PPISR on 14-15, July 2012. The project work was reviewed with the meetings between Dr. ZhongYi and catalysis group of PPISR. GTC USA appreciated the one year project work carried out by catalysis group of PPISR, Dr. Shanbhag, Mr. Vijay Kumar and Mr. Janardhan with a plaque and was awarded by Dr. ZhongYi on behalf of GTC during this visit.
- 4. 9. Dr. G. V. Shanbhag visited Shenyang, China from 16-23, Aug 2012 to carry out scaleup studies of catalyst preparation for GTC project which was arranged by GTC, USA and GTC, Beijing.

# 14.2 In-house seminars

- 1. Ms. Swetha Bhat. "Solar Cell: Towards Advanced Materials"
- Dr. Sanjeev Mardur Biomass utilization/refinery: A sustainable approach to value added products. Date: 29-01-2013
- 3. **Dr. Raghurama P Hegde** Title: Recent Advances in Tuberculosis Research Date: 16.01.2013
- 4. Dr. Raghurama P Hegde

"From a gene to a crystal structure: an overview of protein crystallography" presented in Summer school, PPISR; Date: 26.05.2012

#### 5. Mr. Suhas

Assessment of Membranes and Various Operation Parameters for Pervaporative Separation of Butanol from Aqueous Solution. Date: 17-05-2012

#### 6. Mr. Vijay

Mesoporous materials Synthesis and Applications Date; - 19-03-2013

# 14.3 Invited Talks

- 1. Professor Joel M. Friedman from Albert Einstein College of Medicine, New York delivered talk titled "What to do when you know there is no NO (nitric oxide)" on 21th Febrarury, 2013.
- 2. Dr. A.V.Ramaswamy, Former Head of Catalysis Division, NCL Pune delivered talk titled "ALTERNATIVE SOURCES FOR FUEL AND CHEMICALS" on 5th Febrarury, 2013.
- Dr.Rajakumara Eerappa from FIRC Institute for Molecular Oncology Foundation (IFOM), Milan, Italy delivered talk titled "Mechanistic insights into the histone code and cytosine methylated DNA read-out and interpretation by chromatin associated modules" on 22nd January, 2013.
- 4. 1.Dr. Nagendra, Professor & HOD of Biotechnology, MVIT Engineering college Bangalore delivered a lecture on Essential Bioinformatics for biologists on 7th November, 2012.
- 5. Dr. Shyamprasad, Assistant Professor has delivered a Lecture on "Introduction to Nanobiotechnology" in the department of Biological Sciences, Poornaprajna Institute of Scientific Research, Bangalore on November 2nd, 2012 at Bidalur Campus.
- Dr. Vijay K. Sachdeva, from Centre for mind control Development and relaxation delivered lecture on "Stress management, mind control and health management" during October 12th, 2012.
- 7. Dr. T. S. Suryanarayanan Director of Vivekananda Institute of Tropical Mycology (VIN-STROM), Chennai visited PPISR on 08/10/12 and gave a talk on "Biodiversity in Amazon forests"
- 8. Dr. Mahesh from Materials Research Center, Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, Portugal delivered Lecture titled "Ni-Ti Shape Memory Materials and their Characterization" on 14th September, 2012.
- Dr. Jagjit Nanda, Scientist from Physical Chemistry of Materials group, Materials Science and Technology Division, Oakridge National Laboratory delivered talk titled "High Energy Electrodes and 3D Architectures for Advanced Lithium Batteries and Beyond" on 12th September, 2012.
- Professor Thomas Proffen from Oakridge National Laboratory(ORNL), U.S.A delivered talk titled "Structural Characterization of Complex Materials using Total Scattering" on 5th September, 2012.
- 11. Dr. Balachandra Hegde from University of Southern California, Los Angeles delivered talk titled "Application of Electron Paramagnetic Resonance (EPR) in the Structural Study of Membrane Bound Proteins" on 25th May, 2012.



# 14.4 RAC meetings

- 1. RAC meeting: RAC meeting was held for the first time in PPISR campus on 27-3-2013 to review the research projects of individual faculty of Materials Science. Prof. Guru Row, Prof. K R Krishnamurthy and Prof. T.M. Aminabhavi, the members of RAC attended the meeting. Dr. G.V. Shanbhag and Dr. Sanjeev Maradur presented their ongoing and future research projects. RAC members gave advice on the projects and expressed their satisfaction on the overall progress made in the research during last two and half years.
- 2. The Research Advisory Committee Meeting (RAC) for biological sciences was held on April 3rd, 2013 in the presence of PPISR Director Dr. Anand B. Halgeri and presided by subject experts Dr. A.J. Rao, Professor (Ramanujan Fellow) Department of Biochemisry and Dr. Ramakumar, Professor, Department of Physics, IISc Bangalore.
- 3. The RAC meeting for Theoretical Sciences was held on April 14, 2013 in the presence of PPISR director Dr. Anand B. Halgeri and presided by subject experts Prof. N. Kumar, Distinguished Homi Bhabha Professor, Raman Research Institute, Bangalore, and Prof. C. Sivaram, Professor, IIAP Bangalore, and St. Joseph College.

# 14.5 Academic Outreach Activities

# IAS sponsored Lecture workshop in Introductory Astronomy' at SDM College, Ujire

Dr. Bhargavi was the co-ordinator for this workshop held between 20-22 Dec, 2012. Objective of the workshop was to motivate the students and to expose them to various research facilities in India. It was planned to have 5-6 lectures and equal number of interactive sessions. We covered broad topics like: Cosmology, optical astronomy, radio astronomy, high-energy astronomy and Solar astronomy. Resource persons were from PPISR, RRI and IIA, Bangalore. The lecture workshop was attended by 115 students from Dakshina Kannada. Lodging, Boarding and travel of all outstation students was covered and no registration or tution fee was charged to students. Star-gazing program was included on the second evening using 3 small size telescopes.

## Summer school

PPISR invities undergraduates from rural colleges who has lesser exposure towards fundamental and applied sciences for research training activity. Under this activity two DST INSPIRE fellowship students from Poornaprajna College, Udupi and theree students from Bhandarkar's College, Kundapur did research projects in their respective areas during November, 2012.



### Student visitors from other institutes

- 1. Mr. Poojary and Ms. S. K. Sapthami, final year MSc Industrial Chemistry students, Kuvempu University, Shimoga, completed their project titled "Synthesis and characterization of novel poly-urethanes" under the guidance of Dr. A. V. Raghu.
- 2. Training for Inspire fellow students: Ms. Manasa Tantry BSc, and Ms.Anusha Acharya BSc from Poornaprajna college, Udupi, got training in Microbiology and protein crystallography respectively for two weeks in Oct-Nov, 2012
- 3. Ms. Manasa Tantri, First year BSc student from Poornaprajna college Udupi, secured inspire fellowship and successfully completed a project on lignin degrading enzymes from endophytic fungi from medicinal plants by actively participating for almost five weeks during May 5th -June 10th, 2012
- 4. Three BSc Students from Bhandarkars college Kundapura were also came to PPISR and initiated some project activities and got trained in various techniques in Biological Sciences.
- 5. Ms. Vibha Hande, a II PUC student from Poornaprajna PU college, Udupi is working at PPISR for almost four weeks to get a hands on experience in research in biological sciences.
- 6. Summer Student, Ms. Anusha from Poornaprajna College Udupi was trained in the nanomaterials group at PPISR, under the guidance of Dr. Nalini G Sundaram as part of INSPIRE Scholarship awarded by the Government of India from 2nd May to 18th May 2012

# **Research Facilities** 15.

PPISR has procured several analytical instruments that are vital for the faculty and students to pursue advanced research in basic and applied areas. The Analytical Facility has several instruments 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. Interested individuals can analyze their samples under the guidance of a PPISR staff or submit their sample for analysis.

#### 15.1Sophisticated Instruments

(AAS)

The



facility

Atomic Absorption Spectroscopy

equipments consists of several such as: This instrument from Perkin-Elmer is used for the qualitative and quantitative determination of chemical elements employing the absorption of optical radiation (light) by free atoms in the gaseous state. In analytical chemistry the technique is used for determining the concentration of a particular element (the analyte) in a sample to be analyzed. Specifications:

• Elements analysed in our facility are Iron, Copper, Silicon, Aluminium, Zinc, Calcium, Sodium, Phosphorous and Magnesium.

• Sample in the form of liquids are analysed in this instrument.

• Solid samples are digested using acids (hydrochloric, nitric, sulphuric etc) and made up to required volume using distilled water.



Fourier Transform Infrared Spectroscopy (FTIR)

The Bruker-alpha FTIR spectrophotometer is a compact instrument and measures the infrared spectrum, which represents the molecular absorption and transmission of a sample. Specifications:

- Spectral range 500-4000  $cm^{-1}$  with scan rate of 32.
- Attenuated Total Reflectance available.

• Solid, liquid and gel samples can be analyzed without making pellets.
The UV-Visible spectrophotometer from Perkin Elemer can be routinely used in analytical chemistry for the quantitative determination of different analytes such astransition metalions, highlyconjugated organic compounds, and biological macromolecules.

Specifications:

• Deuterium lamp source for UV region and tungsten halogen lamp for Visible region.

• Both solid and liquid samples can be analyzed by UV-Vis.

• Solid samples in the form of thin films can be analyzed.

• Absorbance, Transmittance, Diffused Reflectance for liquids and Absorbance, Transmittance for solids can be measured.



Ultra Violet Visible Spectroscopy (UV-VIS)



Cold centrifuge

The cold centrifuge is used to separate materials of different density by centrifugal force at low temperatures. Specifications:

- Temperatures: 4° C to room temperature
- High speed of 20,000 rpm.



Powder X-ray Diffractometer (PXRD)

The D2 PHASER table top X-ray Powder Diffractometer from Bruker is ideal for qualitative, quantitative and structure analysis of polycrystalline samples. Specifications:

- Wavelength: Cu Ka ( $\lambda$ =1.5418Å)
- Detector: LYNXEYE(TM) 1-D Solid State Fast Detector
- 2 Theta range: 5-90 degrees
- Sample type: Powder
- Temperature: Room Temperature

TPD analyser is a Chem Labs, Bangalore instrument used for measuring acidic and basic strength of the catalyst. Specifications:

- Catalyst amount: 100-200mg.
- For Acidity measurement gas used: 10 percent ammonia in helium.
- For Basicity measurement gas used: 10 percent  $CO_2$  in helium.
- Detector: TCD
- $\bullet$  Catalyst precondition: 100-500 C at 10/min
- Helium flow: 30ml/min 10 percent ammonia in helium injection at temperature: 100 C
- Equilibrium time : 30 min
- Temp ramp: 100 to 800 at 10/min.



Temperature Programmed Desorption Analyzer (TPD)



NH- 2L Kneader

This machine is procured from China. The Z-blade twin screw mixer particularly adapted to compounds of high viscosity, such as wet mixtures of alumina, zeolites, clays, silica, titanium dioxide.

Specifications:

- Hopper volume : 0.5 kg.
- $\bullet$  Crank speed : 0 40 rpm.

This machine is procured from China. Its a small twin screw extrusion molding equipment, which is mainly used for small-scale banded extruding of catalyst, adsorbent and other powders.

Specifications:

- $\bullet$  Screw external diameter : 26 mm
- $\bullet$  Screw stepless speed regulation : 0 220 rpm
- $\bullet$  Extruding diameter : 0.5 2 mm
- $\bullet$  Production capacity : 1 7kg/h



F-26 Extruder



DGM Abrasion tester

This equipment is used to determine the attrition characteristics of a solid catalyst resulting from inter-particle friction or wall effect when the catalyst is handled. This equipment is dedicated to the determination of attrition and abrasion resistance of catalyst particles. Specifications:

- Rotating rate 30-90 rpm.
- Rotating drum AISI 304
- Reproducibility 5 percent.
- Compliant with ASTM standard method D4058-96.

ZQJ-II Grain Crushing Strength Tester: The GCS Tester consists of an automatic press controlled electronically which allows determination of resistance to crushing of catalyst grains during handling and usage. The grain of catalyst is placed on the anvil of an appropriate transducer and a mobile piston, operated by a stepping motor, crushes the grain. An electronic device measures the peak value when the grain breaks and keeps it displayed on a digital display.

- Specifications:
- Force range : 0 500N
- Precision grade : 1
- Freewheeling speed : about 1mm/sec
- Maximum height : 100

Pervaporation unit consists of stainless pervaporation cell, glass trap connected by Teflon tubing. It is also provided with Telstar-make double stage vacuum, and Grant-make thermostatic bath to maintain field temperature. Specifications:

- Feed capacity: 250 ml
- Feed temperature:  $30-100^{\circ}$  C
- Downstream pressure: < 5 mbar

Crush strength tester



# 15.2 Library

PPISR has a well-maintained library of over 1000 books spanning Maths, Physics, Chemistry, Biology, Materials Science and other interdisciplinary subjects. It is open all 24 hours for reference. Apart from books with scientific and technical content, it houses books of general interest, magazines and daily newspapers. The library also contains a reasonably good collection of Indian and international journals in print and a reasonably large collection of e-journals.



## **15.3** Computers and internet

Each faculty and student is provided with a desktop computer. A central computing facility of two GPU-based supercomputers with Intel Xeon 8 core machines with 32 GB RAM each are available. These are outfitted with multi-core DDR3 based powerfu NVidia GPU's for CUDA computing.

A dedicated 1 MBPS radio link provided by Tulip Inc. from their nearby Dodballapur station, supplemented with an optical fiber link from the local tower to the labs, provides sufficient internet capacity for download and upload.

# 15.4 Other Facilities

Institute is also equipped with emergency generators (2 generators, 50 kVA and 25 kVA) to power the campus, including student and faculty apartments. Additionally, experimental labs are supported by separate UPS-systems. A dedicated tower maintained by Tulip Telecom connects the campus to the world through a dedicated unlimited download link. Thirty desktops/servers and two super-computers used for intensive calculations are also a part of the common facility provided by the institute for scientists. In addition to the above mentioned Analytical Facility, there are also several sophisticated equipment used by each division according to their needs.

The Biological Sciences division is set up in more than 3000 sq. ft lab space equipped with advanced instruments for research in molecular biology, microbiology and crystallography. Major instruments include PCR machine, shaker incubator, phase contrast microscope with attached camera, laminar air flow system, -20C freezer, nitrogen storage dewars, hot air oven, BOD incubators, autoclave, pH and conductivity meter, magnetic stirrer, gel electrophoresis systems, state-of-the art protein crystallization tools and kits and other minor instruments required for everyday laboratory use. In addition to these we also house a powerful computer installed with all crystallography software required for macromolecular crystallography.

The Materials Science division has a well developed, large laboratory which houses furnaces, ovens, a high precision electronic balance, autoclaves, syringe pumps, heating mantles, stirrers and other basic apparatus/ glassware for materials synthesis. In addition to basic synthesis lab, it is also houses the catalytic reactor where gram level catalysis testing is undertaken. A Gas chromatorgraph is also available for analyzing the products of any reaction. The Theoretical Sciences division has sufficient computational facilities for theoretical calculations. The division is equipped with two Supercomputers with Intel Xeon 8 core machines with 32 GB RAM each. These are also outfitted with multi-core DDR3 based powerful Nvidia GPUs for CUDA computing

# 16. Campus life

The Bidalur campus houses hostel rooms for students and faculty apartments with a beautiful view of

the famous Nandi hills. Most selected graduate students working towards their PhD degree stay on campus and are provided with ample and comfortable hostel facilities. Each furnished two-bedroom apartment with a large living area and kitchen is shared by two research scholars.



Various kinds of recreational activities are organized in the PPISR campus to relieve the students from the monotony of day-to-day research studies. Since PPISR is situated in the outskirts of Bangalore, the greenery and clear air, untainted by the hustle and bustle of the city, is a nature lovers paradise. It is a pleasure to witness the sunrise every day while exercising, jogging etc in the campus. The research students have started a Poornaprajna Badminton club which operates between 6-8 am. After a full days work, students also play cricket in quadrangle in front of the main building between 5-6:30 pm. This helps them relieve the stress and tensions of the day. For

students interested in Indoor activities, Table Tennis (TT), Carom, chess games are ideal and provided. Every fortnight movies in various languages are screened in the auditorium; initiative for screening these movies is taken by a couple of students.

Sports facilities, used by faculty members and students alike, include indoor games indoor games like carom board and table tennis, and outdoor games like shuttle badminton.

**Independence Day** was celebrated at Bidlur campus by the PPISR members. The Director Prof. A. B. Halgeri hoisted the flag, with brief talks by him and Financial Advisor, Mr. Sreenivasa Rao.

Sarasvati Pooja and Ayudha Pooja were performed in the Bidlur campus on Oct 20, 2012, during which books, instruments and vehicles were decorated and worshipped. The function was officiated by a priest from a nearby temple.



The beautiful campus away from the busy life of Bengaluru city is a free resort for students and faculty. As a tradition, visitors to the campus are requested to plant a tree of remembrance. We believe that this tradition not only keeps the memory of a visitor but also helps make our campus more greener and

remind us to stay close to Nature.

# 17. Visitors' Views

#### Dr. Rajeshwar Dongara, Reliance Industries Pvt. Ltd, Jamnagar

"Ambience and ambition are integrated in Poornaprajna Institute, a noble place for a scientist's dreams to be associated with. Thanks to Dr. ABH for providing a great opportunity."

Dr. N. Lingaiah, IICT, Hyderabad

"An interesting place with a lot of enthusiasm. The facilities are good and impressive compared to other institutes funded by the public. There is a clear scope for this institute to reach its highest level. All the best to all the dedicated researchers working in this pleasant atmosphere."

#### Prof. Vilas Shirhatti, Birla Research and Life Sciences, Mumbai

"very impressive set in terms of ambience, infrastructure and the great talent and high quality of research being done. In a short span of time, the institute has come a long way. It certainly has a bright future."

## Dr. V. N. Chowdhury, General Manager (R&D) HPCL, Bangalore

"Impressed with the whole place. Labs, building, architecture. The place is quiet and away from the city, but close to Nature. Excellent work is being done at the center, useful for mankind, in line with the vision. Great experience on visiting the institute."

## Prof. M. S. Hegde, IISc, Bangalore

"I feel really hmble in this place. I would like to come and learn more from the young scientists here."

- **Prof. V. Prakash,** Distinguished scientist of CSIR, CFTRI, former Director, Mysore "PPISR is the *KOHINOOR* of the institutions of learning and teaching and research in the materials sciences, life sciences and catalysis."
- Prof. K. C. Patil, (Rtd) IPC, IISc, Bangalore"I am deeply impressed by the infrastructure, experimental facilities in the institute. It is an ideal place to do creative research and development into industrial products."

## Mr. S. Ramesh, Gen. Manager (QC, R&D), MRPL, Mangalore "Excellent environment and facilities for innovative research. Impressed on rightly motivated and young research staff."

## Dr. M. V. Chowdhari, Gen. Manager (R&D), HPCL, Bangalore

"Impressed with the whole place, laboratories, building architecture. The place is quite away from the city, close to Nature. Excellent work is being done at the center, is useful for mankind in line with HH Sri Vibudhesha Theertha Swamiji's vision. Great experience visiting the institute and interacting with Dr. Halgeri and his colleagues."