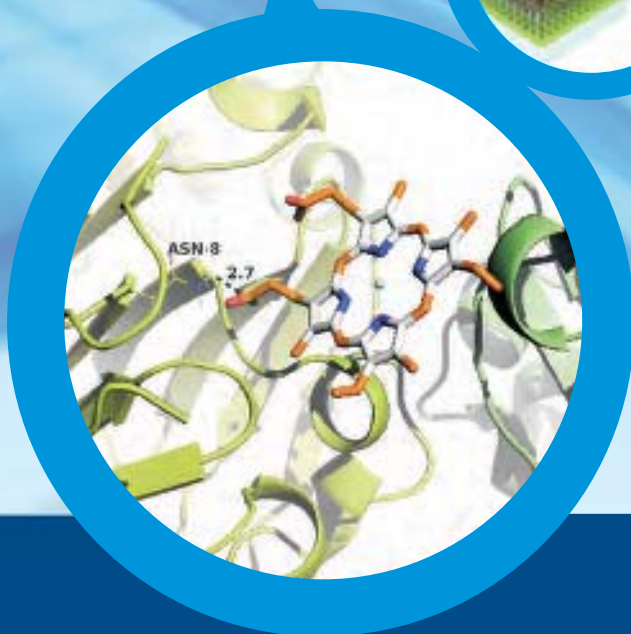
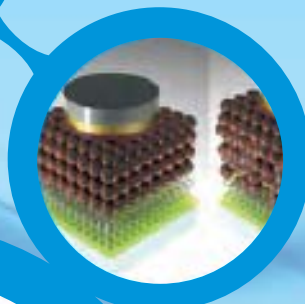
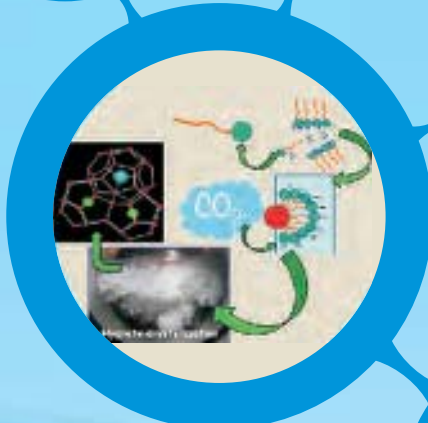




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Dr. Sourav Pal

Director, CSIR-NCL

Compiled and Edited by

Dr. P. K. Ingle

Head

Publication and Science Communication Unit
CSIR-NCL

Editorial Assistance

Mr. G. S. Mane

PSC Unit, CSIR-NCL

Designed by

Ms. Sonali Shinde

PSC Unit, CSIR-NCL

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ANNUAL REPORT

2013 - 14

With Best Compliments from

Dr. Sourav Pal
Director

CSIR-National Chemical Laboratory

Dr. Homi Bhabha Road, Pune 411 008, India
Ph: (Off) +91 20 2590 2600; Fax: +91 20 2590 2601
Email: director@ncl.res.in; URL: ncl-india.org

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CONTENT

निदेशक की कलम से...

वर्ष 2013-14 के लिए सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला का वार्षिक प्रतिवेदन प्रस्तुत करते हुए मुझे अत्यंत हर्ष हो रहा है। वार्षिक प्रतिवेदन हमारी अनुसंधान संबंधी उपलब्धियों तथा हमारे प्रदर्शन के कई मापदंडों को दर्शाता है और मैं यह जानकर अत्यंत प्रसन्न हूँ कि प्रतिवर्ष हमारे प्रदर्शन में निरंतर सुधार आ रहे हैं। पिछले कुछ वर्षों में विशेष रूप से, हमारे प्रकाशनों के साथ ही एकस्व (पेटेंट) प्रस्तुत करने में विशेष बढ़ोतरी हुई है और इस वर्ष भी प्रकाशन और एकस्व की संख्या बढ़ी है। हमने उद्योगों के साथ हमारे सहयोग को मजबूत किया है, जिसका परिणाम अनुकूलित प्रौद्योगिकी हस्तांतरण के रूप में सबके सामने है। वर्ष 2013-14 के दौरान हमारी बाहरी नकद आय भी पिछले वर्ष की आय के अनुरूप बनी हुई है। मैं इस प्रयोगशाला को गौरवान्वित करने के लिए सभी एनसीएल स्टाफ को बधाई देता हूँ।

वर्ष के दौरान बहुत से महत्वपूर्ण कार्यक्रमों का आयोजन हमारे द्वारा किया गया। सीएसआईआर-एनसीएल में विश्व के प्रख्यात वैज्ञानिकों के विभिन्न व्याख्यान इस दौरान आयोजित हुए। भारतीय विज्ञान संस्थान, बेंगलूर के प्रो.ए.के.सूद ने सीएसआईआर-स्थापना दिवस समारोह में 'ड्राइवन सॉफ्ट एंड ग्रेन्युलर मेटर' पर व्याख्यान दिया। प्रो.पियरे एच. डिक्सनेफ, CNRS- Université de Rennes, फ्रांस ने "Tunable Ruthenium Catalysts for Carbene Reactions, C-H Bond Functionalization as Key Steps for Green Chemistry" विषय पर प्रो.बी.डी.तिलक स्मृति व्याख्यान प्रस्तुत किया। प्रो. के.के. बालसुब्रमणियम ने "Atropisomerism of biheterocycles Synthesis and study of atropisomerism in 4-4'-chromenes and a few interesting domino transformations of 4-chloro-benzopyran and 4-chloro-benzothiopyran-3-carboxyaldehydes" विषय पर प्रो. वेंकटरमन स्मृति व्याख्यान प्रस्तुत किया। इसके अलावा प्रो. दीपांकर चटर्जी, अध्यक्ष, भारतीय विज्ञान अकादमी ने सीएसआईआर-स्थापना दिवस पर 'सर्वाइवल अंडर स्टारवेशन' नामक विषय पर व्याख्यान दिया। प्रो. ज्योति चट्टोपाध्याय, रासायनिक जीवविज्ञान प्रमुख, उप्सला विश्वविद्यालय जैवचिकित्सा केंद्र, स्वीडन ने राष्ट्रीय विज्ञान दिवस पर व्याख्यान प्रस्तुत किया। प्रो. दौरास्वामी रामाकृष्णा, पुरड्यू विश्वविद्यालय, यूएसए ने 'डायनामिक मॉडलिंग ऑफ मेटाबोलिक

सिस्टम्स: द साइबरनेटिक एप्रोच' नामक विषय पर एल. के. दोरायस्वामी स्मृति व्याख्यान दिया। इसके अलावा राष्ट्रीय प्रौद्योगिकी दिवस पर डॉ. बी.गोपालन, कार्यकारी निदेशक, आर्किड फार्मा, चैन्नई द्वारा व्याख्यान प्रस्तुत किया गया।

इस वर्ष हमने सीएसआईआर के प्रथम महानिदेशक सर शांति स्वरूप भटनागर की स्मृति में नई व्याख्यान माला आरंभ की है। प्रो.सीएनआर राव ने 'सेलिब्रेशन ऑफ साइंस' विषय पर प्रतिष्ठित सर शांति स्वरूप भटनागर उद्घाटन व्याख्यान प्रस्तुत किया।

वर्ष 2011-12 से एनसीएल के भूतपूर्व शोध-छात्रों द्वारा ग्लोबल एलुमिनी मीटिंग आयोजित की जा रही है। तीसरे ग्लोबल एलुमिनी सम्मेलन के अवसर पर हमने हमारे प्रतिष्ठित भूतपूर्व शोधछात्र तथा डॉ.अंजी रेड्डी लैब के संस्थापक डॉ. के.अंजी रेड्डी की स्मृति में एक नई व्याख्यान माला आरंभ की है। इस अवसर पर भारतीय विज्ञान संस्थान, बंगलूर के प्रो. गोवर्धन मेहता ने 'ए सफारी इन द वर्ल्ड ऑफ केमिस्ट्री' विषय पर डॉ. के.अंजी रेड्डी स्मृति व्याख्यान प्रस्तुत किया।

इस अवधि में प्रयोगशाला के द्वारा आर.एम.मशेलकर प्रतिभा व्याख्यानों के अलावा विभिन्न सम्मेलनों, संगोष्ठियों, कार्यशालाओं का भी आयोजन किया गया। अनुसंधान संबंधी गतिविधियों को बढ़ावा देने की दृष्टि से विभिन्न कार्यशालाएं और संगोष्ठियों का आयोजन किया गया। यह अत्यंत महत्वपूर्ण बात है कि इन सभी कार्यक्रमों में हमारे विद्यार्थियों ने सक्रिय रूप से प्रतिभागिता की। 'इन्टेंसिफिकेशन एंड अप - स्केलिंग ऑफ कंटिन्युस प्रोसेस' विषय पर कार्यशाला, 'बॉयोटेक्नालॉजी बियांड बार्डर' विषय पर इंडो - मेक्सिको कार्यशाला, एंडवांस्ड ग्लायकेशन पर लघु संगोष्ठी, एवं "वंडरलैंड ऑफ मालिक्युलर स्ट्रक्चर्स थू द लुकिंग ग्लास आफ एक्सरे क्रिस्टलोग्राफी" विषय पर संगोष्ठी का आयोजन किया गया। इसके अतिरिक्त एनसीएल - एलुमिनी ग्लोबल मीट 2014 का आयोजन अत्यंत उत्साहपूर्वक किया गया।

हमने प्रौद्योगिकी विकास करने तथा उसे उद्योग जगत को हस्तांतरित करने के अपने प्रयास जारी रखे हैं।

पिछले वर्ष में हमने उद्योग जगत में विभिन्न प्रक्रियाओं के परिचालन हेतु कई प्रौद्योगिकियों/तकनीकी जानकारीयों के उपयोग की अनुमति प्रदान की। प्रौद्योगिकी और प्रक्रियाओं के व्यवसायीकरण में लघु उपकरणों का प्रयोग करते हुए डायरेक्ट यलो 11 डाइ के सतत प्रवाह संश्लेषण, मछली के प्रोटीन, जिसे जिलेटिन कहते हैं, के एन्जाइमेटिक हाइड्रोलिसिस द्वारा पॉलीपेप्टाइड के विकास की प्रक्रियाएं भी सम्मिलित हैं। हमारी प्रयोगशाला द्वारा कार्यात्मक परफ्लूरोपॉलीईथर (PFPE) के यौगिक के निर्माण की प्रक्रिया का व्यवसायीकरण किया गया तथा हॉलो फाइबर मेम्ब्रेन तैयार करने हेतु तकनीकी जानकारी उपयोग करने की अनुमति भी प्रदान की गई।

इस प्रतिवेदन में वर्ष 2013-14 के दौरान हमारे द्वारा विभिन्न क्षेत्रों में किए गए अनुसंधानों की जानकारी प्रस्तुत की गई है तथा मुझे आशा है कि इसमें आपको सीएसआईआर – एनसीएल में हमारे द्वारा

किए जा रहे अनुसंधान तथा विकास कार्यों का परिदृश्य दिखाई देगा। हम रासायनिक अभियांत्रिकी और जैव विज्ञान सहित रासायनिक और संबद्ध विज्ञान के व्यापक क्षेत्र में अपार संभावनाओं को देखेंगे। प्रकाशनों की गुणवत्ता में अनुसंधान की गहराई भी स्पष्ट रूप से परिलक्षित है। हमारे बहुत से सहयोगियों ने विभिन्न सम्मान तथा पुरस्कार प्राप्त किए हैं, इसके लिए मैं उन सबको बधाई देता हूँ।

अन्त में मैं प्रयोगशाला से सभी स्टाफ सदस्यों तथा सीएसआईआर-एनसीएल की अनुसंधान परिषद एवं प्रबन्ध परिषद के सदस्यों की सहायता तथा सहयोग के लिए अपना आभार प्रकट करता हूँ। मैं अपने विभिन्न हितधारकों द्वारा दिए गए सहयोग के लिए भी अपनी कृतज्ञता प्रगट करता हूँ। उनकी सलाह और सहयोग हमारी उपलब्धियों के लिए सहायक है। मुझे पूरा विश्वास है कि हममें उनका दृढ़ विश्वास भविष्य में हमें नई उँचाइयों पर ले जाएगा।

सौरव पाल

(सौरव पाल)



स्वतंत्रता दिवस पर कर्मचारियों को संबोधित करते हुए डॉ. सौरव पाल

From the Director's Desk...

I am happy to present the Annual Report of CSIR-National Chemical Laboratory for the year 2013-14. The report highlights our research achievements and displays several parameters of performance of the laboratory. I am happy to inform that the performances are continuing to improve year by year. For last few years, we have seen a significant increase in publications and patents. This year also we have an improvement in the numbers. We have strengthened our association with the industries resulting in the optimized technology transfer. The external cash earnings for the year 2013-14 have remained steady at the level of the previous year which in stile. I congratulate all the staff for making the laboratory proud.

Several precious events took place during the year. Various talks by eminent scientists from across the world were organized at CSIR-NCL. Prof. A. K. Sood, Indian Institute of Science Bangalore delivered the CSIR-NCL Foundation Day lecture on "Driven soft and granular Matter". Prof. Pierre H. Dixneuf, CNRS- Université de Rennes, France delivered the Prof. B. D. Tilak Memorial Lecture on "Tunable Ruthenium Catalysts for Carbene Reactions, C-H Bond Functionalization as Key Steps for Green Chemistry" and Prof. K. K. Balasubramanian rendered the Prof. K. Venkatraman Memorial Lecture on the topic "Atropisomerism of biheterocycles Synthesis and study of atropisomerism in 4-4'-chromenes and a few interesting domino transformations of 4-chloro-benzopyran and 4-chloro-benzothiopyran-3-carboxyaldehydes".

Prof. Dipankar Chatterji, President, Indian Academy of Sciences delivered the CSIR-Foundation Day Lecture on "Survival under Starvation". Prof. Jyoti Chattopadhyaya, Chair of Chemical Biology, Uppsala University Biomedical Center, Sweden spoke on the occasion of National Science Day Lecture. Prof. Doraiswami Ramkrishna, Purdue University, USA rendered the L. K. Doraiswamy Honor Lecture on "Dynamic Modeling of Metabolic Systems: The Cybernetic Approach". National Technology Day Lecture was given by Dr. B. Gopalan, Executive Director, Orchid Pharma, Chennai.

This year, we initiated a new series of lectures in the memory of our beloved first Director General of CSIR Sir Shanti Swarup Bhatnagar. Prof. C. N. R. Rao delivered the inaugural Sir Shanti Swaroop Bhatnagar Distinguished Lecture on the topic "Celebration of Science".

NCL Alumni has been celebrating global alumni meeting since 2011-12. On the occasion of third global meet, we initiated a new lecture series in memory of Dr. K. Anji Reddy, our distinguished alumni and founder of Dr. Reddy's Lab. Prof. Goverdhan Mehta, Indian Institute of Science, Bangalore delivered the Dr. K. Anji Reddy Memorial Lecture on "A Safari in the world of Chemistry".

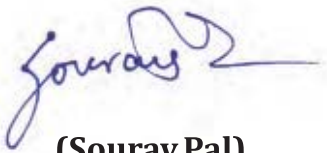
The laboratory hosted several symposia, conferences, workshops besides R. A. Mashelkar Endowment Lectures. Different workshops and symposia were organized to support the research activities. Most important is that students

participated actively in such events. Events like workshop on intensification and up-scaling of continuous processes, Indo Mexico workshop on 'Biotechnology Beyond Borders', mini symposium on Advanced Glycation and Symposium on 'Wonderland of Molecular Structures through the Looking-Glass of X-ray Crystallography' were organized. In addition, NCL AlumniGlobal Meet 2014 was also organized with full enthusiasm.

We have continued our efforts to develop technologies and deliver to the industries. In the last year, we have licensed many technologies/ know-how for various processes. The technologies and processes commercialized included the development of a process for continuous flow synthesis of direct Yellow 11 dye using miniaturized devices, the development of a process for polypeptides by enzymatic hydrolysis of the fish protein called gelatin. The process for the manufacture of functional perfluoropolyether (PFPE) derivative was commercialized and the Preparation was also done.

The Annual Report highlights the research took place in 2013-14 in different areas and hopefully provides you an overview of the research and development that the laboratory has carried. We will notice a very good breadth in broad area of chemical and allied sciences including chemical engineering and biosciences. The depth of research is also evident in the quality of publications. Several of our colleagues received distinctions and laureates. I congratulate all of them.

Finally, I wish to acknowledge the support and co-operation of all staff, members of Research Council and Management Council of CSIR-NCL, DG-CSIR and staff of CSIR, New Delhi. I also acknowledge our various stakeholders. Their advice and cooperation have been helpful in our endeavor. I am sure that their confidence in us will take us forward in the coming years.



(Sourav Pal)

Vision

- To be a globally recognized and respected R&D organization in the area of chemical sciences and engineering
- To become an organization that will contribute significantly towards assisting the Indian chemical and related industries in transforming them-selves into globally competitive organizations
- To become an organization that will generate opportunities for wealth creation for the nation and, thereby, enhance the quality of life for its people

Mission

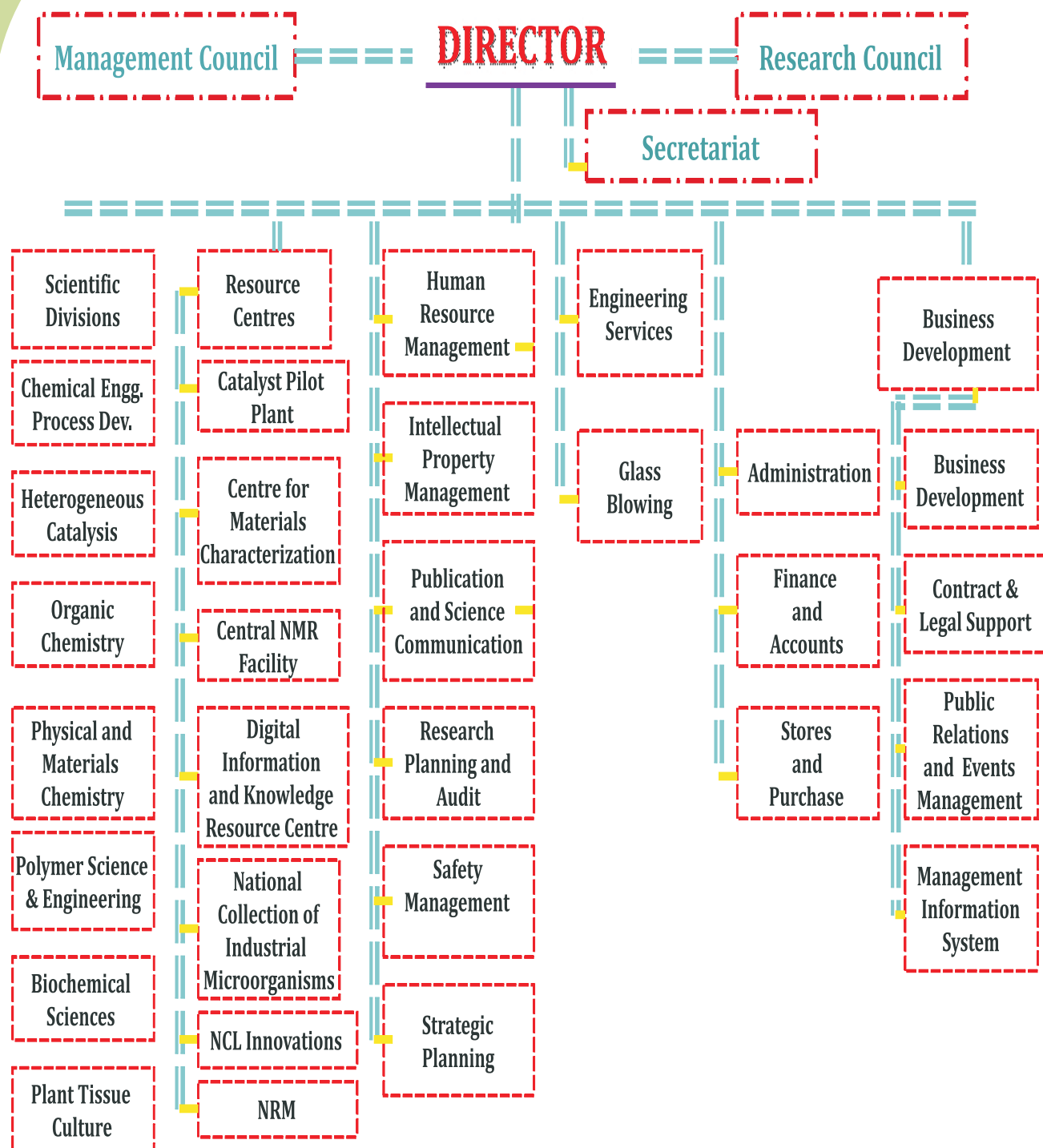
- To carry out R&D in chemical and related sciences with a view to eventually deliver a product, process, intellectual property, tacit knowledge or service that can create wealth and provide other benefits to CSIR-NCL's stakeholders
- To build and maintain a balance portfolio of scientific activities as well as R&D programs to enable CSIR-NCL to fulfill the demands of its stakeholders, present and future
- To create and sustain specialized Knowledge Competencies and Resource Centers within CSIR-NCL which can provide support to all stakeholders of CSIR-NCL
- To contribute to the creation of high quality Ph.D. students with competencies in the area of chemical, material, biological and engineering sciences

Guiding Principles & Values

- To be deeply committed to the success of our stakeholders
- To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency
- To encourage a culture of collective and principle-centred leadership
- To value the dignity of the individual and deal with people with a sense of fairness and without bias, prejudice or favour
- To nurture the highest standards of integrity and ethical conduct

Annual Report 2013-14

Organisation Chart



Annual Report 2013-14 Research Areas

Catalysis

- ✓ Heterogeneous catalysis
- ✓ Organometallic chemistry
- ✓ Surface science

Organic Chemistry

- ✓ Catalysis and new methods
- ✓ Chemical biology
- ✓ Industrial organic chemistry
- ✓ Natural product chemistry
- ✓ Medicinal chemistry
- ✓ Total synthesis

Physical and Materials Chemistry

- ✓ Biomimetic materials
- ✓ Materials for optoelectronics, magnetic and gas storage
- ✓ Quantum electronic and structure theory
- ✓ Soft matter: Theory and simulation
- ✓ Synthesis of materials including nanomaterials

CSIR-NCL serves to various sectors such as

- ✓ Solar Energy,
- ✓ Clean coal
- ✓ Fuel cell
- ✓ Healthcare
- ✓ Agriculture
- ✓ Chemicals & Petrochemicals
- ✓ Water
- ✓ Materials
- ✓ Sustainable environment

Biochemical Sciences

- ✓ Enzymology and microbiology
- ✓ Plant molecular biology
- ✓ Plant tissue culture
- ✓ Proteomics and metabolomics
- ✓ Structure biology

Polymer Science and Engineering

- ✓ Advanced polymeric materials for energy, healthcare, water, security and strategic areas
- ✓ Biomass chemistry and technology
- ✓ Polymer chemistry
- ✓ Polymer engineering
- ✓ Polymer physics

Chemical Engineering Science

- ✓ Bio-chemical & biological engineering
- ✓ Energy & environmental engineering
- ✓ Industrial catalysis and catalytic processes
- ✓ Industrial flow processes
- ✓ Mathematical & computational modeling
- ✓ Process development and scale-up
- ✓ Process intensification & engineering

Centers of Excellence

During the last few years, CSIR-NCL has initiated five Centers of Excellence to encourage and carry out excellent research in specified areas by bringing in like-minded people from various divisions together through discussions and to train staff and students in doing quality research using the best infrastructure and facilities.

- ✓ Micro reactor Engineering
- ✓ Scientific Computing
- ✓ Solar Energy
- ✓ Surface Science
- ✓ Sustainable Polymer Industry through Research Innovation & Training

Chairperson

Prof. D. D. Sarma
Solid State & Structural Chemistry
Indian Institute of Science
Bengaluru



Members

Prof. Uday Maitra

Department of Organic Chemistry
Indian Institute of Science
Bengaluru

Prof. V. Chandrasekhar

Centre for Interdisciplinary Sciences
Tata Institute of Fundamental Research
Hyderabad

Dr. Sumit Bhaduri

Department of Chemistry
Indian Institute of Technology, Mumbai

Shri Yogesh M. Kothari

Alkyl Amines Chemicals Ltd.
Dr. Annie Besant Road, Worli, Mumbai

Dr. R. Brakaspathy (Agency Representative) **Dr. Pushpito K. Ghosh (DG Nominee)**

Department of Science and Technology
New Mehrauli Road, New Delhi

Director,
CSIR- CSMCRI, Bhavnagar

Dr. Rajesh S. Gokhale (Sister Laboratory)

Director, CSIR- IGIB,
Delhi

Head or His Nominee (Permanent Invitee)

Planning & Performance Division
CSIR, New Delhi

Dr. Suresh Das (Cluster Director)

Director, CSIR - NIIST
Thiruvananthapuram

Dr. Sourav Pal (Director)

Director, CSIR - NCL
Pune



Dr. G. S. Grover
Member Secretary
CSIR - NCL, Pune

Chairperson

Dr. Sourav Pal
Director, CSIR-NCL



Dr. Anil Kumar
Scientist

Dr. G. J. Sanjayan
Scientist

Dr. (Ms) Sarika Maitra Bhattacharyya
Scientist

Dr. Meitram Niraj Luwang
Scientist

Dr. (Mrs) A. A. Prabhune
Technical Officer

Mr. G. Prabhakaran
Scientist

Dr. B. D. Kulkarni
Distinguished Scientist

Dr. V. V. Ranade
Outstanding Scientist



Representative from sister Laboratory

Dr. S. R. Wate
Director,
CSIR-NEERI,
Nagpur



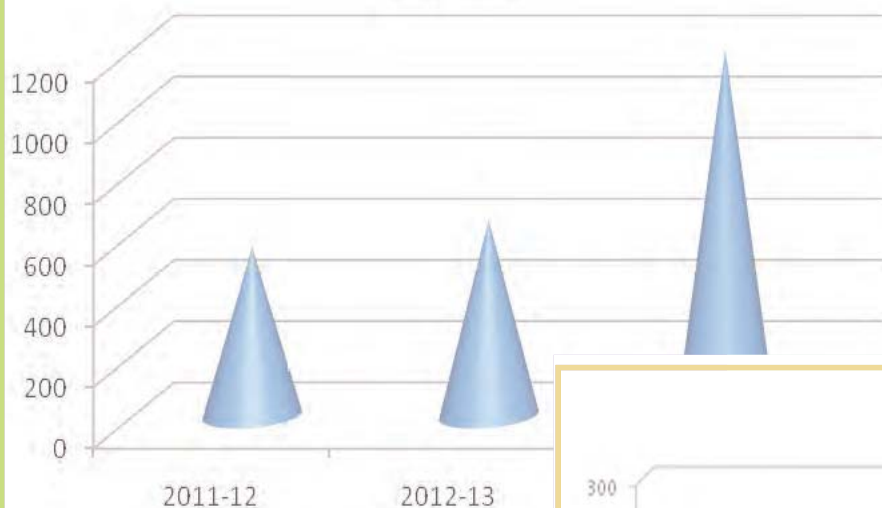
Member Secretary

S. K. Gupta
Controller of Administration, CSIR-NCL

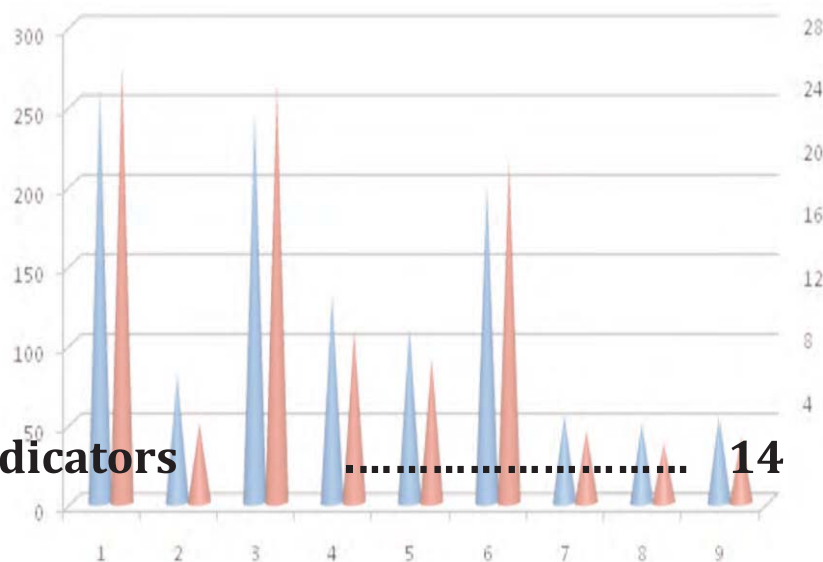
PERFORMANCE

INDICATORS

₹ in Lakhs

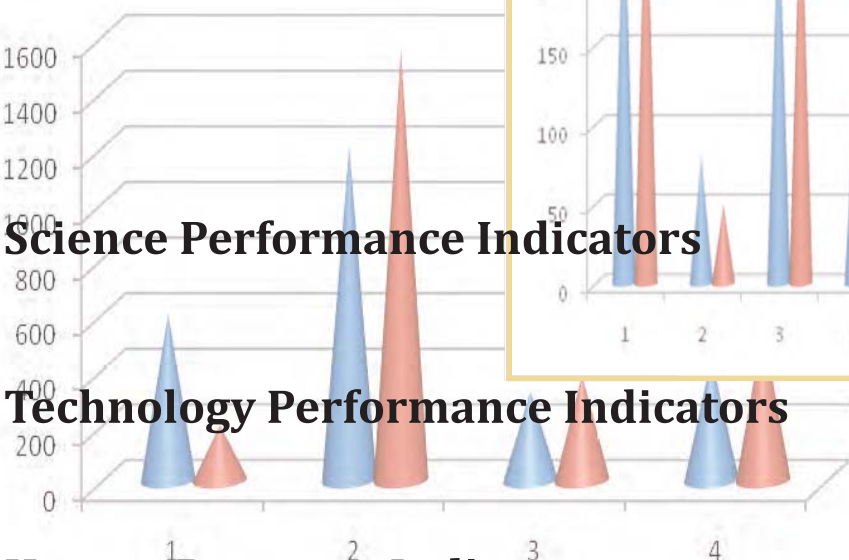


Science Performance Indicators



14

Technology Performance Indicators



15

Human Resource Indicators

Financial Performance Indicators

Outputs and Outcomes

16

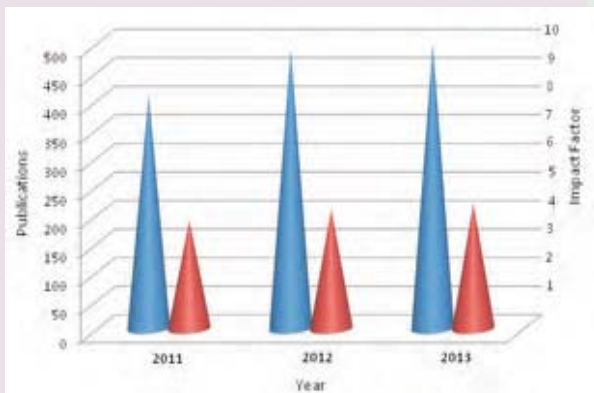
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23

Annual Report 2013-14

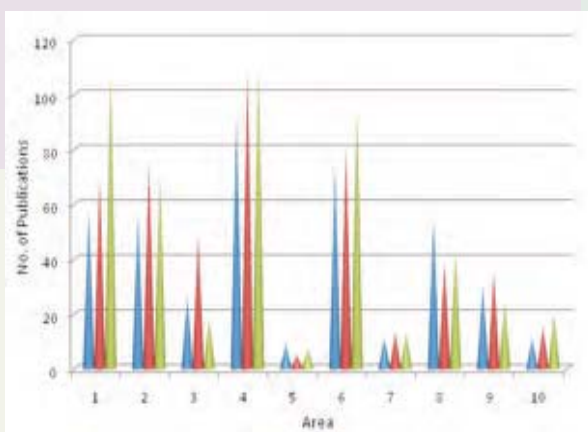
Science Performance Indicators

Research Output: Publications



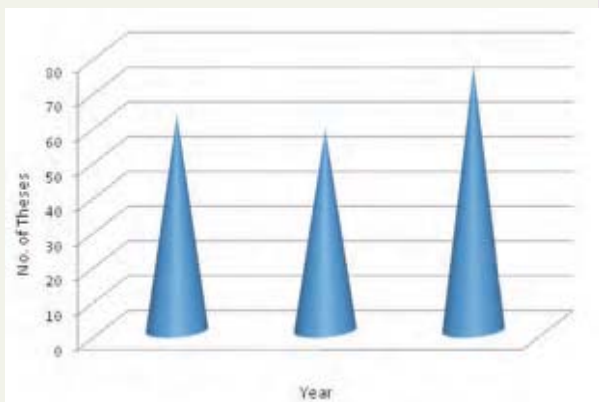
Year	2011	2012	2013
Total Papers	389	460	467
Average Impact Factor	3.29	3.69	3.96

Areawise Publications



Year	2011	2012	2013
1. Biological Sciences and Engineering	57	69	101
2. Catalysis and Surface Science	56	65	64
3. Chemical Engineering Sciences	26	46	18
4. Materials Chemistry	89	109	109
5. NMR	6	2	3
6. Organic Chemistry	65	75	85
7. Physical Chemistry	7	8	8
8. Polymer Science and Engineering	50	39	40
9. Structural Chemistry	25	32	21
10. Theory and Computational Science	07	10	17

Ph. D. Theses

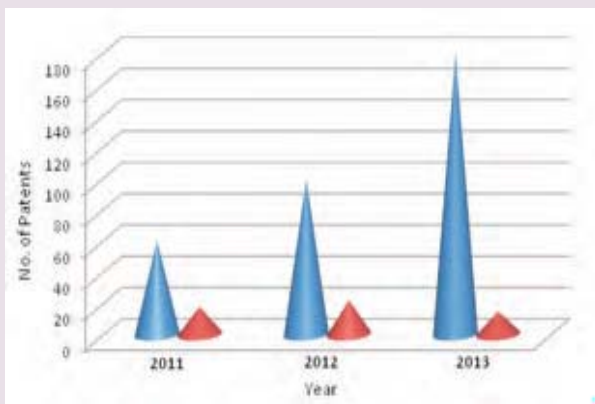


Year	2011	2012	2013
No. of Theses	58	52	70

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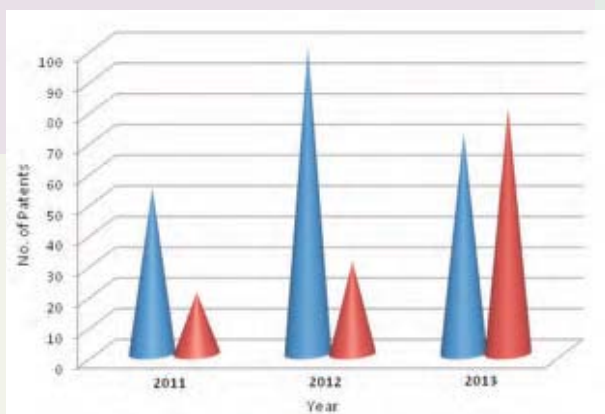
Technology Performance Indicators

Indian Patents: Filed and Granted



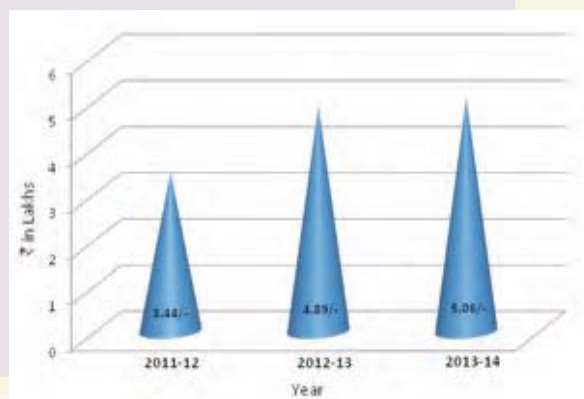
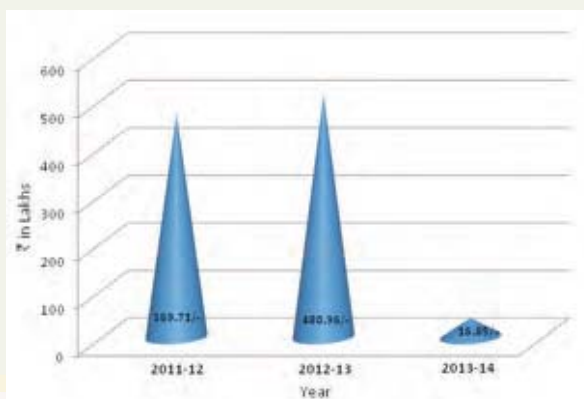
Year	2011	2012	2013
Filed	56	86	173
Granted	12	19	10

Foreign Patents: Filed and Granted



Year	2011	2012	2013
Filed	49	96	67
Granted	13	22	72

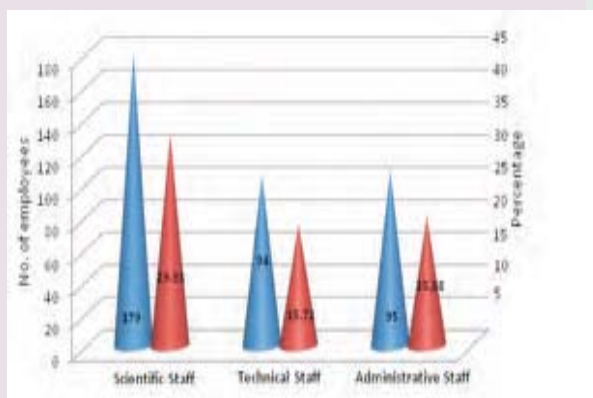
Revenue Generated from CSIR-NCL's IP (Revenue Trends Report)



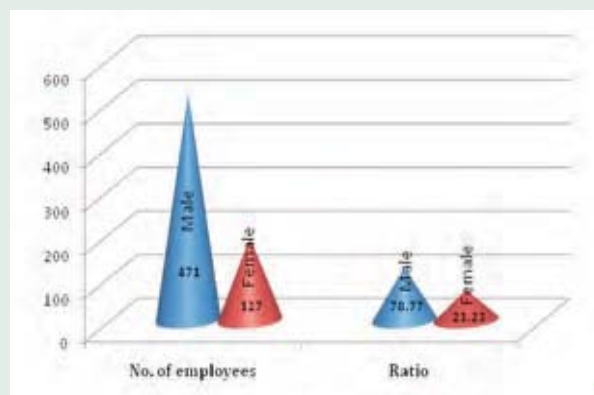
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Human Resource Indicators

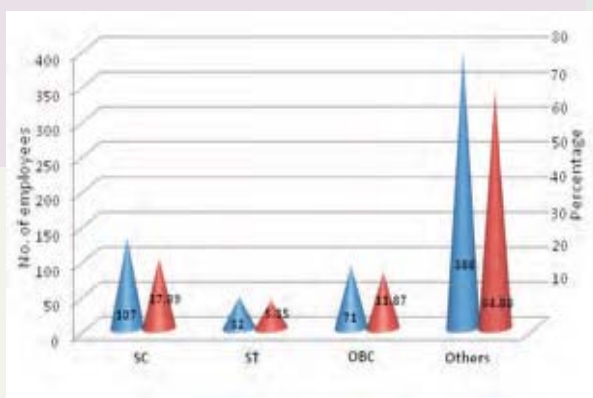
Total Staff: 598



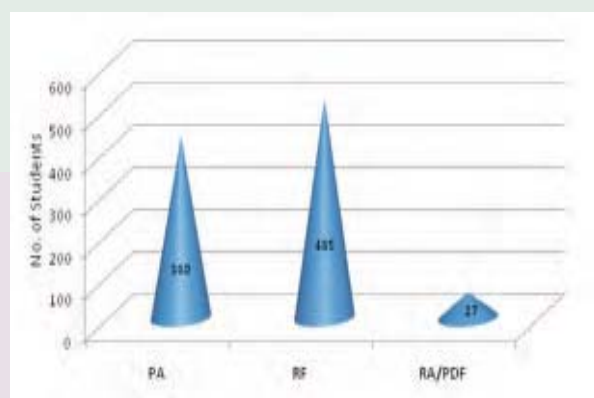
Male and Female Employees



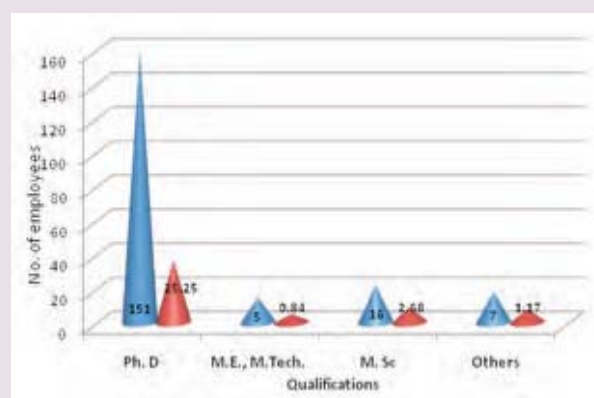
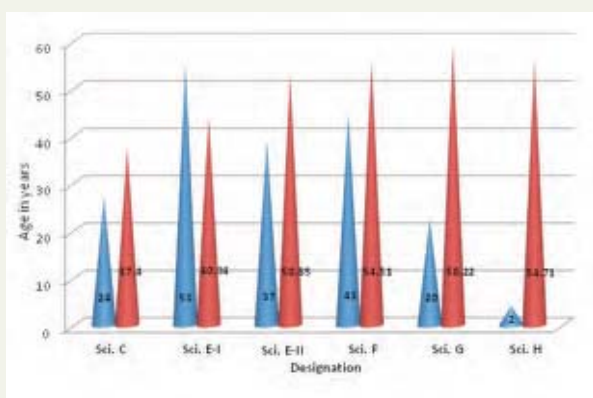
SC, ST, OBC and Others



Students and Project Staff



Scientific Staff: Age wise distribution





Dr. Amitava Das
(03.04.13)

Molecular recognition & biomarkers, Supramolecular chemistry and assembly interfacial electron transfer, Designing dye for solar cell application

- Ph. D., Jadavpur University, Kolkata (1989)
- M. Sc., Jadavpur University, Kolkata (1985)



Dr. S. Mhaske
(16.05.13)

Total synthesis and methodology development

- DST-Ramanujan Fellow Scientist, CSIR-NCL, Pune (June 2010 - May 2013)
- Post-doctoral Research Fellow, Alexander von Humboldt Foundation, University of Hannover, Germany (Feb 2008 - Mar 2010)
- Post-doctoral Research Associate, School of Medicine, Wayne State University, Michigan, USA (2007)
- Post-doctoral Research Scholar, Illinois Institute of Technology, Chicago, USA (2006) Ph. D., Organic Chemistry, CSIR-NCL, Pune (2005)



Dr. A. Ambade
(16.05.13)

Polymer synthesis, Supramolecular chemistry

- Fellow Scientist, CSIR-NCL, Pune (Oct 2010 - May 2013)
- Post-doctoral Research Fellow, New York University, USA (Aug 2007 - Nov 2008)
- Post-doctoral Research Fellow, Georgia Tech, USA (Mar 2007 - Jul 2007)
- Post-doctoral Research Fellow, University of Massachusetts, Amherst, USA (July 2004 - Feb 2007)
- Ph.D., Indian Institute of Technology, Bombay (2004)
- M. Sc., Organic Chemistry, University of Pune (1998)



Dr. Dhanasekaran
(16.05.13)

Molecular parasitology, Metabolomics, Apicomplexan parasite genomics, Anti-malarial and anti-toxoplasma chemical/Genetic screening

- CSIR Quick Hire Fellow, CSIR-NCL, Pune (Feb 2012 - May 2013)
- Post-doctoral Fellow, University of Pennsylvania, Philadelphia, USA (Mar 2004 - Dec 2011)
- Ph. D., Biochemistry, Indian Institute of Science, Bangalore (Aug 1997 - Mar 2004)
- M. Sc., Medical Biochemistry, Pondicherry University, Pondicherry (1994 - 1997)



Dr. Nilesh Mali
(01.07.13)

Process modeling and simulation, Process intensification, Thermally coupled distillation systems, Energy & exergy engineering, Vapor liquid equilibrium of fluids

- ✎ Ph. D., Chemical Engineering, Institute of Chemical Technology, Mumbai (2011)
- ✎ M. Tech., Chemical Engineering, Dr. Babasaheb Ambedkar Technological University, Lonere (2006)
- ✎ B. E., Chemical Engineering, Pune University (2004)



Dr. E. Balaraman
(15.07.13)

Organometallics & sustainable catalysis

- ✎ Research Assistant Professor, SRM Research Institute, Chennai [Jan 2012 - Jul 2013]
- ✎ Post-doctoral Fellow, Weizmann Institute of Science, Israel [Jul 2008 - Jan 2012]
- ✎ Ph. D., Chemistry, University of Hyderabad [Jul 2002 - May 2008]
- ✎ M. Sc., University of Madras, Chennai (2002)



Dr. S. Chinnathambi
(01.08.13)

Neuroscience and biochemistry, Mis-folded protein conformation and microtubule dynamics

- ✎ Post-doctoral Training at the German Center for Neurodegenerative Disease (DZNE)-Bonn and Max Planck Institute for Neurobiological Research (Hamburg-outstation), Hamburg, Germany
- ✎ Ph. D., Biochemistry, Max Planck Institute for Structural Molecular Biology, Hamburg, Germany
- ✎ M. Sc., Microbiology, Bharathidasan University, Tiruchirappalli



Dr. Nitin Patil
(14.08.13)

Metal catalysis and organocatalysis, Total synthesis of natural products

- ✎ Ph.D., University of Pune (2002)
- ✎ Post-doctoral Fellow, University of Göttingen, Germany (2002)
- ✎ JSPS Fellow, Tohoku University, Japan (2005)
- ✎ Assistant Professor, Tohoku University, Japan (2006)
- ✎ Research Fellow, Institute of Chemical and Engineering Sciences, Singapore (2007)
- ✎ Research Fellow, The Scripps Research Institute, USA (2008)



Dr. Arup K. Rath
(21.10.13)

Nanoscience & technology

- ✎ Post-doctoral Fellow, Institute of Photonic Sciences, Barcelona, Spain (Oct 2010 - Sep 2013)
- ✎ Ph. D., Indian Association for the Cultivation of Sciences, Kolkata (Jan 2006 - Sep 2010)
- ✎ M. Sc., Physics, Jadavpur University (2003-2005)



Dr. S. K. Jha
(10.01.14)

Protein folding; unfolding and aggregation, Enzyme catalysis, Spectroscopy

- ✎ Post-doctoral Scholar, University of California, Berkeley, USA (Apr 2012 - Jan 2014)
- ✎ Post-doctoral Scholar, Stanford University, Stanford, USA (Feb 2010 - Mar 2012)
- ✎ Ph. D, Biophysical Chemistry, National Centre for Biological Sciences, TIFR, Bangalore (Oct 2003 - Nov 2009)
- ✎ M. Sc., Chemistry, Indian Institute of Technology, Delhi (Aug 2001 - Aug 2003)



Dr. Sakya S. Sen
(31.01.14)

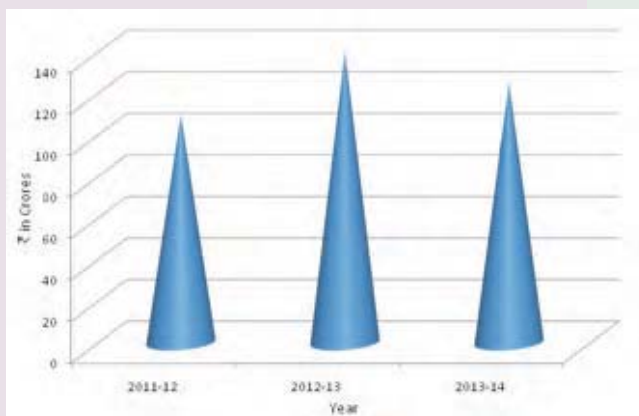
Organometallic chemistry, Homogeneous catalysis

- ✎ Alexander von Humboldt Post-doctoral Fellow, University of Würzburg, Germany (2011-2013)
- ✎ Post-doctoral Research Fellow, University of Göttingen, Germany (2010-2011)
- ✎ Ph. D., Chemistry, University of Göttingen, Germany (2006-2010)
- ✎ M. Sc., Chemistry, IIT Kharagpur (2004-2006)

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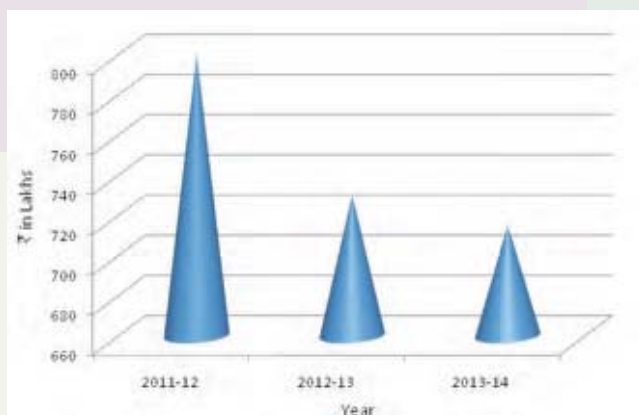
Financial Performance Indicators

CSIR Budget



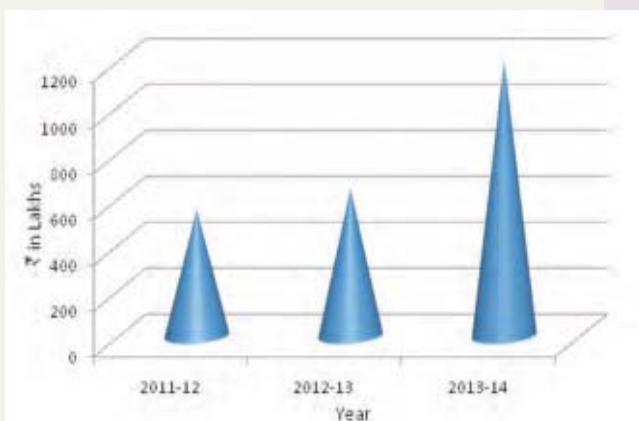
Year	₹ in Crores
2011-12	109.63 (CSIR Budget : 85.32 + Network Project : 17.70 + NMITLI Projects : 06.60)
2012-13	131.72 (CSIR Budget : 89.12 + Network Project : 37.86 + NMITLI Projects : 4.74)
2013-14	115.17 (CSIR Budget : 68.70 + Network Project : 41.26 + NMITLI Projects : 5.21)

Laboratory reserve: Receipts



Year	₹ in Lakhs
2011-12	795
2012-13	719
2013-14	712

Laboratory reserve: Expenditure

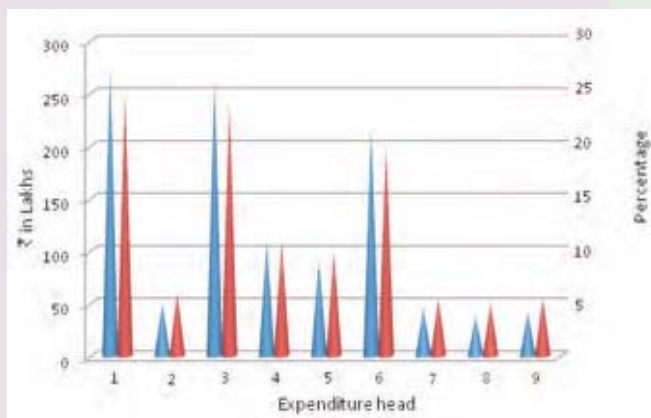


Year	₹ in Lakhs
2011-12	433
2012-13	483
2013-14	1128

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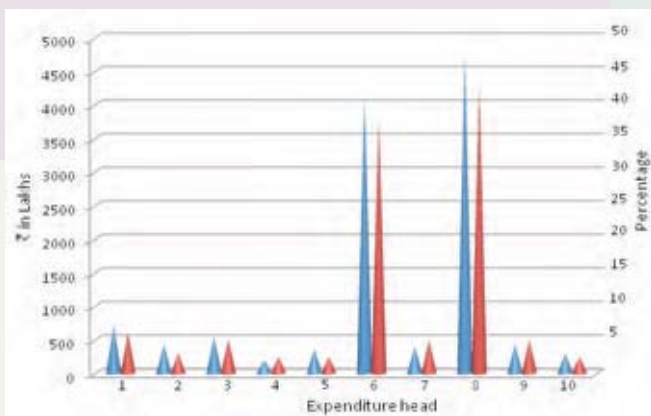
Financial Performance Indicators

Expenditure: Laboratory reserve



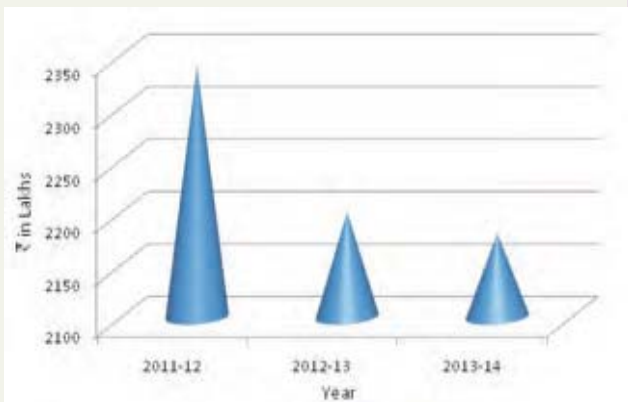
Expenditure head	Amount	%
1. Salary linked allowances	274.655	24
2. Library	49.866	5
3. Appliances and equipment + Comp. equip.	263.653	23
4. Contingencies	108.332	10
5. Maintenance (Lab. + Staff quarter)	90.952	8
6. Chemicals & Consumables	216.307	19
7. Work and services	45.189	4
8. Furniture	37.546	3
9. Construction of Staff Quarters	41.209	4

Expenditure: CSIR and Network Projects



Expenditure head	Amount	%
1. Appliances and equipment + Comp. equip.	612.50	5
2. Chemicals	225	2
3. Contingency	494.596	4
4. Library (Books, Journals and Electronic Journals)	90.213	1
5. Maintenance (Lab. + Staff quarter)	166.929	1
6. Network projects	4114.286	36
7. NMITLI projects	396.546	4
8. Salaries (Pay & Allow.)	4745.203	42
9. Staff quarter: construction	428.850	4
10. Work and services	100	1

External Income

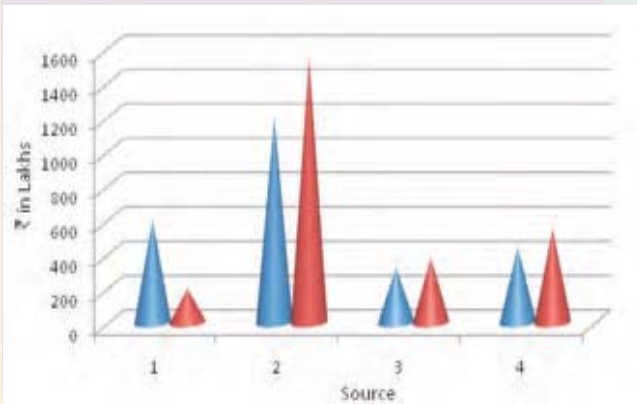


Year	₹ in Lakhs
2011-12	2335
2012-13	2191
2013-14	2151

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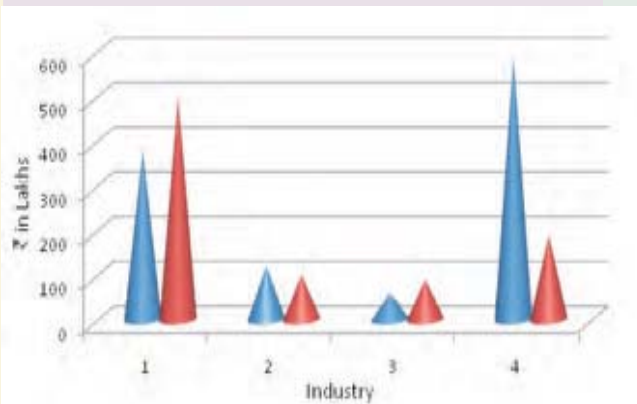
Financial Performance Indicators

ECF by Source



Source	2012-13 ₹ in Lakhs	2013-14 ₹ in Lakhs
1. Knowhow & Royalty/IP	481	22
2. Grant-in-aid-projects	1176	1409
3. Consultancy / technical services	204	281
4. Sponsored / collaborative projects	330	439
Total	2191	2151

ECF from Industry



Industry	2012-13 ₹ in Lakhs	2013-14 ₹ in Lakhs
1. Indian Industry (Private)	352	488
2. Indian Industry (Public)	96	80
3. Government Sector	05	14
4. Foreign Sector	565	159
Total	1018	742

			20	20	20
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in foreign journals / publications (Calendar year)	370	431	455
		Number of papers published in Indian journals (Calendar year)	19	26	8
		Average Impact Factor	3.29	3.69	3.96
		Number of invention disclosure (Calendar year)	84	116	176
		Number of patents filed in India (Calendar year)	56	86	118
		No of foreign patents filed ** (Calendar year)	46	96	66
		Number of PCT applications filed (Calendar year)	28	36	55
		No of US applications filed	14	26	24
	Highly trained man-power	Number of PhDs produced (Calendar year)	59	52	73
		Number of NET/GATE qualified students joined (including DBT JRF)	140	90	118
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	NA	NA	NA
		Number of national and regional workshops, seminars organized	6	9	4
	Pride and standing among nations; National image	Number of international awards won	-	-	-
		Memberships of major international academies and learned societies	12	12	12
		Memberships of editorial boards of international peer-reviewed journals (Cumulative membership years)	NA	NA	NA
		Number of papers in foreign journals	370	431	455
		Number of IF research papers	355	434	419
		Number of foreign patents granted** (Calendar year)	13	22	62
	Representation in global affairs	Official(s) in global/ trans-national organizations like the UN, WHO etc - IUPAC	6	6	6

Annual Report

2013-14

Outputs and Outcomes

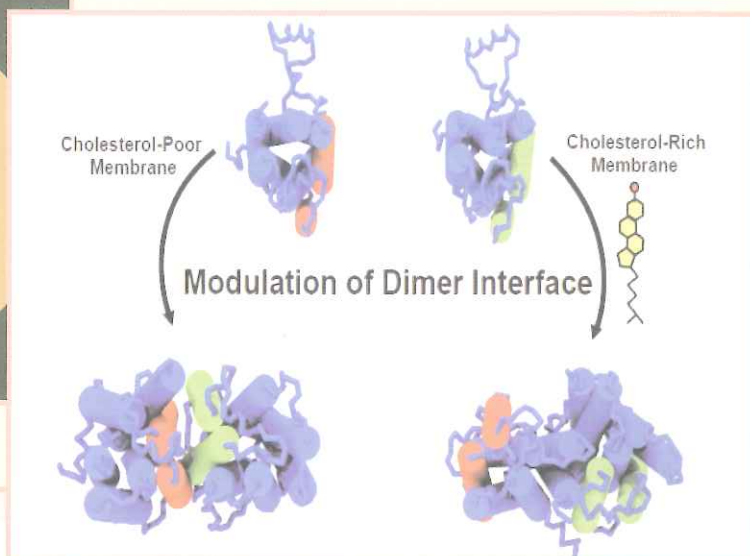
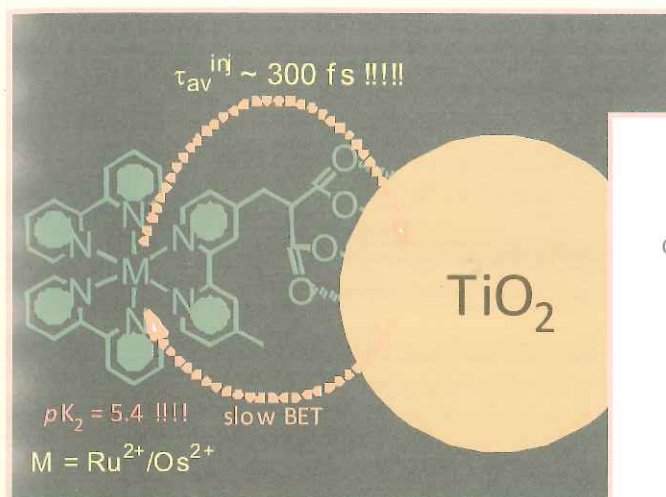
			20	20	20
Private goods	Research, consulting, teaching and analytical services	Total earnings from projects done for Indian & Foreign businesses/ industry (₹ in Crore) (Industrial ECF, excluding Grant-in-Aid)	11.03	10.18	7.42
	Continuing education	Total earnings from continuing education/ training programs (₹ in Crore)	NA	NA	NA
Strategic goods and options	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (₹ in Crore)	3.70	4.81	0.22
	Other tactical and strategic developments	Total earnings from patent related transaction (₹ in crore)	3.44	-	-
		No. of patents in new Licensing /assignment/ option arrangements	7	-	1
		No. of unique Licensing /assignment/ option cases	1	-	1
		No. of Indian patents granted (Calendar year)	12	19	10
		No of foreign patents granted** (Calendar year)	13	22	68
	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (₹ in Crore)	8.95	4.74	5.21
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (₹ in Crore)	12.31	11.73	14.09
Intellectual assets and reputation	Quality, reputation and standing of scientific manpower	No. of Indian patents granted (Calendar year)	12	19	10
		No. of foreign patents granted** (Calendar year)	13	22	68
		Number of papers in foreign peer-reviewed journals	370	431	455
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	NA	NA	NA
		Number of PhDs granted where lab scientists were research guides	58	52	73
		Number of staff who are members of National academies (Cumulative)	31	32	32

* - Individuals who are members of more than one academy have been counted only once

** - Foreign means all filings other than IN & WO

1 Crore = 10 Million

RESEARCH & DEVELOPMENT REPORTS



Functional Materials including Nanomaterials	26
Polymer Materials	37
Organic Chemistry	41
Chemical Biology	52
Biological Sciences	60
Catalysis and Surface Science	73
Chemical Engineering Science	85
Physical Chemistry	89
Structural Chemistry	90
Theory and Computational Science	91
Centers of Excellence	96

Magnetostrictive smart materials

The objective was to enhance the magnetostrictive performance parameters of sintered cobalt ferrite by simple and novel processing techniques. Magnetostriction studies on sintered polycrystalline cobalt ferrite derived from nanocrystalline powders were made after sintering the material under different conditions to evaluate the effect of processing and the related microstructure on the magnetostriction characteristics. It was found that best magnetostriction characteristics were obtained after sintering at 1450°C for very short durations, and the changes in the value of magnetostriction were somewhat correlated with the microstructure. Magnetic field annealing was very effective to enhance the magnetostriction and strain derivative of the sintered cobalt ferrite samples. Especially higher magnetostriction as well as relatively larger strain derivative was obtained for samples sintered at lower temperatures after magnetic field annealing. The higher magnetostriction was achieved after sintering at relatively lower temperatures with magnetic field annealing for sintered cobalt ferrite derived from nanocrystalline powders.

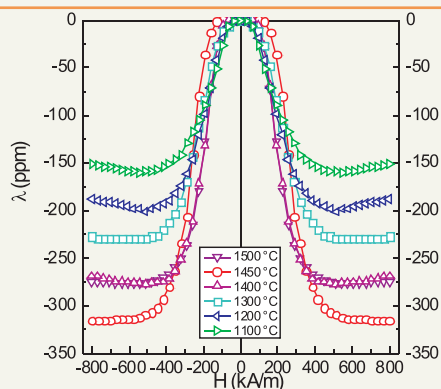


Fig. 1: Magnetostriction curves of cobalt ferrite sintered at different temperatures

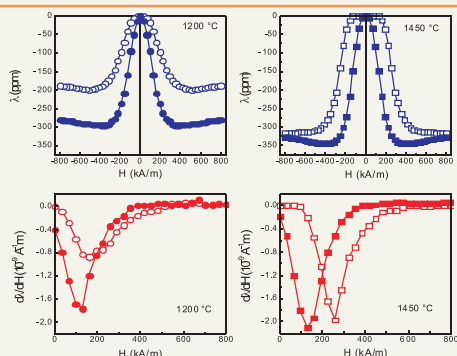


Fig. 2: Magnetostriction and the corresponding strain derivative curves of the samples sintered at 1200 and 1450°C

Curcumin is a promising candidate for coating on iron oxide nanoparticles for biomedical applications. Curcumin coated

Publications: Phys. Chem. Chem. Phys., 2013, 15, 20808; J. Eur. Ceram. Soc., 2014, 34, 677; Solid State Commun., 2014, 177, 89; J. Nanofluids., 2014, 3, 1

superparamagnetic iron oxide nanoparticles (SPIONs) were synthesized and characterized using various techniques; the effectiveness of direct coating of curcumin on the nanoparticles was also confirmed. The anti-oxidant property of curcumin was found to be retained after coating on their on oxide nanoparticles. Relaxivity measurements using nuclear magnetic resonance (NMR) technique showed the values similar to that reported for other established superparamagnetic iron oxide based contrast enhancement agents in magnetic resonance imaging (MRI). The curcumin coated ultra small iron oxide based nanofluids were expected to be a suitable multifunctional probe in biomedical applications because of its superparamagnetic nature and very small size of the particles along with the medicinal, radical scavenging and fluorescence properties.

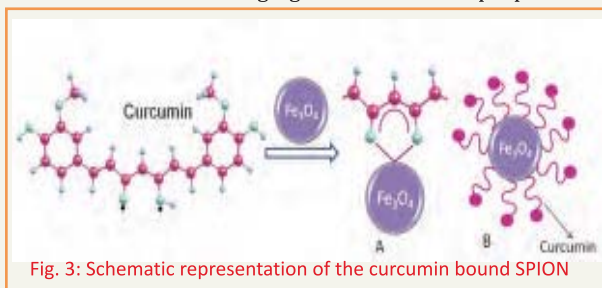


Fig. 3: Schematic representation of the curcumin bound SPION

Magnetic properties of disordered carbon were investigated as a function of the extent of graphitization. It was found that the magnetization of the disordered carbon decreased with increasing degree of graphitization. Treatment with acid modified the magnetic characteristics considerably and the original magnetic characteristics were retained upon further heat treatment. The results showed that the intrinsic magnetic behavior of the disordered carbon depended on the microstructure and the edge states played a critical role to decide the magnetic interactions in the amorphous carbon system. The results showed that a disordered magnetic state with random strengths, previously observed in nanographite and graphene nanoribbons, also existed in amorphous carbon.

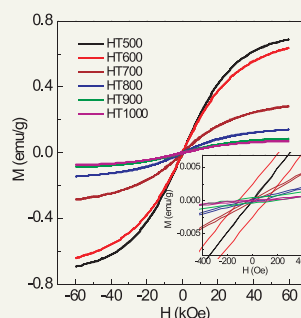


Fig. 4: Magnetization curves of the carbon pyrolyzed at different temperatures

Multifunctional materials for energy conversion and storage devices

Publications: *Nanoscale*, 2014, 6, 11, 5944; *Small*, 2014, DOI: 10.1002/smll.201303892; *ACS Appl. Mater. Inter.*, 2013, 5, 24, 13397; *Chem. Commun.*, 2014, 50, 54, 7188

The aim was to develop the materials for variety of applications such as oxygen reduction reaction (ORR), hydrogen evolution reaction (HER), oxygen evolution reaction (OER) and charge storage. Development of few materials such as nitrogen doped carbon nanohorns (NCNH), nitrogen doped graphene-transition metal core shell nanostructures, MOF derived, nitrogen doped carbon was done.

Synthesis of platinum free electrocatalysts for energy applications

Various low-Pt electrocatalysts were explored for different energy applications like metal-air batteries, fuel cells, and water oxidation. Development of a cost-effective Pt-free electrocatalyst was done by shielding an Au core with N-doped graphene (NGr) by simple water-in-oil emulsion technique for oxygen reduction reaction (ORR). The change in the electronic configuration of NGr shell resulted into higher ORR activity with reduced overpotential compared to their individual counterparts. A 3-dimensional (3-D) hollow, symmetrical NGr interpenetrated Ni-nanocage structure was engineered for oxygen evolution reaction (OER). A beautiful 3-D structure of Ni-NGr was achieved by changing the transition metal from Au to Ni.

Surface modified single wall carbon nanohorns for oxygen reduction reaction

Platinum-free PEM fuel cell was achieved by using nitrogen doped carbonaceous materials based on graphene and carbon nanotubes. The electrocatalysts based on these materials lack high surface area and good electrical conductivity. Simple annealing process of a mixture of single walled carbon nanohorns and urea provided nitrogen doped carbon nanohorns (NCNH) with high surface area ($1800\text{m}^2/\text{g}$). NCNH showed the improved ORR activity in alkaline condition with 50mV overpotential compared to 20% wt Pt/C. The materials showed improved electrochemical stability with efficient fuel selectivity. A maximum power density of $30\text{mW}/\text{cm}^2$ was obtained from a single cell derived from NCNH as the cathode catalyst.

Nanostructuring of pseudocapacitive materials for enhanced ionic accessibility

A simple electrochemical method was developed to achieve the deposition of uniform MnO_2 nano-wall forest over a conducting carbon fiber substrate. Vertical MnO_2 wall assembly having uniform micro-porosity was grown electrochemically that provided spacious and accessible corridors along the surface to act as facile channels for ion transport. The carbon fiber backbone helped the system to

overcome the issue of the inherent electrical resistance associated with MnO_2 . This led to a high specific capacitance of $1149\text{F}/\text{g}$, of which $565\text{F}/\text{g}$ was retained even at a high current dragging condition of $100\text{A}/\text{g}$. Cycle stability was observed excellent for the material and the structure was found to be stable even after 10000 cycles.

Solid-state supercapacitors with enhanced electrode-electrolyte interface

All-solid-state supercapacitor having close matching charge storage characteristics with its liquid-state counterpart was developed under extreme temperature and humidity conditions. The prototype supercapacitor devices were made by electro-depositing polyethylenedioxythiophene (PEDOT) onto the individual carbon fibers of a porous carbon substrate. Improved electrode-electrolyte interface was established by using polyvinylalcohol-sulphuric acid ($\text{PVA-H}_2\text{SO}_4$) gel electrolyte, which was intercalated into the electrode matrix. The established electrode-electrolyte interface nearly mimics the interface of the counterpart based on the liquid electrolyte. Consequently, the solid-state device attained very low internal resistance ($1.1\ \Omega\ \text{cm}^{-2}$) and a high specific capacitance ($181\ \text{F g}^{-1}$) for PEDOT at a discharge current density of $0.5\ \text{A g}^{-1}$ (Fig. 2).

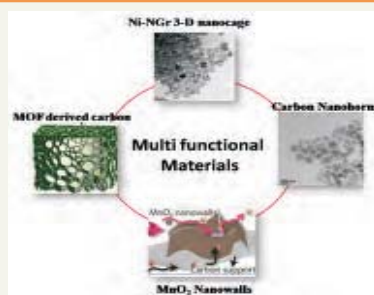


Fig. 1: Schematic representation of multifunctional materials used for different energy applications

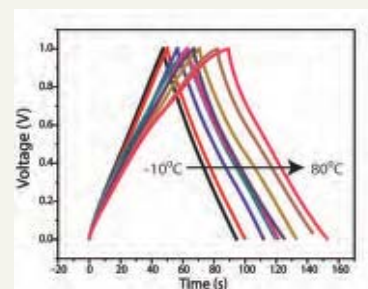


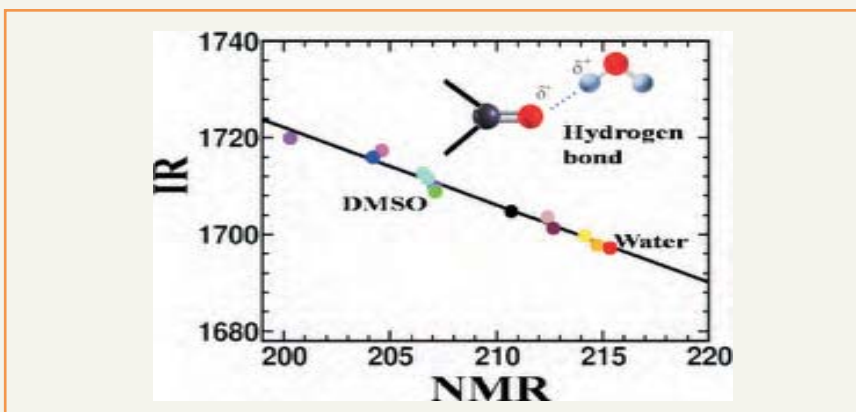
Fig. 2: Charge-discharge profile of PEDOT based all-solid-state supercapacitor at different temperatures

Electrostatic nature of carbonyl hydrogen bond interactions

Publications: J. Phys. Chem. Lett., 2014, 3211; J. Spectrosc. Dyn., 2014, 22; J. Am. Chem. Soc., 2013, 11181

The electrostatic nature of carbonyl hydrogen bond interactions was experimentally verified. Previous works regarding this fundamental physical chemistry issue involved theoretical research; this work is the experimental proof of the concept.

A project on cold denaturation of proteins using calculations of infrared spectra from MD simulations was completed.



Atomically thin 2D nanomaterials for novel device systems

Publications: Chem. Phys. Chem., 2014, 15, 1592; Nanoscale, 2014, 6, 3550; ACS Appl. Mater. Inter., 2014, 6, 1158; 15881; Appl. Phys. Lett., 2014, 104, 81911; 105, 43109; 233101; 233103

The objective was to synthesize the single layer and few layers of various TMDCs including MoS_2 , MoSe_2 , WSe_2 etc. over 300 nm SiO_2/Si using micromechanical and hydrothermal method.

Synthesis of 2D materials

The synthesis of transition metal dichalcogenides (TMDCs) possessing crucial electronic properties was aimed. The synthesis and characterization of these materials and fabrication of devices was of high interest. Fabrication of transistor, gas sensor photodetector, field emitter arrays of various atomically thin inorganic layered materials was undergone successfully.

The Pulsed Laser Deposition (PLD) technique rendered stoichiometric transfer of atomic species to a thin film from a bulk target under controlled, ambient classes of systems. The film on flexible substrates showed greater prospects for flexible smart devices such as photodetector, transistor, sensor etc. Emission current density was drawn as large as $30\text{mA}/\text{cm}^2$ at an applied voltage of 3.8 kV. The nonlinearity observed in the F-N plot was a direct consequence of the semiconducting nature of MoS_2 . The MoS_2/W -tip emitter exhibited the capability to deliver large emission current density due to the presence of nanometric protrusions on the surface. This hetero-structure device showed good photo response.

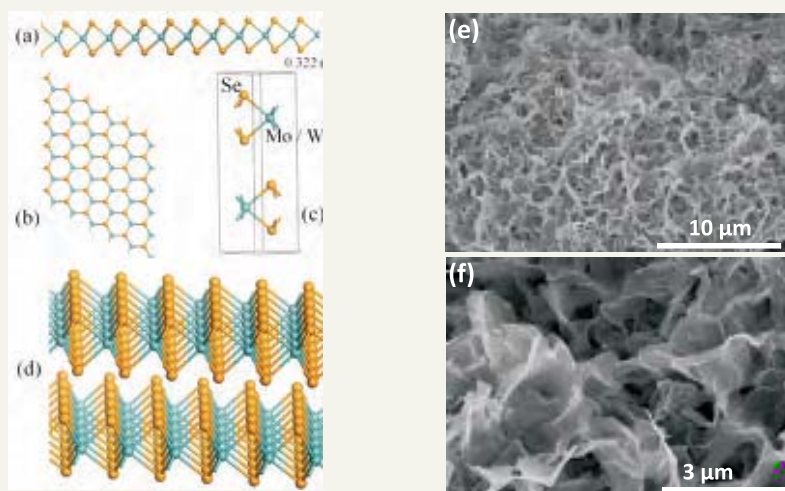


Fig. 1: Crystal structure of MoSe_2 / WSe_2 : (a, c) side, (b, d) top views and (e, f) FESEM images of few layered WS_2 nanosheets synthesized by hydrothermal method

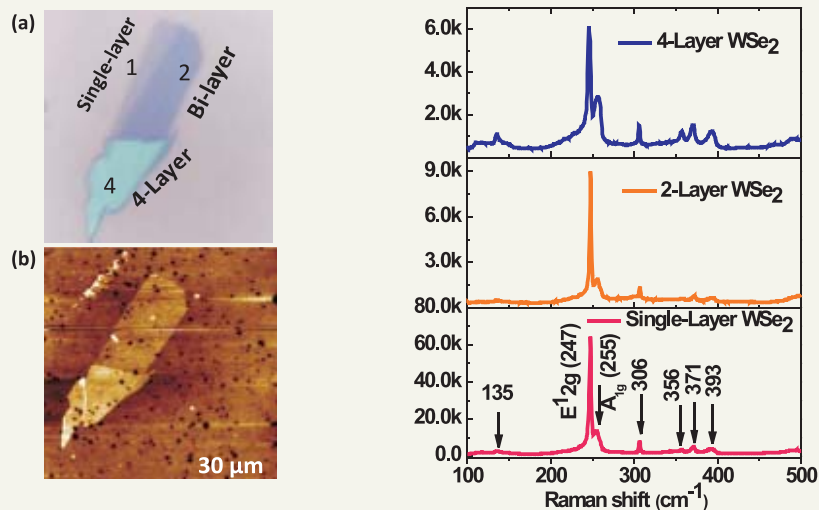


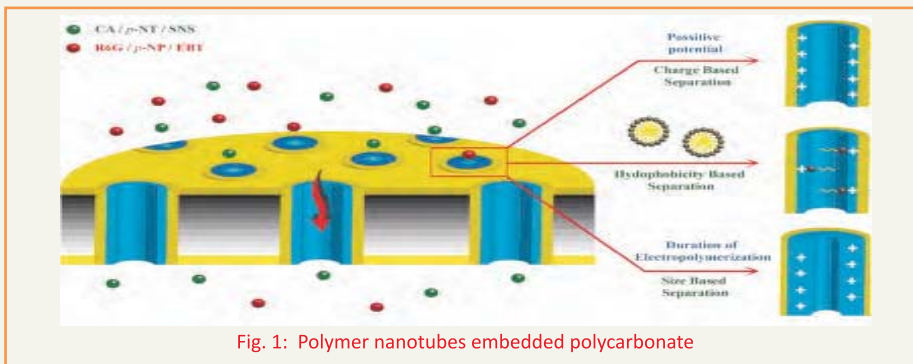
Fig. 2: Single-layer and few layers WSe_2 sheet (a) Optical image (b) AFM (c) Raman spectra

Variable hydrophobic nanotubes

Publication: Chem. Commun., 2014, 50, 5905

The preparation of nanotubes was reported with variable hydrophobic interiors by taking advantage of the electrostatic polyvalent attraction between anionic micelles and the inner walls of positive charge bearing rigid conjugated polymer nanotubes. This attractive interaction resulted in the disassembly of anionic micelles. The surfactants adhered to the positive charges of the polymer converted the hydrophilic and positive charge containing polymer nanotube interiors into hydrophobic and neutral surface. The supervision of the number of surfactants

adhering to the polymer surface was undergone by controlling the number of positive charges on the polymer, which is a function of applied potential. This potential was varied for the modulation. The hydrophobicity variation was studied using transport of hydrophobic and hydrophilic molecules through these nanotubes. It was also demonstrated that nanotubes before filtration of anionic micelles can differentially transport molecules based on charge. It is possible to differentially transport molecules based on size using these nanotubes.



Photoresponsive materials for organic photovoltaics

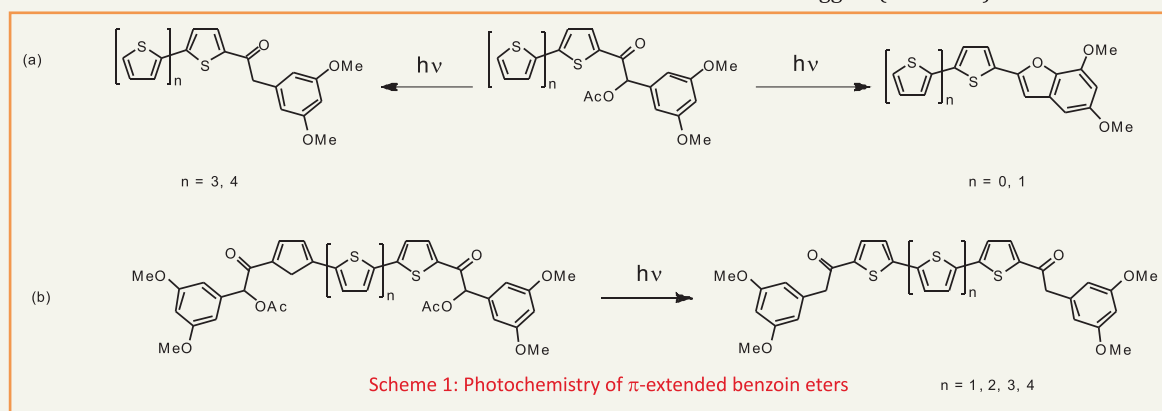
The efforts were made to process the organic semi-conducting molecules by photo activation. It was focused on the synthesis of dyes for dye sensitized solar cells Spiropyran based photo-responsive materials.

Photochemistry of benzoin esters: Effort towards processing organic semiconducting molecules

Solution-based processing methods were imparted and controlled the nano-scale morphology of the required thin film to achieve the high efficient devices. A masked

functional group from several photo-labile protecting groups was activated when irradiated by light. A photolabile protecting group 3,5-dimethoxy benzoin was used as protecting acid as an ester which upon irradiation released acid in very high yield (>90 %) with good quantum efficiency ($\phi = 0.64$).

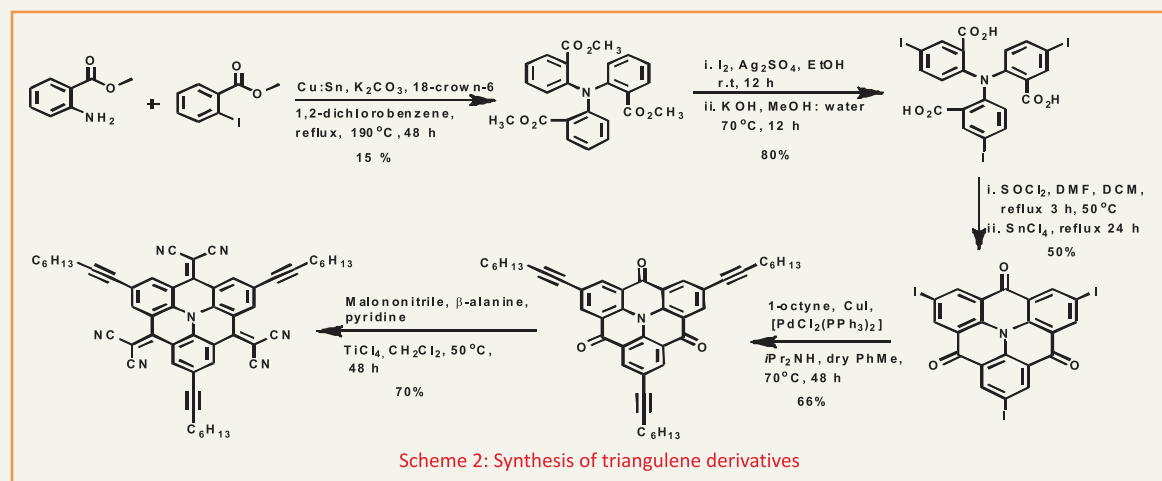
π -Extended benzoin esters were synthesized by invoking metal catalyzed C-H activation methods and observed distinctive photochemical reactivities with respect to the structures of the triggers (Scheme 1).



Synthesis of dyes for dye sensitized solar cells

Synthesis of dyes for the dye sensitized solar cells (DSSC) required the design of panchromatic absorption, that avoids the dye aggregation and torsional distortion upon photo-activation. The dyes utilized in DSSC possessed Donor- π Bridge-Acceptor configuration in order to increase absorption towards visible region of solar spectrum. An effort was made to synthesize the planar nitrogen donor for

the DSSC for the effective charge delocalization. Triangulene based donor core molecules were synthesized and functionalized with malanonitrile to afford the hexacyano derivative (Scheme 2). Cyclic voltammetry was investigated to find out the HOMO (-5.83 eV) and LUMO (-3.63 eV) energy levels. Field effect transistor study revealed that the hexacyano derivative can transport electron with the mobility of $1 \times 10^{-2} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.



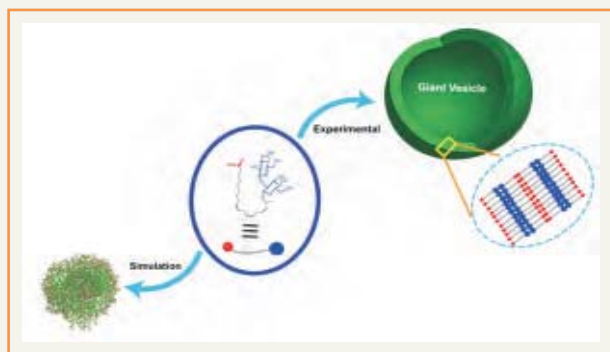
Synthesis assemblies and applications of functional nanoparticles

Publications: Chem. Eur. J., 2014, 20, 6246; Chem. Mater., 2014, 26, 3436; Langmuir, 2014, 30, 10143

The work involved the development of new methods for material synthesis, bio-nanoparticle conjugates and their applications, surface modification of nanoparticles and their assemblies and molecular assemblies etc.

Giant vesicle from bolaamphiphilic biosurfactants: Dynamics simulation studies

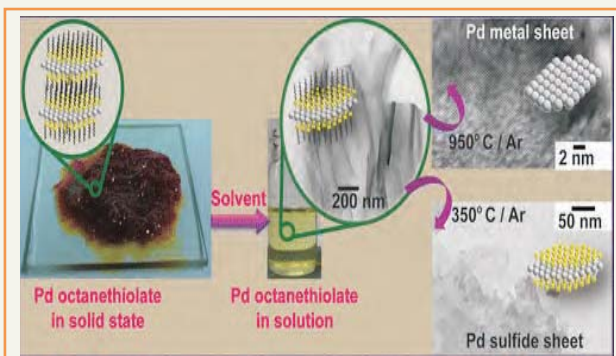
Sophorolipids from different fatty acids consisting one oleic acid, two linoleic acid and three linolenic acid *cis*-double bonds were considered. Linolenic acid SLs were self-assembled to form giant vesicle like structures as evidenced by different microscopic techniques including confocal whereas no structure was seen to be formed by SLs of linoleic acid. Dye encapsulation result suggested that the presence of aqueous compartment inside the vesicle like structures were formed by LNSLs. Molecular Dynamics Simulations (MD) studies were performed to obtain deeper insights into the formation of these structures. MD studies showed the existence of two possible conformations for linolenic acid SLs and the head sophorose groups are mostly buried inside the layer structures. These conformations were predominantly arranged into tail-head-head-tail fashion. MD simulation and experimental data confirmed the presence of double bilayer arrangement in the assembled structure.



Ultrathin sheets of metal or metal sulfide from thin sheets of metal thioliates in solution

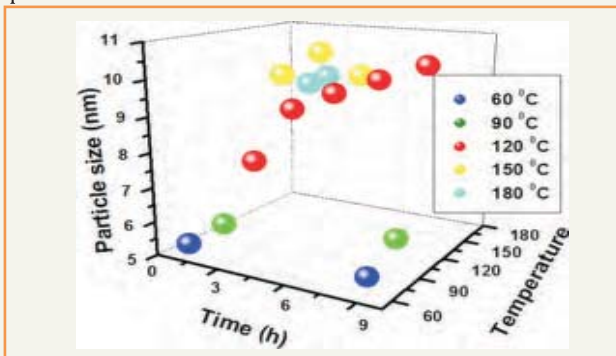
A demonstration was done to confirm that metal thioliates existing as lamellar assemblies in the neat state can be disassembled into individual molecular sheets simply by dilution in a polar organic solvents and form ultrathin metallic layers on substrates upon heat treatment. The pathway to the disassembly of metal thioliates in solution was established using a combination of techniques, including X-ray diffraction, light scattering, FTIR, and TEM. The results indicated that the lamellar structure of Pd-thioliates was preserved in toluene up to a concentration of 300% w/v and the average inter sheet distance was unchanged.

The dynamics of the Pd-thiolate sheets remained correlated even on diluting them up to 30% w/v, though the disorder within the lamellar stacks increases with a decrease in their coherence length. Finally, at dilutions less than about 5% w/v, individual sheets of these structures were accessed, isolated and directly observed using TEM. Heat treatment of the ultrathin films of metal thioliates deposited on appropriate substrates resulted in the formation of metal or metal sulfides with retention of sheet like morphologies.



Time and temperature effects on the digestive ripening of gold nanoparticles

The effects of time and temperature on the gold nanoparticles size obtained by digestive ripening were investigated. Digestive ripening cleared that upon refluxing a polydisperse colloid with a surface active ligand in a solvent got converted in monodisperse one. A polydisperse gold nanoparticle system was heated in 4-tert-butyltoluene with hexadecanethiol at different temperatures, viz., 60, 90, 120, 150, and 180°C for different time periods and the trends in particle size variations were recorded. After the initial narrowing of the size distribution, the particle sizes remained constant even though the refluxing step was continued for 24 h, substantiating the prevalence of the digestive ripening process at lower temperatures such as 60 and 90°C. At elevated temperatures (120, 150, and 180°C) particle size grow continuously, indicating a deviation from the digestive ripening behavior to an Ostwald ripening-type phenomenon.



Synthesis and applications of multifunctional nanomaterials

Publications: Surf. Sci. Rep., 2014, 4, 4897; J. Mater. Chem. A, 2014, 2, 2152; Carbon, 2014, 68, 175; RSC Adv., 2013, 3, 21390

New electrode materials for charge storage

Carbon nanomaterials were extensively researched, either in an electric double layer capacitor as the carbon electrode or in pseudocapacitors that employed a composite of highly conducting carbon with a material such as metal oxides. Nanoporous carbon supercapacitors counter ions entered pores to form endohedral supercapacitors having negative surface curvature. Graphene based materials showed zero curvature, one-dimensional capped CNTs exhibited a positive surface curvature whereas counter ions resided on

the outer surfaces, leading to exohedral supercapacitors. These positive surface curvature carbon electrodes were charged at a high rate. A cheaper and green approach was developed for the synthesis of CNOs and demonstrated a supercapacitor based on these CNOs which provided a higher specific capacitance than conventional graphitic/mesoporous/activated carbons. A composite of CNOs with MnO_2 was synthesized showing high enhancement in specific capacitance of the supercapacitor with high rate capability and long cycle life.

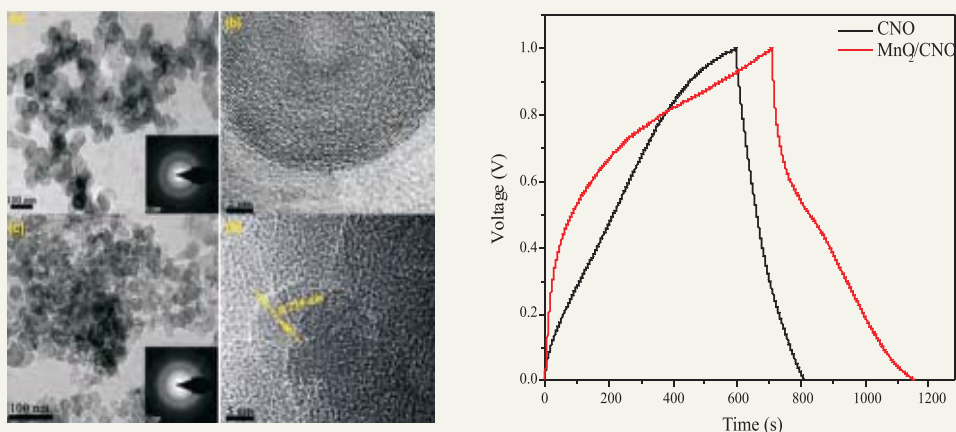


Fig. 1: Multilayer fullerene- MnO_2 nanoparticle composite supercapacitor electrodes

Development of multifunctional nanostructured materials

The hybrid nanomaterials like semiconductor-metal composites showed enhanced physical properties such as low reflection, high absorption and dielectric strength. The

effect of the surface plasmon of gold nanoparticles was demonstrated on SiNWs/ TiO_2 heterojunctions. These hybrids showed the enhanced optical absorption, emission and photocurrent generation.

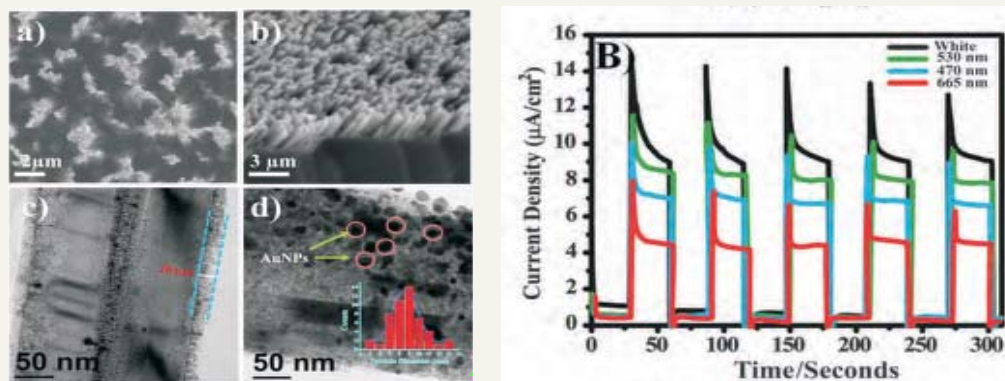


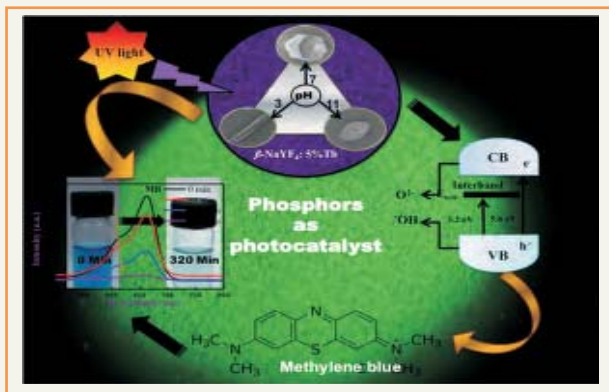
Fig. 2: SEM, TEM images and wavelength-dependent photoresponse of AuNP decorated SiNW/ TiO_2 heterojunctions

Phosphors and plasmonic superstructures for molecular detection and catalytic applications

Publications: J. Mater. Chem. A, 2014, 2, 19189; J. Phys. Chem. C, 2014, 118, 4016; 13268; 19363; Nano Res., 2014, DOI: 10.1007/s12274-014-0572-2

Photoluminescence and photocatalytic properties of β -NaYF₄ phosphor microcrystals

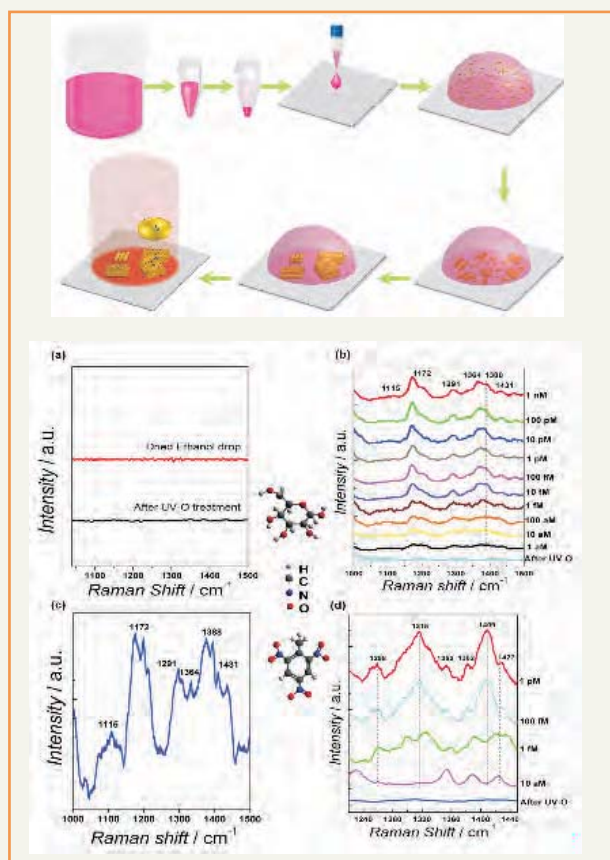
The fabrication was undergone for the Lanthanide-ion-doped, single-crystalline hexagonal phase NaYF₄ microcrystals with multiform morphologies; including microrods, hexagonal micro-prisms, and spindle-like structures. It utilized the cationic/anionic binary capping agents like CTAB and tri-sodium citrate-assisted hydrothermal route. The influence of synthesis conditions on the crystalline morphology was studied to present the possible growth mechanisms. The photoluminescence (PL) properties of β -NaYF₄: Ln³⁺ (Ln=Tb, Yb/Er, and Yb/Tm) were investigated. The static and dynamic PL studies of β -NaYF₄:5% Tb³⁺ showed strong dependence of photoluminescence properties on the crystalline morphology. The β -NaYF₄:5% Tb³⁺ phosphors exhibited efficient photocatalytic activity under UV as well as solar light irradiation and showed enhanced selectivity towards methylene blue. The morphological effect on the photocatalytic activity of β -NaYF₄:5% Tb³⁺ crystals was studied. The high luminescence efficiency and strong photocatalytic activity of β -NaYF₄:5% Tb³⁺ made them a potential phosphor material and promised to provide a gateway into other applications as in biology and material sciences.



Self-assembled gold nanorod superlattices for ultra-high sensitive detection of molecules

Self-assembled vertically aligned gold nanorod (VA-GNRs) superlattices served as substrates for ultra-high sensitive detection of various molecules. D-glucose and TNT (2,4,6-trinitrotoluene) were chosen as model systems due to their very low Raman cross sections ($5.6 \times 10^{-30} \text{ cm}^2 \text{ molecule}^{-1} \text{ sr}^{-1}$ for D-glucose and $4.9 \times 10^{-31} \text{ cm}^2 \text{ molecule}^{-1} \text{ sr}^{-1}$ for TNT) to show that the VA-GNR superlattice assembly offers as low as yoctomole sensitivity. Self-assembled superlattices of VA-GNRs were achieved on a silicon wafer by depositing a drop of solvent containing the GNRs and subsequent solvent evaporation in ambient conditions. The advantage of VA-

GNR monolayers and its superlattices is its extremely high reproducible morphology accompanied by ultrahigh sensitivity useful in many fields where very small amount of analyte is available. The assembly can be reused number of times after removing the already present molecules. The method of obtaining VA-GNRs is simple, inexpensive and reproducible. Simulations showed that super lattices achieved the better sensitivity than the monolayers assembly of VA-GNRs.



Development of efficient and cost effective photovoltaic devices based on inorganic quantum dots and nanocrystals

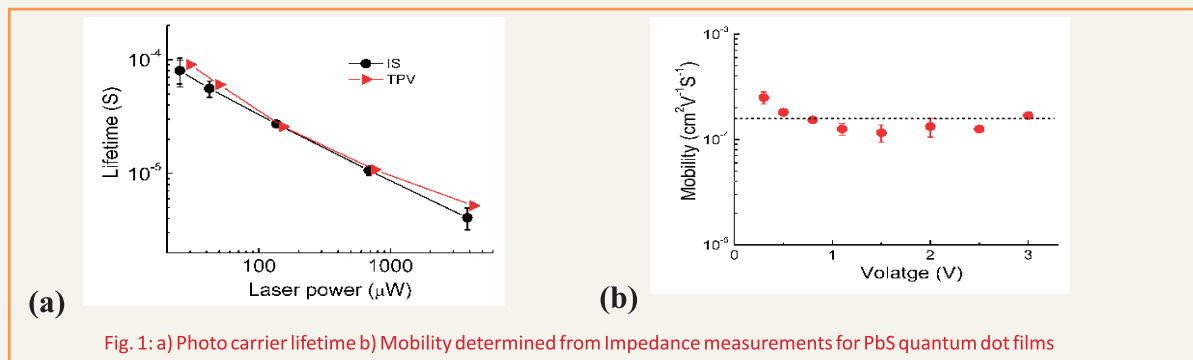
Publications: App. Phys. Lett., 2014, 104, 63504; Adv. Mater., 2014, 26, 443, 4741

The research was aimed to develop the inorganic quantum dots and nanostructures with tailored electronic and optical properties from chemical root for renewable energy and other optoelectronic applications. It was focused to develop next generation solar cells by employing quantum dots and nanostructures as active materials for low cost and high efficiency applications.

Determination of carrier lifetime and carrier mobility of quantum dot based solar cell devices

Sophisticated experimental set up and specific device architectures were utilized to determine these parameters in thin films of inorganic quantum dots and organic semi-

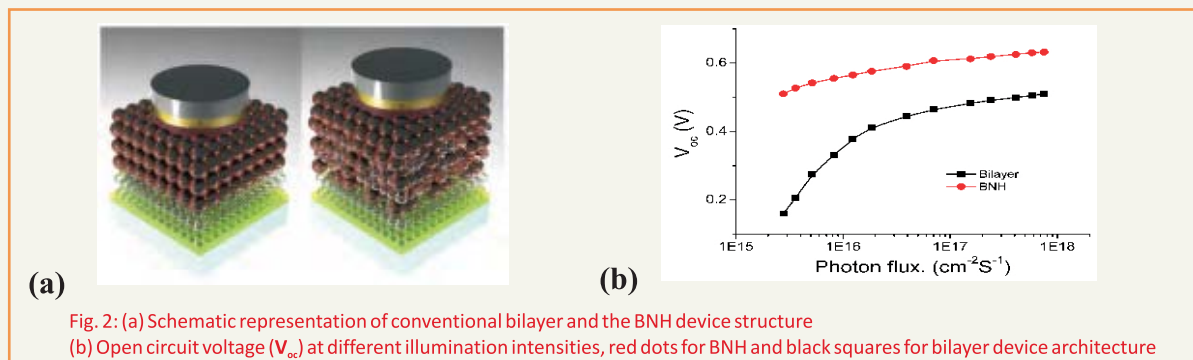
conductors. It was observed that the measured values of mobility sometimes do not corroborate with the experimental results of solar cells due to change in device structure and measuring conditions. It was showed that both carrier lifetime and mobility of a solar cell can be determined conveniently and accurately from impedance spectroscopy measurements without changing the device structure. It will save the energy, time and cost of expensive experimental infrastructure. Impedance spectroscopy is widely used in industry to determine frequency dependent phenomena of devices, where this technique can be easily integrated for quality checking of the materials.



Advance device engineering for remote trap passivation and enhanced efficiency in quantum dot solar cell

An effort was made to show that an alternative device structure-based methodology that offers higher charge collection efficiency, higher photocurrents and a trap passivation mechanism results in higher attainable V_{oc} in quantum dot based photovoltaic devices. An architectural platform called bulk nano-heterojunction (BNH) was employed for this typical demonstration, in which the p-type PbS quantum dots and n-type ZnO nanocrystals were

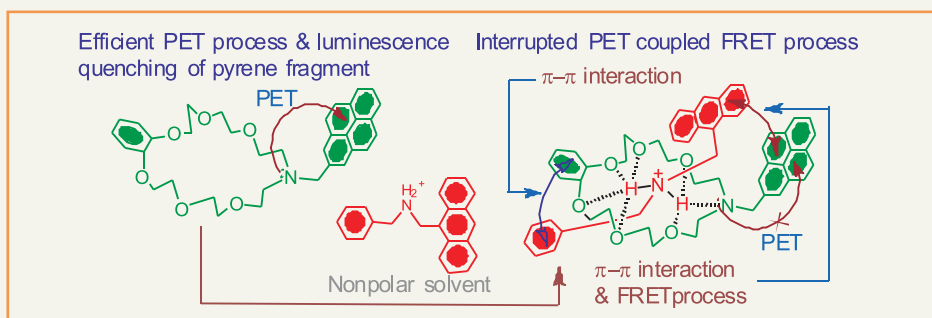
Blended on the nanometer scale. It was hypothesized that by bringing ZnO NCs in the vicinity of PbS QDs x minority carrier trap passivation can be achieved, by charge transfer from the abundance of electrons in the ZnO NCs to the deep electron acceptor sites of PbS QDs, which are also known as recombination centres. The average power conversion efficiency produced by BNH devices was observed 5.24% compared to 2.64% in the best performing bilayer device, under 1 Sun condition.



Spectroscopic signature for molecular recognition and inclusion complex formation

Appropriate aza-crown ether based host and secondary ammonium ion ($R^1R^2NH^+$) based guest molecules were functionalized with suitable fluorophore; that led to the formation of a supramolecular assembly by utilizing various non-bonding (H-bonding and π -stacking) interactions. Reversible

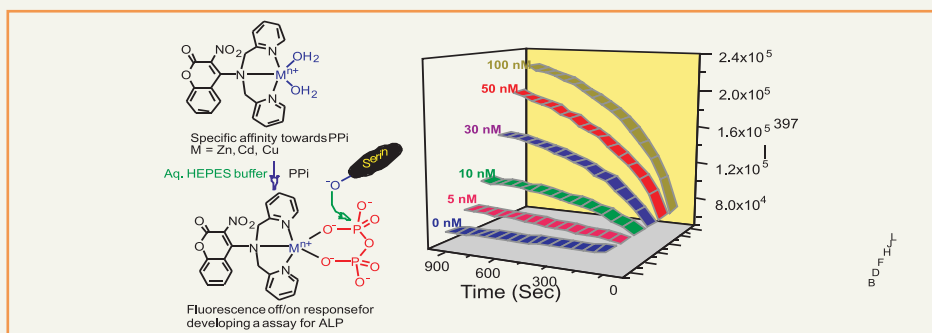
change in conformation of the host molecule was induced by the formation of the inclusion complex with $R^1R^2NH^+$. Associated change in luminescence gave response due to a two step FRET process, which was utilized for predicting the changes in conformation of the host molecule.



Molecular recognition for application in sensing and as imaging reagent

A new purpose-built reagent was synthesized for specific recognition of biologically significant pyrophosphate ion in

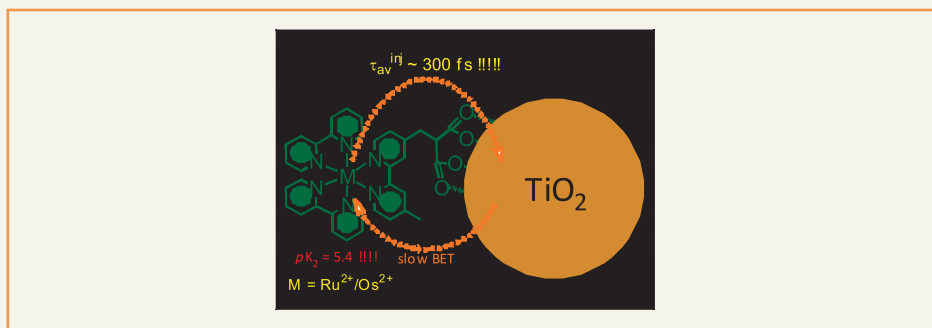
physiological condition. The reagent was utilized for developing an enzymatic assay for an alkaline phosphatase, an important enzyme for mammals.



Designing sensitizer molecule for DSSC application

Interfacial electron transfer rates for newly designed geminal dicarboxylate bound ruthenium(II)- and osmium(II)-polypyridyl complexes on nanoparticulate TiO_2 surfaces were studied by using time resolved absorption studies in the ultrafast time domain. It revealed that slow

back electron transfer (BET) from the conduction band ($[CB]e^-_{TiO_2}$) to the photooxidized Ru(III) is most important to achieve the higher efficiency in DSSC. It has crucial role to develop a better insight to design molecules for DSSC application.



Self-assembly of amphiphilic linear-dendritic copolymers in dilute aqueous solution

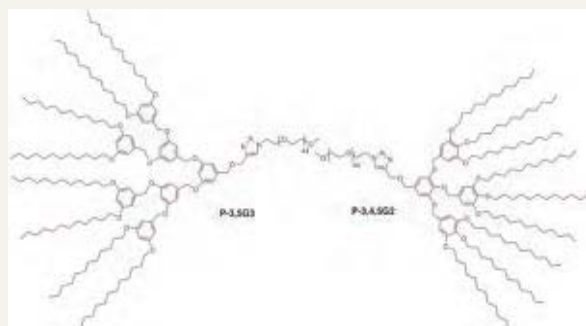
Publication: Macromol. Chem. Phys., 2014, 215, 1456

The aim was to achieve the self-assembly of amphiphilic block copolymers with its desired micellar properties. The factor of polymeric architecture such as Linear-dendritic copolymers of anisotropic shape was applied.

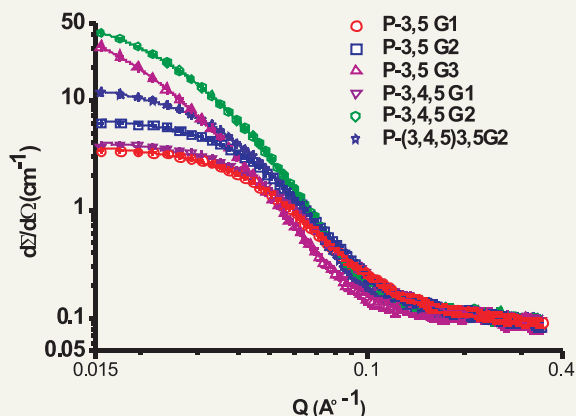
Effect of dendron branching pattern on micellar core properties

Hydrophobic benzyl ether dendrons based on different branching patterns viz. 3,5-di- and 3,4,5-trisubstituted phenyl rings were synthesized and attached to linear poly ethylene glycol.

Core properties of the resultant copolymer micelles were investigated in THF/water mixtures by small-angle neutron scattering (SANS). Aggregation numbers for 3,4,5-based dendron copolymers were lower with more THF molecules of solvation compared to 3,5-based dendron copolymer; due to different size and hydrophobic density of the two branching patterns as well as different shape at higher generations. Micellar core size also increased in small steps with dendron size so that dye encapsulation is tuned.



Dendron-PEG linear-dendritic copolymers



SANS profiles for 1wt% solutions of copolymers in THF/D2O (10/90) at 30°C

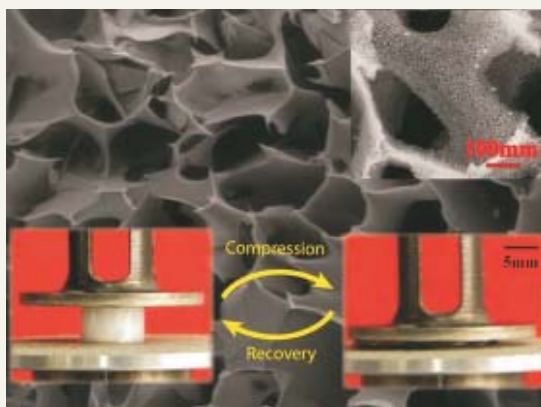
Elastic scaffolds from macroporous scaffolds of colloid-polymer hybrids

Publication: Chem. Mater., 2014, 26, 3436

The aim was to create centimeter-size macroporous monoliths which were accomplished using a general strategy that comprised primarily of colloidal particles that recover elastically after large compressive strains.

The ice-templating of an aqueous dispersion of particles, polymer and cross-linker was achieved leading crosslinking in the frozen state. The method yielded elastic composite scaffolds for starting materials ranging from nanoparticles to micron-sized dispersions of inorganics or glassy latices. The mechanical response of the monolith was qualitatively independent of polymer type, molecular weight and crosslinking chemistry.

The results suggested that the monolith mechanical properties arise from the formation of a unique hybrid microstructure, generated by crosslinking the polymer during ice templating. A remarkable consequence of this microstructure is that the monolith mechanical response is entropic in origin. The modulus of these scaffolds increased with temperature over a range of 140K. This microstructure showed the monolith mechanical response entropic in origin. The interparticle connections formed by crosslinking during ice-templating determined the monolith modulus; and also allowed relative motion between connected particles, resulted in entropic elasticity.



Insertion copolymerization of polar olefins and sustainable polyacetals

Publications: Coord. Chem. Rev. 2014, 262, 1; 265, 52; J. Polym. Sci. Part A Polym. Chem. 2014, 52, 1; Green Chem. 2014, 16, 3810

The objective was to undergo the insertion copolymerization of functional olefins and the catalytic synthesis of enantiopure p-stereogenic supramolecular ligands and its implications in asymmetric catalysis. The research also involved the isomerizing hydroformylation and metathesis of plant oils to feedstock chemicals and the renewable and sustainable polymers.

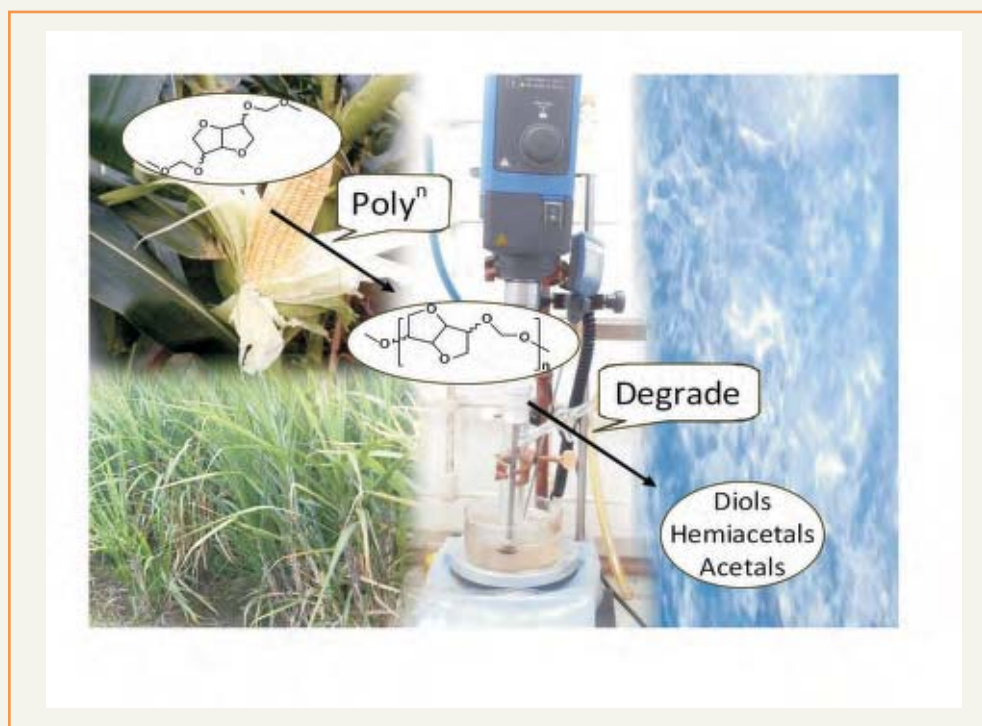
Insertion copolymerization of functional olefins

A method for the synthesis of acetonitrile ligated Pd-phosphinobenzene-sulfonate complex as catalyst for insertion-copolymerization of mono and 1,1-disubstituted functional olefinic monomers with ethylene was developed. The palladium complex was fully characterized using combination of spectroscopic and analytical tools. The prepared complex was tested in the insertion copolymerization of ethylene with methylacrylate, acrylonitrile and ethyl-2-cyanoacrylate. The final copolymers displayed

Functional olefin incorporation of 25.8% (methylacrylate), 17.2% (acrylonitrile) and 6.5% (ethyl-2-cyanoacrylate).

Renewable and degradable polyacetals from isohexides

A single step synthetic protocol was established to access a small family of renewable diacetals. The resultant chiral diacetals are valuable building blocks for pharmaceuticals and material science. Its synthetic competence was demonstrated by subjecting isohexide-diacetal to acetal metathesis polymerization and corresponding polymers were isolated as white solids with molecular weights in the range of 3200-27600 (g/mol). The semi-crystalline polymers showed glass transition temperatures between 38 to 65°C and melting temperature in the range of 103 to 156°C. The isohexide derived polyacetals were stable towards practical washing and rinsing conditions but degraded in slightly acidic media.



Shape and size selective functional nanoparticles from cellulose

Publications: Chem. Commun., 2013, 49, 8818; Carbohydr. Polym., 2014, 104, 135

The objective was to synthesize spherical shaped nanoparticles from agricultural residue. Obtained nanoparticles showed good antimicrobial activity that proved to be useful for the drug delivery.

A very simple method to obtain spherical shaped polymer nanoparticles was reported. Generally spherical shaped nanoparticles were used to obtain by maintaining very specific conditions such as prolonged sonication in acidic condition, high temperature, mechanical stirring, centrifugation, extensive washing, etc. A superior method was developed which took only 15 minutes ultrasonication to produce stable aqueous dispersion of nanoparticles with high yield. The method was reported for the first time which showed less utilization of the time.

The nanoparticles were obtained exhibiting spherical shape and narrow size distribution near 25-32 nm. These nanoparticles showed uniform range of size and carboxy groups on the surface. It was proved to have good potential in the field of nanotechnology and applications in biology, medicine, bioimaging and drug delivery. Cellulose was utilized to convert into the nanocellulose because of its abundance in the nature; it led to various new high end applications. The application of the nanoparticles was controlled by engineering their shape, size and surface functionality. Surface functionalization of nanoparticles was effective to control the interface between nanoparticles surface and the biological systems. The spherical shaped nanoparticles of carboxycelluloses were significantly improved as compared to currently available analogs.

Easily available low molecular weight agricultural residue derived cellulose and higher molecular weight cotton cellulose were utilized to prepare 6-carboxycellulose nanoparticles (6-CCNP); which proved to be a good method for the agricultural residue management. A specific enhancement was reported in the antimicrobial activity against microorganisms such as *Escherichia coli*, *Bacillus subtilis*, *Staphylococcus aureus*, and *Mycobacterium tuberculosis*. The polymer was found effective against tuberculosis and was likely to be, due to its spherical nanoparticle shape and small size of 25-35 nm. The spherical shape provided the greater surface area as well as spherical nanoparticles were more stable in aqueous suspension than nanofibers. A demonstration was carried out to prove that functionalized nanoparticles were extremely efficient in the stabilization of carbon nanotubes with minimal ultrasonication that led to save the energy. 6-CCNP helped to achieve the highly stable dispersions of both single-walled and multi-walled carbon nanotubes for several days. Cellulose nanomaterial substrates were investigated to use in the fabrication of recyclable organic solar cells. Further development in this field by use of 6-CCNP proved to be beneficial to increase its use in energy production technologies.

Chemistry of inositols

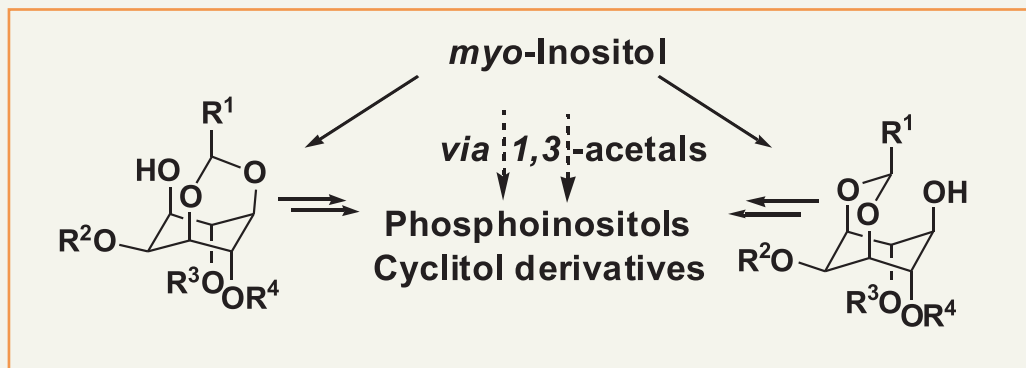
Publication: Chem. Eur. J., 2013, 19, 12867

The aim was to search different methods for synthesis of natural and unnatural cyclitol derivatives with biological significance. The synthetic strategy for polyols requires methods for the regioselective reactions of the hydroxyl groups of cyclitols.

Use of 1,3-acetals

Synthetic sequences starting from commercially available *myo*-inositol necessarily involved the protection or deprotection strategies of its six hydroxyl groups. Many

strategies were developed over the last several decades leading to the synthesis of naturally occurring phosphoinositols, their analogs and cyclitol derivatives. The *myo*-inositol, 1,3-acetals obtained by the reductive cleavage of *myo*-inositol orthoesters are the early intermediates for the synthesis of phosphorylated and other inositol derivatives. Several syntheses were carried out that illustrate the economy and convenience of using 1,3-acetals as early intermediates during syntheses from *myo*-inositol.



Reactions in molecular crystals

Investigation of the intermolecular acyl-transfer reactivity in molecular crystals of *myo*-inositol orthoester derivatives and its correlation with crystal structures enabled to identify the essential parameters to support efficient acyl-transfer reactions in crystals. These parameters were used to identify another reactive crystal of 2,3-naphthalene diol and its di-

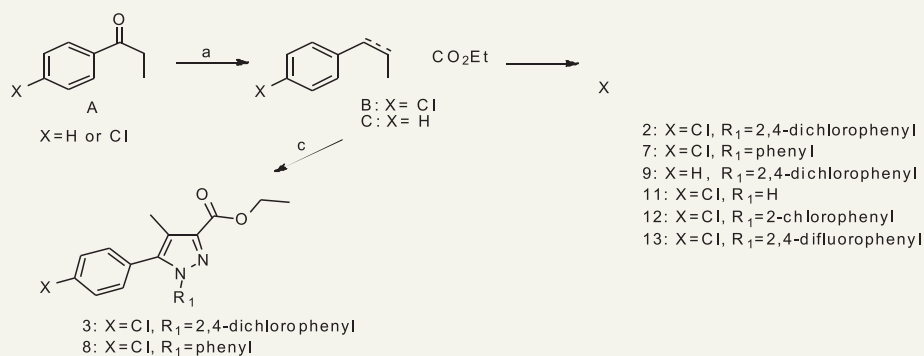
toluate through a data-mining study of the Cambridge Structural Database. A facile intermolecular thermal p-toluoyl group transfer was observed in presence of sodium carbonate, as predicted. A new method involving the reactive crystals was identified for the detection of molecular crystals capable of exhibiting acyl-transfer reactivity.

Discovery of rimonabant and its potential analogues as anti-TB drug candidates

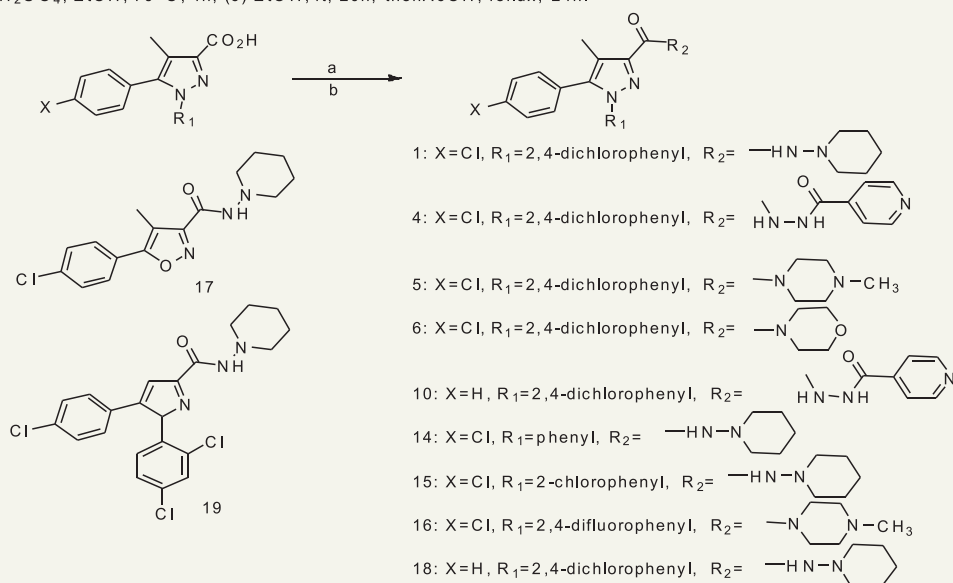
The research was aimed to synthesize rimonabant and its analogues which were achieved in moderate to good yields implying simple synthetic routes.

The synthesized compounds were subjected to *in vitro* screening against *Mycobacterium tuberculosis* and *M. smegmatis*. The most potent analogue JMG-14 exhibited MIC value of 3.13 compared to 3.25 and 50 µg/ml for ethambutol and pyrazinamide, respectively. The molecular docking revealed that pyrazole ring, number and position of halogen atoms played crucial role to decide interactions with MTCYP-121. These findings opened up a new avenue in the search of potent anti-TB drugs with rimonabant and its novel analogue JMG-14 as lead molecules. The synthesis of compounds 2, 3, 7, 8, 9, 11, 12, and 13 was carried out as

outlined in the scheme1. 4-chloro propiophenone (A) on condensation with diethyl oxalate in the presence of LiHMDS gave lithium salt of ethyl 4-(4-chlorophenyl)-3-methyl-4-oxido-2-oxobuten-3-oate (B). This on condensing with 2, 4-dichloro phenyl hydrazine hydrochloride and phenyl hydrazine hydrochloride in ethanol gave hydrazones, which on refluxing in acetic acid for 24 h gave esters 3 and 8, respectively. Subsequent reaction of B with suitable hydrazines in 50% sulfuric acid and ethanol at 79°C for 14 h yielded desired acids (2, 7, 9, 11, 12, and 13). These acids on subsequent treatment with thionyl chloride afforded acid chlorides. The amidation was executed at last to afford the target compounds 1, 4, 5, 6, 10, 14, 15, 16, 17, 18, and 19 (Scheme 2). The structures of newly synthesized compounds were established on the basis of spectral and physico-chemical profiles.



Scheme 1. Reagents and conditions: (a) LiHMDS, diethyl oxalate, methyl cyclohexane, 15-25 °C, 6h; (b) 50% aq. H₂SO₄, EtOH, 79 °C, 4h; (c) EtOH, rt, 20h, then AcOH, reflux, 24h.



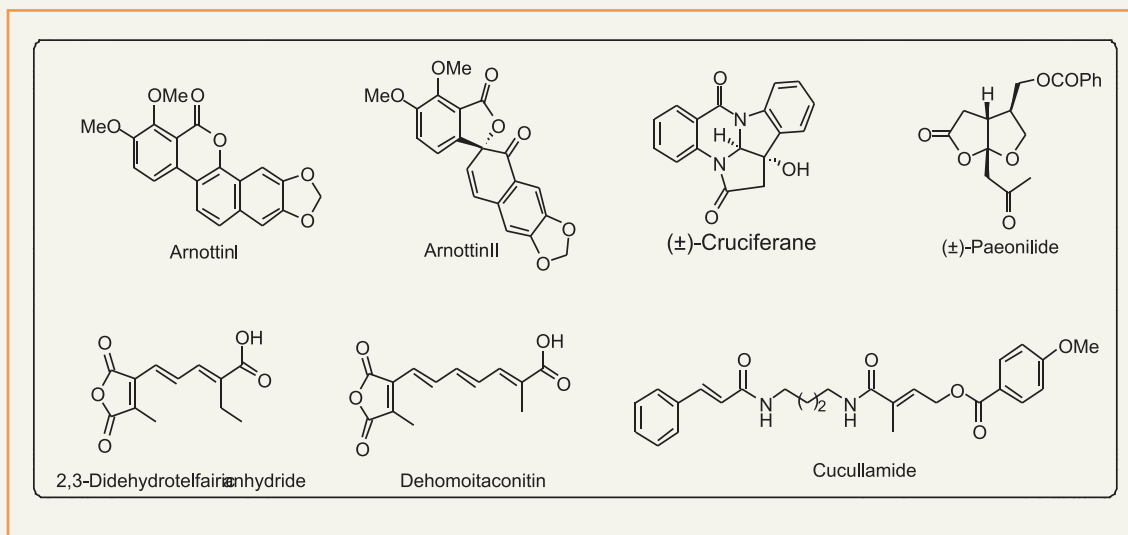
Scheme 2. Reagents and conditions: (a) thionyl chloride, DMF(cat), toluene, 100 °C, 4h; (b) Et₃N, suitable amide, 0°-rt, 12h

Total synthesis of recently isolated bioactive natural products

Publications: Org. Lett., 2013, 15, 5826, 4006; J. Org. Chem., 2014, 79, 2538

Total syntheses of several desired, complex bioactive, natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors were undergone employing variety of new synthetic strategies. The natural products synthesized included cruciferane, arnottin I, arnottin II, paeonilide, 2,3-

di-dehydrotelfaric anhydride, dehomitaconitin and cucullamide. The products were synthesized applying different avenues like the aryne insertion reactions, intramolecular one-pot double cyclization, diastereoselective reactivity umpolung and remarkable base stimulated 1,2-/1,4-/1,6-eliminations.



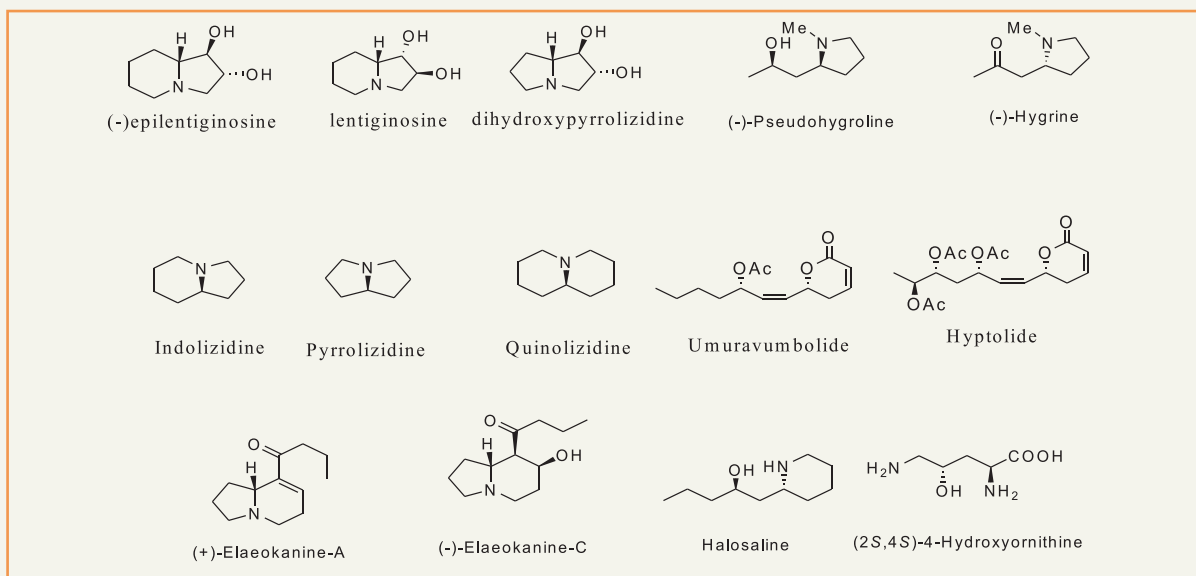
Methodologies for asymmetric synthesis of biologically active compounds

Publications : RSC Adv., 2013, 2, 18288, 2014, 4, 3238; Adv. Synth. Catal., 2013, 355, 1719; J. Org. Chem., 2013, 8, 11756; Tetrahedron Asymmetr., 2013, 24, 305; Synlett, 2014, 25, 1089

Research was focused on asymmetric synthesis of biologically active natural products which included mainly the naturally occurring lactones and amino alcohols. A proline catalysed organocatalytic route to the enantiopure synthesis of *syn/anti*-1,3-polyols was recently developed. The protocol developed was further extended to the synthesis of *syn/anti*-1,3 amino alcohol which was successfully utilised for the synthesis of a variety of natural

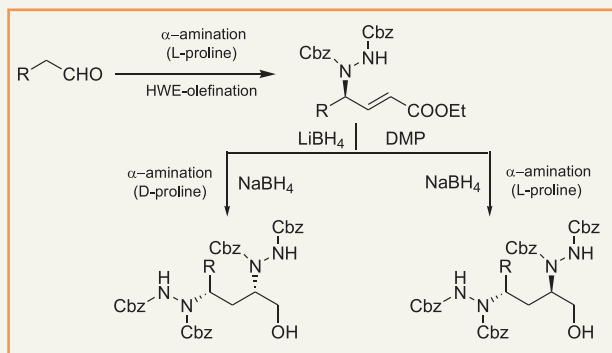
products of biological and pharmaceutical importance such as halosaline, hydroxyornithine, pseudohygroline, lentiginosine, hyptolide and umuravumbolide etc. Above protocol helped to synthesize the indolizidine, pyrrolizidine and quinolizidine ring system.

The total syntheses of molecules mentioned below were accomplished using the above reactinos.

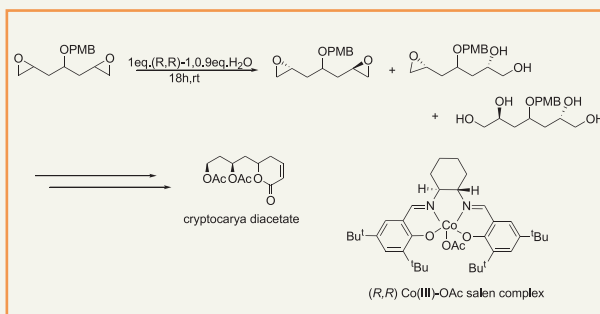


Synthetic strategy for the synthesis of 1,3-diamines

A general organocatalytic strategy for asymmetric synthesis of *syn/anti*-1,3 diamine was developed. The strategy employed a proline catalysed sequential α -aminoxylation and Horner Wadsworth-Emmons (HWE) olefination of aldehydes as the key steps where *syn*-1,3-diamines were obtained as the most favourable product.



A desymmetrisation approach was used for the synthesis of enantiopure *syn/anti*-1,5diols via hydrolytic kinetic resolution (HKR) of functionalised meso bis-epoxide which was further elaborated to the synthesis of *syn/syn*-1,3-5-triols and subsequently applied to the formal synthesis of cryptocarya diacetate.



Development of synthetic methods and total synthesis of natural products

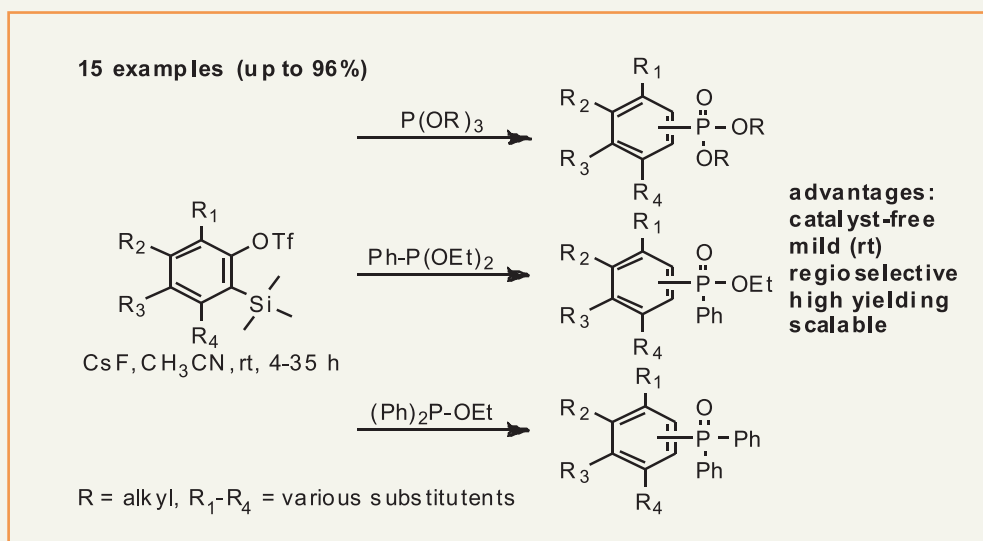
Publications: Org. Lett., 2013, 15, 2218; Synth. Commun., 2013, 43, 1; Angew. Chem. Int. Ed., 2014, 53, 7038

The development of novel methodologies and their application in the total syntheses of drugs and bioactive natural products were highly targeted in the research.

P-arylation: Arynes to aryl-phosphonates, aryl-phosphinates, and aryl-phosphine oxides

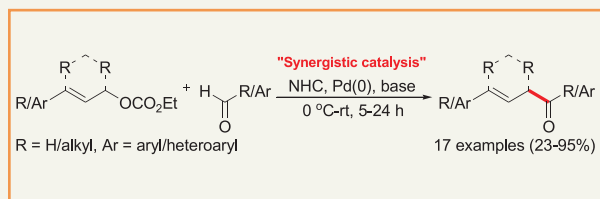
Michaelis-Arbuzov reaction is the most extensively utilized method for the preparation of organo-phosphorous com-

pounds, which works well only with aliphatic halides. Hence, relatively harsh reaction conditions using transition-metal-catalyzed P-arylation (Arbuzov/Hirao reaction) were used for the preparation of aryl-phosphorus compounds. A competent process for the synthesis of aryl-phosphonates, aryl-phosphinates and aryl-phosphine oxides was developed by making an efficient use of arynes for CP bond construction.



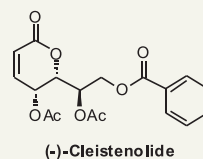
Direct allylation of *in situ* generated aldehyde acyl anions by synergistic NHC- and Pd-catalysis

The first, direct and regioselective allylation of *in situ* generated aldehyde acyl anions was achieved by synergistic NHC- and Pd-catalysis. This provided an efficient access to valuable β,γ -unsaturated ketones under milder reaction conditions starting from easily accessible allylic carbonates and aldehydes without any pre-activation. The synergistic catalysis method was demonstrated to add new dimension to the area of metal mediated C-allylation.



Diastereoselective chemoenzymatic total synthesis of 6-epi-(-)/(+)-cleistenolide

A short, efficient, practical and protecting group-free diastereoselective total synthesis of 6-epi-($\pm$)-cleistenolide was achieved in five steps with 60% overall yield. An application of the chemoenzymatic approach also furnished both the enantiomers of 6-epi-cleistenolide. Achmatowicz reaction, chemoselective oxidation of secondary alcohol, diastereoselective 1,3-*anti* reduction of β -hydroxy ketone and enzymatic resolution of 1,3-diol were the key features of this linear total synthesis. Such synthetic strategy can be extended for an asymmetric total synthesis of (-)-cleistenolide and related bioactive natural products.



Anti-tuberculotic

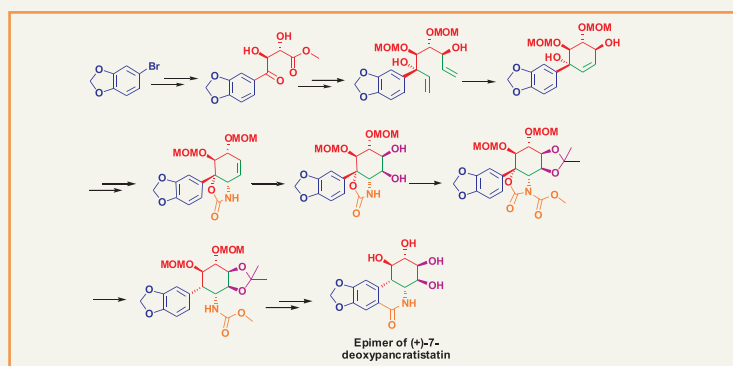
Synthesis of natural products and biologically active compounds

Publications: Tetrahedron Lett., 2013, 54, 4851; 4789; 5562;
Tetrahedron Asymmetr., 2013, 24, 1473; Synthesis, 2013, 45, 3399

The research work involved the organic synthesis of biologically active molecules like commercially important drugs and natural products. The targets included 7-epideoxypancratastatin, vitamin H (D+)-Biotin, antihistaminic drug Olopatadine, synthetic route towards Tamiflu drug, antidepressant drug Venlafaxine and alkaloids berberis and miltefosine.

Synthesis of epimer of (+)-7-deoxypancratistatin

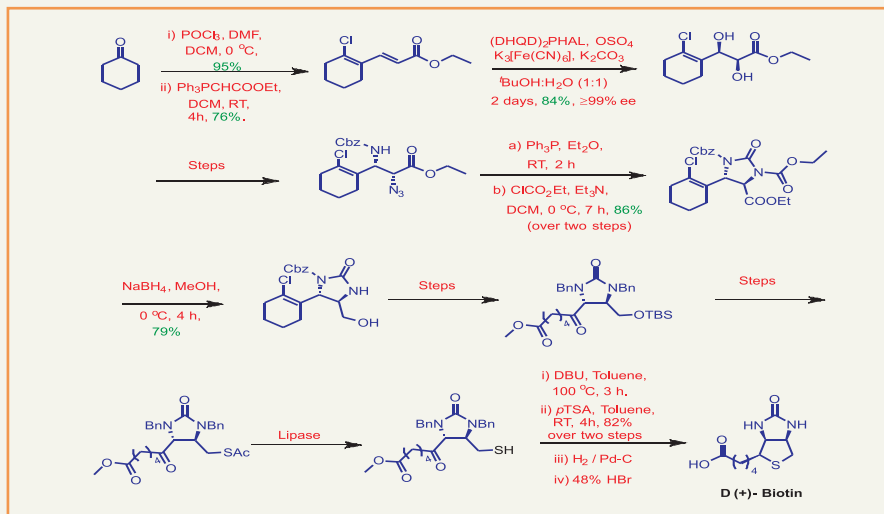
A highly stereocontrolled asymmetric total synthesis of epimer of (+)-7-deoxypancratistatin was achieved from readily available starting materials via unified strategy employing sharpless asymmetric dihydroxylation, ring closing metathesis, overman rearrangement, hydrogenolysis and Bischler-Napieralski reaction in 15 purification steps with 15% overall yield.



Enantioselective synthesis of D-(+)-biotin via a sharpless asymmetric hydroxylation strategy

A novel and enantioselective synthesis of (D)-(+)- biotin using asymmetric approach to install the chiral centers was accomplished starting from commercially available cyclohexanone. The key steps in the sequence were the sharpless asymmetric dihydroxylation of (*E*)-ethyl 3-(2-

Chlorocyclohex-1-en-1-yl) acrylate which was transformed to vicinal diamine derivative to establish the stereocenters of D-(+)-biotin. The carboxyalkyl side chain was revealed by unmasking the cyclohexene by ozonolysis and enzymatic hydrolysis of a thioacetate. Further cyclisation and functional group transformations led to the target molecule.



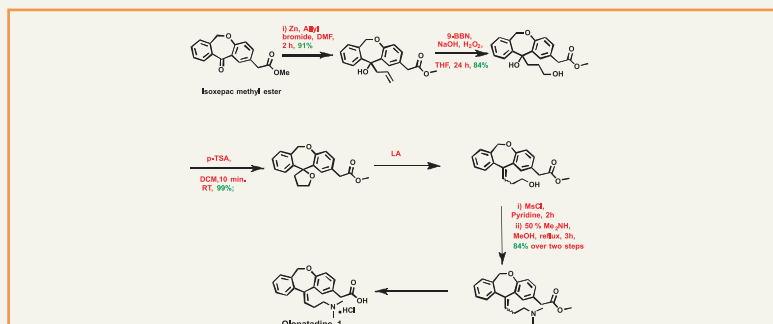
Synthesis of antihistaminic drug olopatadine hydrochloride

A new and simple synthetic route for the synthesis of olopatadine was undertaken. Isoxepac methyl ester was subjected to Barbier reaction with allyl bromide in the presence of zinc powder in DMF as the solvent furnished the allylic alcohol. Hydroboration with 9-BBN followed by

quenching with sodium hydroxide and hydrogen peroxide afforded the diol. The diol was treated with both protic as well as lewis acids. It was found that inorganic protic acids led to the formation of cyclic spiro ether as the exclusive product. Spiro ether on treatment with 2.5 equivalents of AlCl_3 resulted in the formation of homoallyl alcohol with an E/Z ratio of 2:3. The ratio was improved to 1:9 by using the

Synthesis of natural products and biologically active compounds

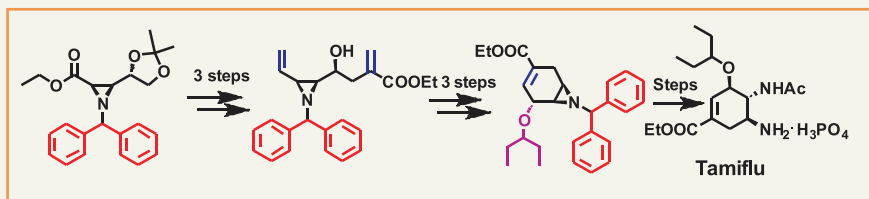
recrystallization. This synthetic route was simple to operate and completed in seven steps with 59% overall yield.



A concise synthetic approach towards Tamiflu

The key synthon cis-aziridine was synthesized from (D)-mannitol efficiently and utilised for the synthesis of the

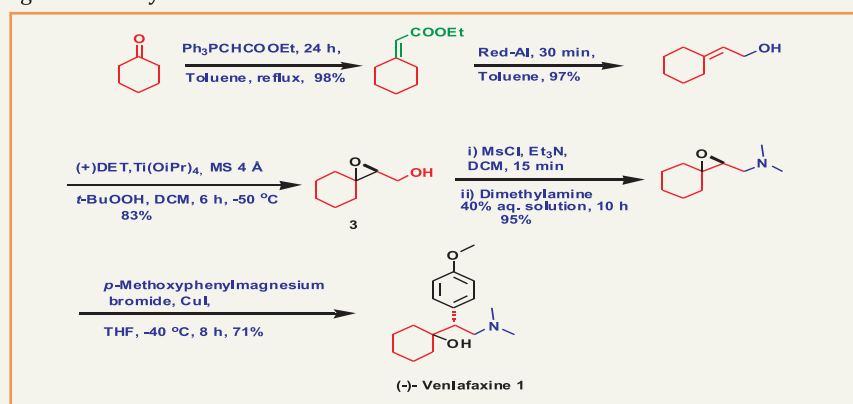
Oseltamivir phosphate, using Wittig olefination, Barbier addition, Mitsunobu reaction and ring closing metathesis (RCM) as key essentials.



Asymmetric synthesis of antidepressant venlafaxine

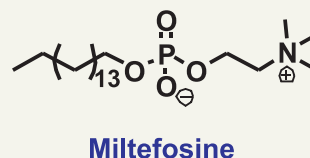
An asymmetric total synthesis of (-)-venlafaxine was achieved from commercially available, cheap starting material by using an eco-friendly proline-based catalyst. A novel protocol for gram scale synthesis of venlafaxine was

Developed which involved sharpless asymmetric epoxidation as a key chirality inducing step and regiospecific opening of epoxide with aryl Grignard reagent. This synthetic approach provided a high overall yield (53%) in 6 steps.



Process development for miltefosine

Miltefosine (Impavido), the drug clinically used for the treatment of Visceral Leishmaniasis (Kala-Azar, black fever). A process was developed on lab scale and demonstrated to an Indian company.

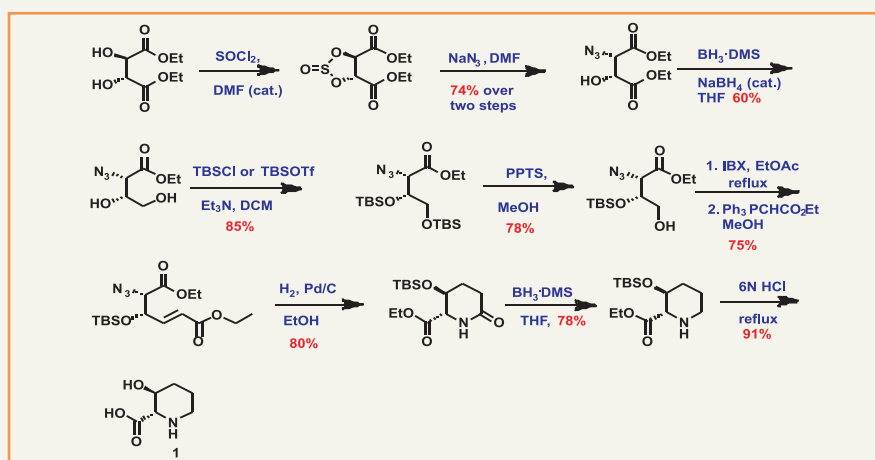


Synthesis of natural products and biologically active compounds

Synthesis of (2S,3S)-3-hydroxypipelicolic acid

An enantiopure synthesis of 3-hydroxypipelicolic acid was targeted. The formal synthesis of 3-hydroxypipelicolic acid was accomplished starting from L(+)-tartaric acid and total synthesis from *cis*-2-butene-1,4-diol using sharpless asymmetric di-hydroxylation. Tartaric acid was converted to cyclic sulphite and opened with azide to furnish azido alcohol. The ester adjacent to hydroxyl group was selectively

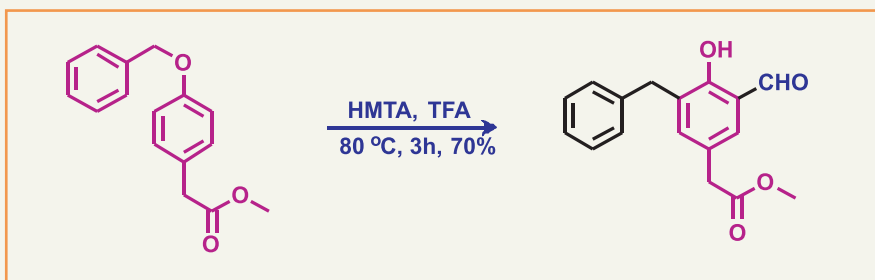
reduced to furnish diol to form its derivative bis TBS ether. This primary alcohol was selectively deprotected and the alcohol was oxidized and subjected to 2 carbon homologation to furnish unsaturated ester which was subjected to hydrogenation and it underwent 3 step transformation led to the formation of lactam. The lactam was reduced to amine and further TBS and ester were globally deprotected to furnish (2S,3S)-3-hydroxypipelicolic acid.



Development of synthetic methodologies: One-pot migration-formylation of benzyl aryl ethers under Duff reaction condition

The reaction was performed with HMTA (hexamethylene tetramine) and TFA (trifluoroacetic acid). Under the optimal

reaction conditions, a variety of Bn and PMB ethers underwent *ortho* rearrangement. Thus, a novel one-pot synthetic route to access substituted salicylaldehyde from benzyl aryl ether involving migration of benzyl group and formylation in moderate to good yields was developed.



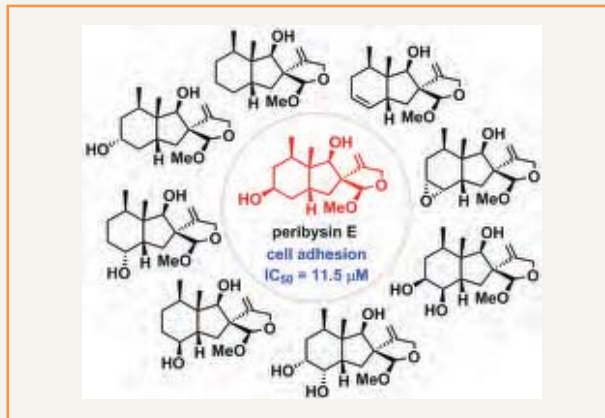
Total synthesis of biologically active compounds and medicinal chemistry

Publications: Org. Lett., 2013, 15, 1894, 4556; J. Org. Chem., 2013, 78, 6281, 8149; RSC Adv., 2013, 3, 20291; Synthesis, 2013, 45, 1689

The work was aimed to undergo the total synthesis of biologically active compounds and study different aspects of its medicinal chemistry. The products with the properties of cell adhesion inhibitors, insect repellents, antibacterial, anti-inflammatory and anti-cancer agents were targeted.

Total syntheses of potent cell adhesion inhibitor Peribysin E analogs

A group of natural products called peribysins (A-G) was isolated from a strain of *Periconia byssoides* OUPS-N133 separated from the sea hare, *Aplysia kurodai*. This natural product, peribysin E attracted the attention owing to its potent cell adhesion inhibitory activity. The total synthesis of ($\pm$)-peribysin E was accomplished in less than ten steps starting from readily accessible materials. Eight new analogs of the natural product were also synthesized by means of "diverted total synthesis". The synthesis highlights the use of sequential Diels- Alder/ Aldol strategy, Semipinacol type rearrangement and a protecting group free approach to access these functionally embellished hydrindanes.

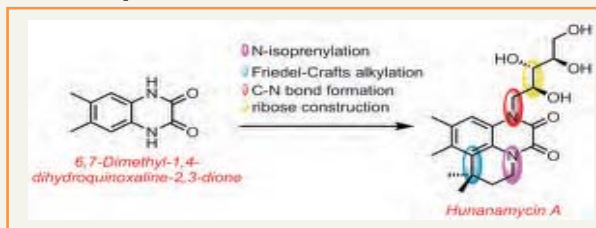


The sequential Diels-Alder/ aldol approach was further explored and utilized for the efficient synthesis of functionalized cis-hydrindanes and cis-decalins in a highly diastereoselective manner. Several new cis-hydrindanes/ cis-decalins loaded with orthogonal functional groups were synthesized which serve as key intermediates in the synthesis of complex molecules. A protecting group-free total synthesis of an insect repellent Nootkatone and the first synthesis of a Noreremophilane using the shortest sequence were achieved.



First total synthesis of hunanamycin A

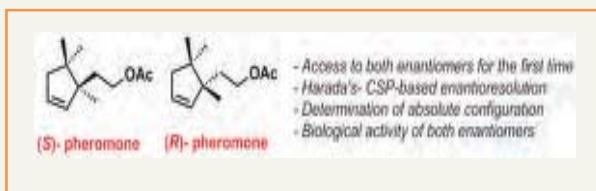
Hunanamycin A is a perfect drug candidate for lead optimization in drug discovery, as it complies with the Lipinski rule of five. First total synthesis of hunanamycin A and several analogues using simple and scalable chemistry were accomplished.



Synthesis of the enantiomers of the longtailed mealybug pheromone

The synthetic sex pheromone isolated from *Pseudococcus longispinus* was proved to be biologically active. Its racemate 25 μ g remained active for several months under field conditions. The preparation of both the enantiomers of the pheromone was done by converting an advanced intermediate into its diastereomeric derivative. The absolute configuration was determined unambiguously by X- ray crystal structure and biological activities of both synthesized enantiomers and the racemate were tested in field trials.

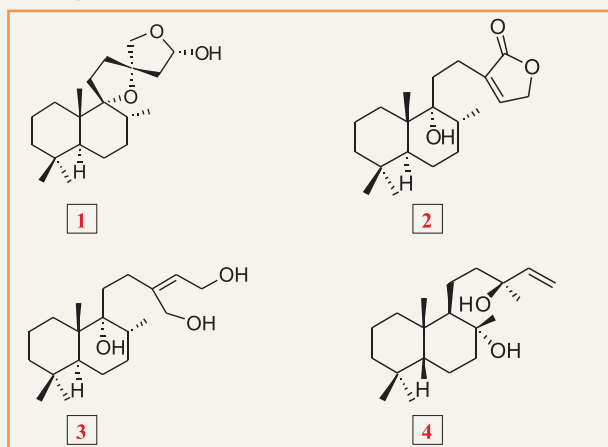
The field trials showed that the (S)-(+)-enantiomer was highly attractive to male mealybugs, strongly suggesting that female longtailed mealybugs produce this enantiomer. The (R)-(-)-enantiomer was benign, neither attractive nor inhibitory. This work was done in collaboration with J. G. Miller of California University, United States.



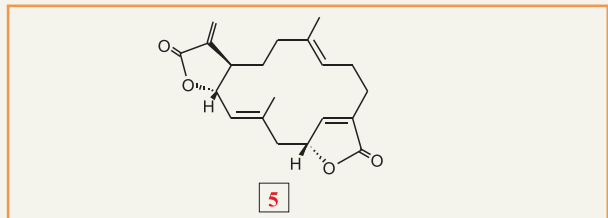
Identification of novel phytochemicals with biological activities

Compounds with anti-mycobacterial activity

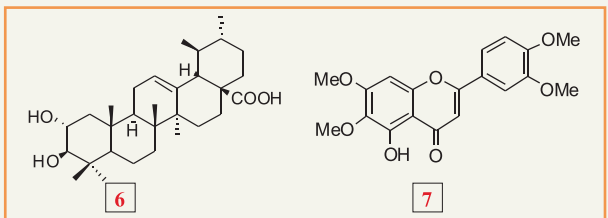
Diterpenoids, triterpenoid and flavonoid with anti-TB activity were isolated from three *Lamiaceae* plant species. Isolation of new labdane diterpenoids (1), (2), (3) and (4) with selective activity against *Mycobacterium tuberculosis* H37Ra and IC_{50} 5.02-9.8 $\mu\text{g/ml}$ was carried out from the species *Leucas stelligera*. These compounds were non-toxic to species *M. smegmatis*, *E. coli* and cell lines MCF-7, THP-1 and HepG-2.



Cembrane diterpenoid ovatodioid (5) with selective activity against IC_{90} 6.53 $\mu\text{g/ml}$ and *M. tuberculosis* H37Ra was isolated from *Anisomeles heyneana*.



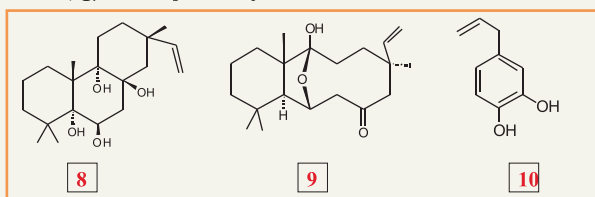
The phytochemical investigation of *Plecthranthus mollis* led to the isolation of anti- *M. tuberculosis* H37Ra compounds, triterpenoid corosolic acid (6) (IC_{50} 4.47 $\mu\text{g/ml}$) and flavonoid 3'-O-methyleupatorin (7) (IC_{50} 4.93 $\mu\text{g/ml}$).



Compounds with anti-cancer activity

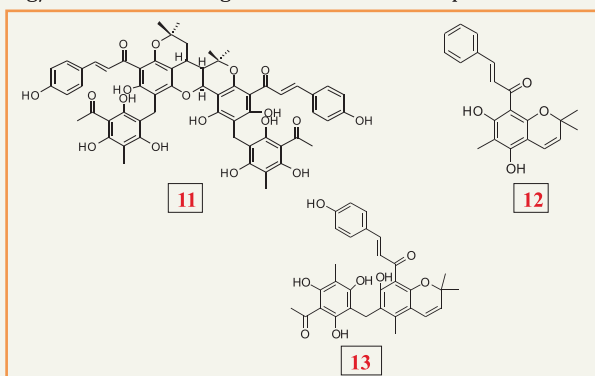
Phytochemical investigation of *Anisochilus verticillatus* resulted in the isolation of a new isopimarane diterpenes (8), a new 8,9-secopimarane diterpene (9) and hydroxychavicol

(10). Compounds (8), (9), and (10) inhibited the growth of *M. tuberculosis* H37Ra, with IC_{90} values of 35.00, 20.00, and 12.50 $\mu\text{g/ml}$, respectively.



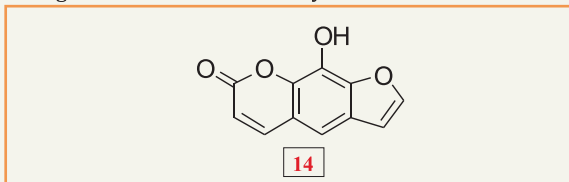
Compounds with anti-fungal activity

One new dimeric chalcone kamalachalcone E (11) along with known compounds as 1-(5,7-dihydroxy-2',2,6-trimethyl-2H-1-benzo-pyran-8-yl)-3-phenyl-2-propen-1-one (12), and 4'-hydroxyrotyllerin (13) from the red colored extract of Kamala (*Mallotus philippinensis*) were isolated. Compounds (11) and (12) exhibited IC_{50} of 8 and 16 mg/mL against food spoilage fungi *Cryptococcus neoformans* and *Aspergillus fumigatus*, respectively. Compound (13) at 100 mg/mL showed 54% growth inhibition of Thp-1 cell line.



Compounds with anti-glycation activity

A coumarin xanthotaxol (14) was isolated from fruits of *Aegle marmelos* with antiglycation activity, IC_{50} 0.43 mM by BSA-glucose fluorescence assay.



Purified extracts with anti-STI activity

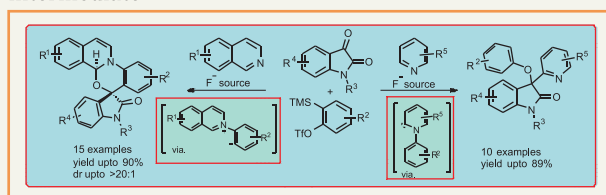
Four purified extracts were developed with good anti-STI activity such as anti-HIV and anti-HSV-2 and are under process for preparation of new microbicidal herbal product.

Transition-metal-free carbon-carbon bond-forming reactions using aryne chemistry and NHC organocatalysis

Publications: Angew. Chem. Int. Ed., 2013, 52, 10040; Org. Lett., 2013, 15, 4620, 5202, 5452, 2014, 16, 676, 1728, 5202; J. Org. Chem., 2014, 79, 4245; Synlett, 2014, 25, 608

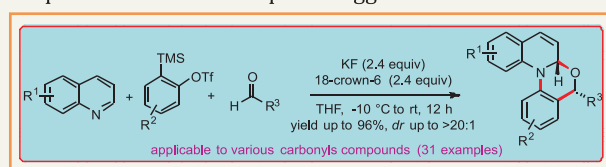
Transition-metal-free multicomponent reactions involving arynes, N-heterocycles and isatins

The reaction afforded the spirooxazino isoquinoline derivatives with isoquinoline as the nucleophilic trigger proceeding via 1,4-dipolar intermediates. The utility of pyridine as nucleophile furnished indolin 2-one derivatives and the reaction is likely to proceed through a pyridylidene intermediate.



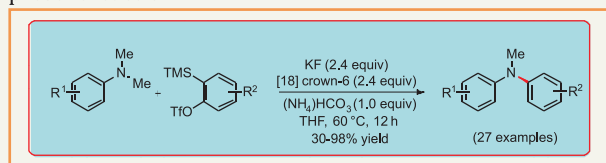
Multicomponent reactions involving arynes, quinolines and aldehydes

The MCR involving arynes, quinolines and aldehydes were developed leading to the diastereoselective synthesis of benzoxazino quinoline derivatives in good yields proceeding via 1,4-zwitterionic intermediates. The synthetic potential of various carbonyl compounds as well as the utility of isoquinoline as the nucleophilic trigger was examined.



Arynes in transition-metal-free monoarylation of aromatic tertiary amines

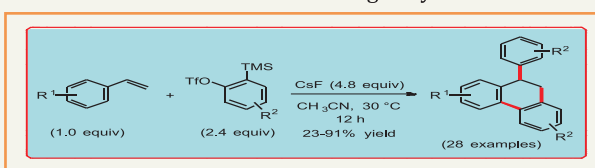
The highly monoselective N-arylation of aromatic tertiary amines was developed using a transition-metal-free approach by arynes. The reaction afforded functionalized diaryl amines in moderate to excellent yield. High levels of functional group compatibility especially with halogen containing substrates, dyes and donor-acceptor systems, as well as high yields of products are the notable features of the present reaction.



Efficient synthesis of 9-aryl dihydrophenanthrenes by a cascade reaction involving arynes and styrenes

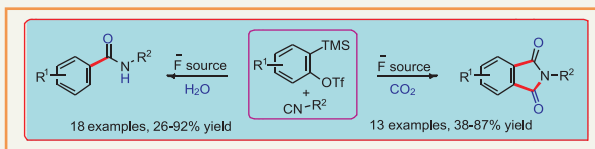
A mild, general and transition-metal-free protocol for the synthesis of 9,10-dihydrophenanthrenes was developed.

The aryne generated by the fluoride-induced 1,2-elimination of 2-(trimethylsilyl)aryl triflates undergone the Cascade reaction initiated by the Diels-Alder reaction leading to the formation of 9-aryl- 9,10-dihydro phen anthrene derivatives in moderate to good yields.



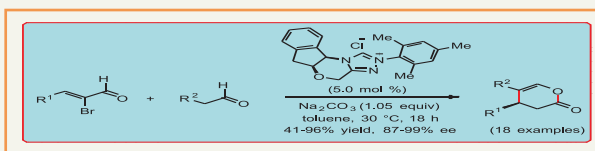
Practical synthesis of phthalimides and benzamides by a multicomponent reaction involving arynes, isocyanides and CO2/H2O

The transition-metal-free multicomponent reactions involving arynes and isocyanides with either CO2 or H2O were developed. The reactions resulted in the formation of N-substituted phthalimides where CO2 was the third component. The utility of water as the third component furnished benzamide derivatives in moderate to good yields. The reactions took place under mild conditions.



Asymmetric NHC-catalyzed annulation of modified enals with enolizable aldehydes

The NHC-catalyzed highly enantioselective lactonization of modified enals with enolizable aldehydes was undergone proceeding via the, -unsaturated acylazolium intermediates. The reaction resulted in the asymmetric synthesis of synthetically important 4,5-disubstituted dihydro pyranones.



Synthesis of functionalized coumarins and quinolinones by NHC-catalyzed annulation of modified enals with heterocyclic C-H acids

NHC-catalyzed lactonization and lactamization of 2-bromo enals with heterocyclic C-H acids proceeding via the α , β -unsaturated acylazolium intermediates were reported. The reaction furnished coumarin or quinolinone fused the lactone/lactam derivatives.

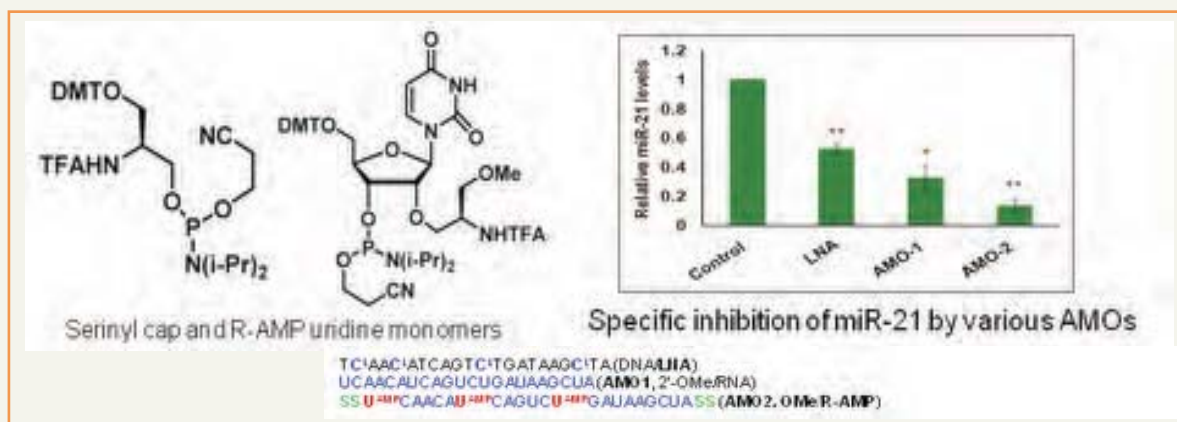
Synthetic functional nucleic acids for regulation of mRNA, miRNA, siRNA and as aptamers

RNA sequences were targeted by synthetic oligonucleotides (ON) to substitute protein as a therapeutic strategy. It developed the DNA/RNA aptamers.

MiRNA targeting and splice correction to encounter deadly diseases

A chirally substituted *R*-AMP-DNA (*R*-2'-amino-methoxy-propyl-substituted DNA) analogue was developed which is highly resistant to nucleases that form very stable

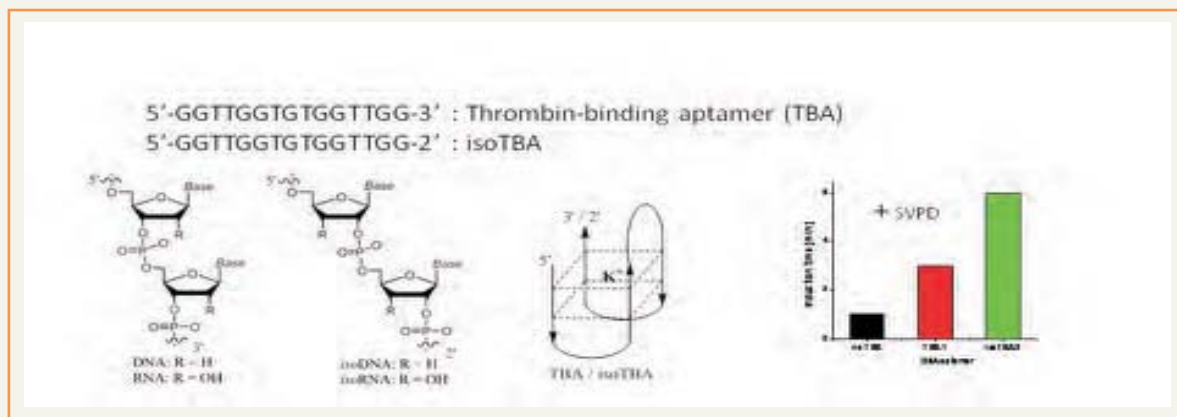
duplexes with RNA. The serinyl capped *R*-AMP/OMe mixmers were tested for splice correction assay and were found better than the OMe/LNA mixmers in the splice correction assay. It was developed to correct the mutation of β -globin aberrant gene responsible for thalassemia. It has high potential against miR-21 and miRNA found to be over-expressed in cancer cells. The miRNA inhibition studies were done at CSIR- IGIB, New Delhi. The splice correction assay was done by Dr. Mike Gait at MRC-LMB, Cambridge, UK.



2'-5'-sugar-phosphate backbone as enzymatically stable functional alternate to 3'-5'-DNA aptamers

The application of this aptamer was not optimum due to the enzymatic instability of the 3'-5'-linked oligomer in biological systems. Several chemical modifications of this aptamer were studied. It led to the instability of tertiary quadruplex structure or loss of thrombin binding activity.

A homosequential 2'-5'-linked isoDNA sequence, an enzymatically stable isoTBA that retained the functional ability to bind thrombin which showed better clotting induction time in presence of SVPD, a phosphodiesterase hydrolytic enzyme. Thrombin acted as a chaperone to induce the quadruplex structure with a different backbone identity in isoTBA compared to the natural 3'-5'DNA backbone.

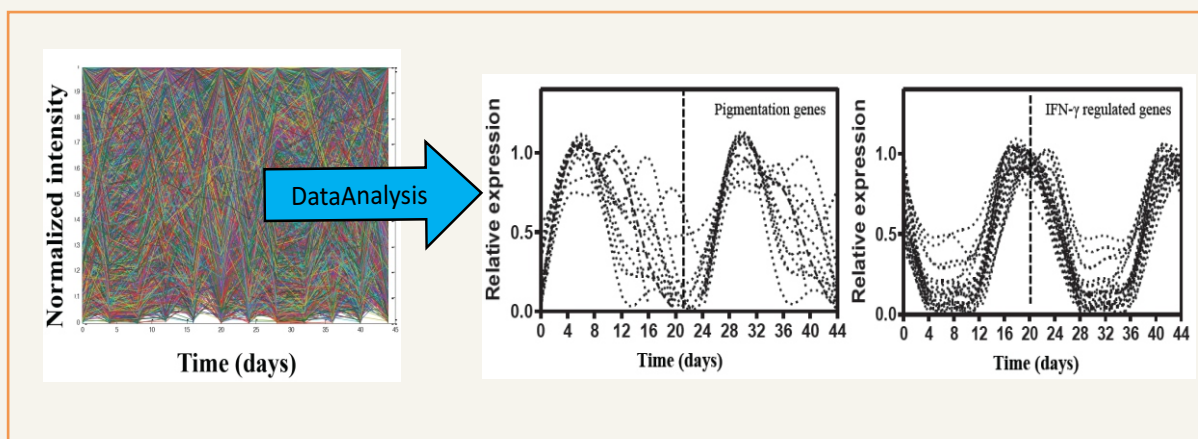


Analysis of high-throughput data for deciphering pigmentation

Publication: Proc. Natl. Acad. Sci. U.S.A., 2014, 111, 2301

Skin pigmentation has implications in healthcare and cosmetology. It is a dynamic process with the skin constantly undergoing tanning followed by a return to basal pigmentation levels, or de-tanning. Defects in the pigmentation machinery lead to diseases with very serious social implications such as vitiligo. With the aim of understanding normal and aberrant pigmentation, a team of experimental biologists led by Rajesh Gokhale from CSIR-IGIB has been investigating pigmentation in various systems ranging from in vitro cell culture to clinical studies using skin samples from vitiligo patients. Using high-throughput measurements, a lot of data is generated. For instance, analysis of one sample (one of the replicate measurements for one treatment, at one time) gives about 40,000 values for the expression of each fragment of expressed RNA that is tested. Given the multiple treatments, few replicates, and multiple time-points at which samples are taken, analysis of this data is challenging.

At CSIR-NCL, we have developed the capability of carrying out such high throughput data analysis. The results are used to develop hypothesis about the mechanism that can be experimentally tested, and also used for developing a reaction network for melanin synthesis, transport and control of these processes. In one such project, we developed a simple but new method based on a modified periodogram analysis for mining of noisy time-course expression data (figure on left below). This analysis led to the identification of interferon-gamma regulated genes (figure on right) as regulators of the depigmentation process. Extensive experimentation including cellular assays and animal models were used by experimental collaborators to verify this hypothesis.

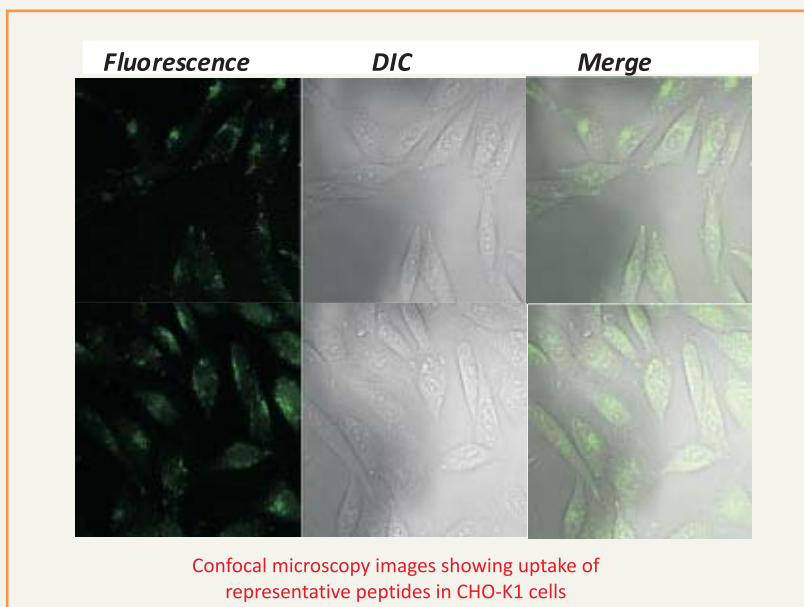


Design and synthesis of novel molecular transporters for efficient cargo delivery to cells

The objective was to develop novel molecular transporters for efficient cargo delivery, especially to skin cells. It exhibit less barriers to traverse for such transporters to evaluate the efficiency to transport cargo molecules such as drugs and siRNA for different applications.

The previously designed and synthesized penetrating oligomers were taken up by mammalian cells (CHO-K1 and HeLa) far more efficiently than control cell penetrating peptides (CPPs). These oligomers possess low cytotoxicity which is an additional attractive feature. A series of cell pene-

trating peptides based on the (R-X-R)-motif and containing N-aminoalkyl proline-derived spacer amino acids (X) was further developed. An enhanced cell uptake was demonstrated by FACS analysis and the oligomers were shown to be efficient at transporting pDNA into cells. The chirality together with the hydrophobicity and flexibility derived from the spacer amino acid were found to have a marked influence on the cell-penetrating and cargo delivery properties of the CPPs. The peptides containing *N*-(3-aminopropyl)-D-proline spacers were found to be the best at cell penetration and cargo delivery.



pH effects in small scale culture platforms and solutions

Publications: J. Ind. Microbiol. Biotech., 2014, 41, 647;
J. Chem. Tech. Biotech., 2014, 90, 166; WO 2014020617 A1

pH effects in small scale culture platforms and solutions

Shake flasks are widely used to culture animal cells and microorganisms, but do not allow for pH control without additional infrastructure. In the presence of a carbon source like glucose, culture pH typically decreases due to overflow metabolism and can limit growth in shake flasks. We have demonstrated the use of magnesium hydroxide loaded pH managing hydrogels (m-pHmH) for in situ base release to counter the decrease in culture pH in shake flasks using *E. coli* as a model organism, and previously also shown their application in animal cell culture. We demonstrate one application of such in situ pH management to increase the volumetric plasmid yield from *E. coli* in shake flask culture. In situ glucose release through a hydrogel to mimic fed batch culture along with the addition of m-pHmH resulted in a 395% increase in volumetric plasmid yield to 38 µg/ml in shake flask culture.

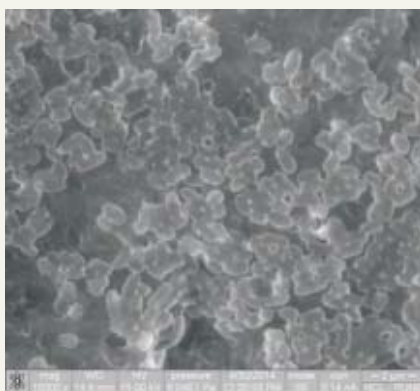
Mathematical models currently used to simulate animal cell growth and metabolism do not simulate changing culture pH and its effect on metabolism, and hence cannot accurately model culture behavior in the absence of pH control. Animal cell cultures are however widely cultured at a small scale without pH control, e.g., for clone screening during cell line development. A mathematical model for animal cell growth without pH control was developed and applied to design optimal conditions for clone screening without pH control. The model was used to simulate clonal heterogeneity and predict relative clone performance in different culture conditions. Correlation coefficients predicted by the model between clone titers in batch and fed batch screening conditions and the pH controlled fed batch are in good agreement with experimentally reported values. Fed batch mode is predicted to result in better screening outcomes than batch, but only for clones able to consume lactate. Model simulations reveal that culture duration of the screening assay has a large effect on the predictive ability of the screen and optimal durations differ based on the ability or inability of clones to consume lactate.

A novel method for the immobilization of bacterial whole cell containing penicillin G acylase

The aim of the research was to develop a stable and economical immobilized preparation method to obtain Penicillin G acylase which acts on the side chains of penicillin G and related antibiotics to produce β -lactam antibiotic intermediates such as 6-aminopenicillanic acid.

A new methodology for whole cell immobilization using cellulose based modified polymer was developed. The SEM

image of immobilized whole cells containing penicillin G acylase is shown in the figure. The immobilized whole cell flat sheet polymer showed 25% less K_m than the free whole cells. In addition, 92% operational stability after 20th cycle of successive runs and 90% storage stability at 4°C for twenty days were obtained using immobilized preparation. Initial studies indicated a high potential of immobilized preparation for commercial exploitation.



SEM image of immobilized bacterial whole cells

Study of biochemical pathways in human cells

The aim was to study biochemical reaction pathways both small and large networks using mathematical modeling, computational approaches and optimization techniques. The progression of complex diseases and the identification of potential treatment strategies were understood to bring out many potential drug targets to counteract and control the disorders.

Reconstruction of human cell specific pathways

Hedgehog and Notch, two comprehensive human cell signaling pathways were reconstructed for further *in-silico* analysis. The resulted pathway data was collated which is the largest data not present in any of the available major and widely used databases. The newly reconstructed Hedgehog map comprised of 57 proteins, 6 cellular or phenotypic expression and 96 hyper-interactions, which is the largest Hedgehog pathway map of human. The manually curated Notch pathway contains 115 molecules including proteins and organic compounds and 231 molecular interactions.

Modeling and computation of pathways

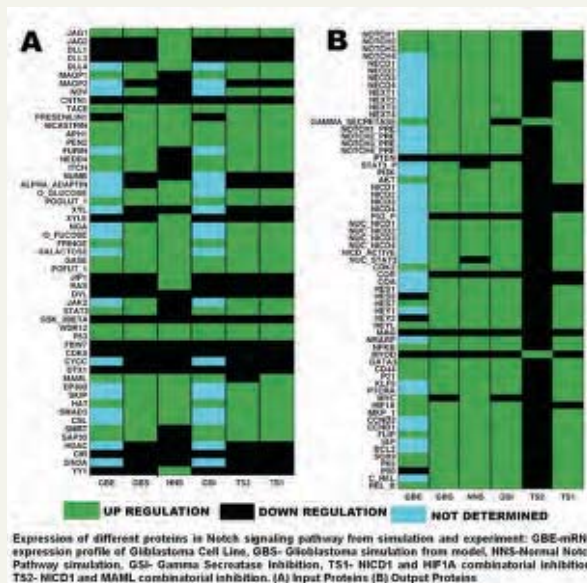
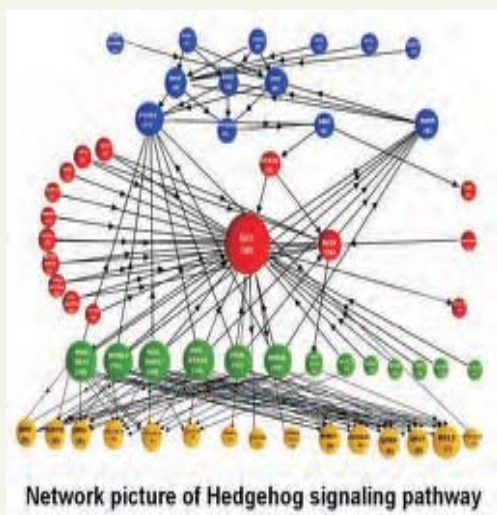
The structural and logical analysis of these pathways was performed using the recently developed computational techniques. The connectivity and centrality parameters were calculated to identify the important proteins from the

Publications: Clin. Exp. Pharmacol., 3, 137. Doi:10.4172/2161-1459.1000137 PLoS ONE, 8(7): e69132. Doi:10.1371/journal.Pone.0069132

network. Master Boolean models of all the interactions between the proteins of the pathways were developed to capture the regulations of the molecules. Normal as well as different cancer scenarios were created, such as Glioma, Colon and Pancreatic. Perturbation analysis on these cancer conditions were performed to identify the important and minimal combinations of proteins and to propose suitable treatment strategy.

In silico identification of key target metabolites

The computational strategies helped to predict the optimal yield and behavior of the pathways as well as identifying important target molecules. The novel combinations of drug targets SMO, GLI1, and GLI2 were identified to treat Glioblastoma cell line in the Hedgehog pathway. In Notch signaling pathway two alternative scenarios were proposed that included the partial suppression of Notch target proteins by NICD1 & HIF1A and complete suppression by NICD1 & MAML, in Glioblastoma cell line. The newly identified minimal combinations of oncoproteins probably used as the drug targets for further in-vitro and in-vivo analysis to control different cancers. It can be used specifically in treatment of Glioma, Colon and Pancreatic cancers and paves the way for newer biomarker identification and also for therapeutic marker identification.

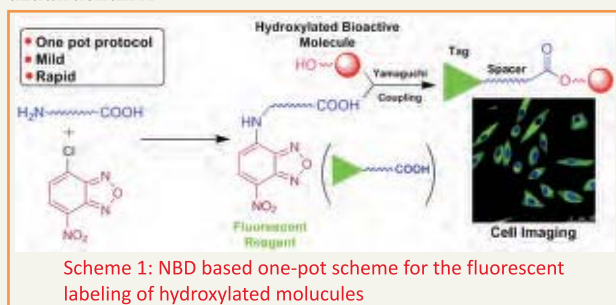


Chemistry and biology of natural products

The research was focused on different aspects of chemistry and biology of natural products.

One-pot fluorescent labeling protocol for complex hydroxylated bioactive natural products

A 7-nitrobenzo-2-oxa-1,3-diazole (NBD) based high yielding, one-pot labeling protocol was investigated for multi-functional and sensitive hydroxylated molecules using Yamaguchi coupling as the key reaction with comprehensive demonstration of optimization and applicability of the protocol. It involved the aromatic nucleophilic substitution on NBD-Cl by amine functionality of amino acids in the initial step to generate fluorescent reagent followed by Yamaguchi coupling between free carboxylic end and hydroxylated bioactive molecule in the same vessel (Scheme 1). The methodology was successfully applied on several sensitive and complex hydroxylated bioactive compounds including 7-deacetylazadi-radione, simvastatin, camptothecin, andrographolide, cinchonine, β -dihydroartemisinin and azadirachtin A.



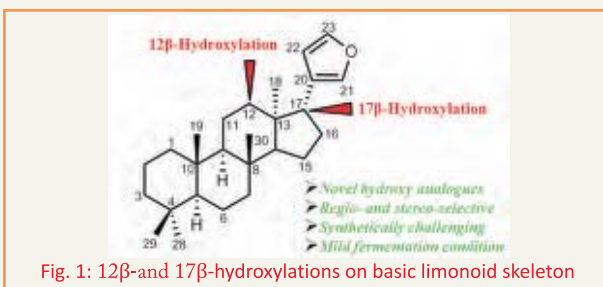
Azadiradione derivatives and their labeled analogues were evaluated for cytotoxic activity against several cancer cell lines by cancer cell viability and motility assay, thus the applicability of NBD tagged bioactive molecules was assessed. The qualified fluorescent probes such as 1 were imaged successfully within cancer cell-lines to investigate cellular uptake and localization. Sub-cellular localization of 1 was investigated by co-localization studies (Fig. 1).

Biocatalyst (fungi) mediated regio- and stereo-selective hydroxylations of basic limonoids

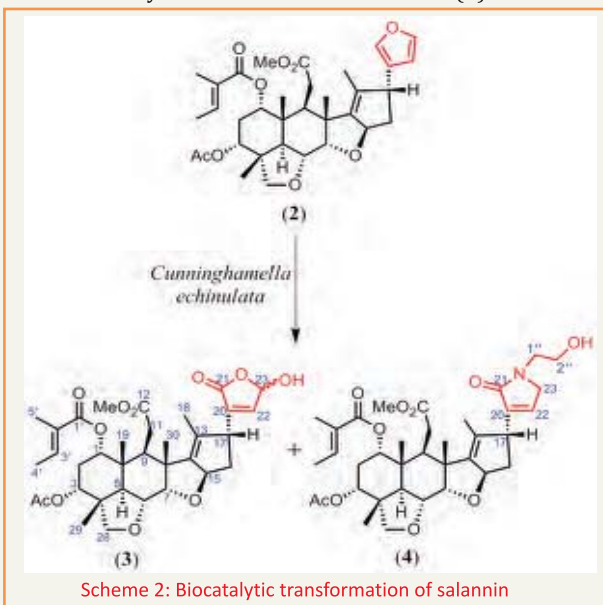
The fungal system belonging to the genera of *Mucor* efficiently converted basic limonoids such as azadiradione, epoxyazadiradione, gedunin and their derivatives into its synthetically challenging novel 12 β - and 17 β -hydroxy analogues (Fig. 1). The connectivity and stereochemistry of selectively introduced hydroxyl functionality was established through extensive spectroscopic (1D and 2D NMR, MS) and crystallographic studies. Selectivity among 12 β - and 17 β -hydroxylations was achieved through certain modifications of skeletal functional groups or choice of

Publications: Green Chem., 2013, 15, 1311; J. Org. Chem. 2013, 78, 10192; J. Med. Chem. 2013, 56, 8468; Org. Biomol. Chem. 2014, 12, 1048

Various whole-cell fungal biocatalysts.

**Biocatalyst (*C. echinulata*) mediated functionalization of salannin**

Biocatalyst assisted functionalization of salannin was studied due to its pronounced insecticidal activity and inefficiency of synthetic methods for selective modification. Among various fungal system screened, *Cunninghamella echinulata* was able to convert salannin to furan modified metabolites efficiently (Scheme 2). The major metabolite salanninolide (3) was γ -hydroxybutenolide analogue of C-17 furan and isolated previously from Neem seed extract. The minor metabolite was structurally novel and characterized as N-(2-hydroxyethyl)- α,β -unsaturated- γ -lactam analogue of furan moiety and named as salanninactam (4).

**Biocatalyst mediated regio- and stereo-selective hydroxylation and epoxidation of (Z)- α -santalol**

The biotransformation of (Z)- α -santalol (5) was studied using different fungal cultures. The (Z)- α -santalol was converted to its ester derivative, (Z)- α -santalyl acetate (6), which was further utilized to study its mode of biotransformation with a versatile, soil isolated fungal

Chemistry and biology of natural products

culture, *Mucor piriformis*. Followed by isolation and purification, the metabolites were spectrally characterized using 1D, 2D-NMR, GC, GC-MS and IR. The efficient regio- and stereo-selective functionalization of **6** into four novel metabolites through **5** was observed using the versatile fungal system *M. Piriformis*, which were identified as 10,11-cis- β -epoxy- α -santalol (**7**), 5 α -hydroxy-(Z)- α -santalol (**8**), 10,11-dihydroxy- α -santalol (**9**) and 5 α -hydroxy-10,11-cis- β -epoxy- α -santalol (**10**) (Scheme 3).

***Mucor hiemalis* mediated 14 α -Hydroxylation on steroids**

Transformation of testosterone and progesterone into synthetically challenging 14 α -hydroxy derivatives was achieved by using fungal strain *Mucor hiemalis*. Prolonged incubation led to the formation of corresponding 6 β /7 α , 14 α -dihydroxy metabolites. The position and stereochemistry of newly introduced hydroxyl group was determined by detailed spectroscopic analyses. The time course experiment indicated that fungal strain initiated transformation by hydroxylation at 14 α -position followed by at 6 β - or 7 α -positions (Scheme 4). It was suggested that

the 14 α -hydroxylase activity is NADPH dependent and belonged to the cytochrome P450 family.

Design, Synthesis, and Broad Spectrum Anti-microbial Properties of Short Hybrid E-Vinylogous Lipopeptides

Nonribosomal E-vinylogous γ -amino acids are widely present in many peptide natural products and have been exploited as inhibitors for serine and cysteine proteases. The broad spectrum antimicrobial properties and self-assembled nanostructures of various hybrid lipopeptides composed of 1:1 alternating α - and E-vinylogous residues were reported. Analysis of the results revealed that self-assembled nanostructures also play a significant role in the antimicrobial and hemolytic activities. In contrast to the α -peptide counterparts, vinylogous hybrid peptides displayed excellent antimicrobial properties against various bacterial and fungal strains. Peptides that adopted nano fiber structures displayed less hemolytic activity, while peptides that adopted nano needle structures displayed the highest hemolytic activity.

Characterization of protease inhibitor genes

Research was aimed to understand and decipher economically important traits in agriculturally important plants using omics based approaches.

Molecular responses of *Helicoverpa armigera* to plant protease inhibitors (PIs) and recombinant PIs

Molecular responses of *H. armigera* were investigated for different natural diets containing complex defense molecules and specific plant defensive protease inhibitor. The expression of phylogenetically diverse, 8 trypsin-like and 4 chymotrypsin-like mRNAs from different life stages of *H. armigera* reared on nutritionally distinct host plants was profiled to investigate the functional intricacy of serine proteases. The analysis revealed the diet- and stage-specific protease expression patterns. Expressed trypsins showed structural variations which resulted in differential substrate with inhibitors. Another approach was reported to investigate the optimal dose of recombinant CanPI-7 (rCanPI-7) and other inhibitory repeat domain peptides for effective antibiosis to *H. armigera*. Further responses of digestive proteases were characterized. The growth retardation upon exposure to rCanPI-7 and IRDs was more prominent in neonates as compared to third instar larvae. Influence of dosage of rCanPI-7 or IRDs was noticed on the expression and regulation of candidate trypsin and chymotrypsin genes in *H. armigera*. The transcript accumulation pattern correlated with the protease activity in rCanPI-7 or IRD exposed the larvae. It was also evident that the regulation and expression of *H. armigera* gut proteases were specific to the stage of PI exposure. Upregulation of the energy metabolism and redox processes was noticed in unbiased proteomic analysis.

Plant secondary metabolic pathway analysis and its significance in biotic stress

Comparative co-expression analysis between tomato and potato coupled with chemical profiling revealed an array of 10 genes that partake in SGA biosynthesis. Six of them existed as a cluster on chromosome 7, whereas additional two were adjacent in a duplicated genomic region on chromosome 12. A revised SGA biosynthetic pathway starting from cholesterol up to the tetra-saccharide moiety linked to the tomato SGA aglycone was suggested after the systematic functional analysis. Silencing GLYCOALKALOID METABOLISM 4 prevented accumulation of SGAs in potato tubers and tomato fruit. This phenomenon said to be utilized for the removal of unsafe, antinutritional substances present in these food crops. Metabolites related to defense from *Ocimum kilimandscharicum* were investigated. The biochemical and metabolic changes in *Ocimum kilimandscharicum* occurred in response to the feeding of

Publications: Insect Mol. Biol., 2013, 22, 258; J. Biomol. Struct. Dyn., 2014, 32, 13; Phytochemistry, 2014, 101, 16; Science, 2013, 341, 175

Helicoverpa armigera larvae. Metabolic analysis revealed that the primary and secondary metabolism of local and systemic tissues in *O. kilimandscharicum* was severely affected following larval infestation. The levels of specific secondary metabolites like camphor, limonene and β -caryophyllene were significantly increased in leaves upon insect attack. Choice assays were conducted by exposing *H. armigera* larvae on *O. kilimandscharicum* and tomato leaves. It demonstrated that *O. kilimandscharicum* significantly deters larval feeding. Larvae fed on artificial diet supplemented with *O. kilimandscharicum* leaf extract, camphor, limonene and β -caryophyllene showed growth retardation, increased mortality rates and pupal deformities. Digestive enzymes of *H. armigera* like amylase, protease and lipase showed variable patterns after feeding on *O. kilimandscharicum* that implied striving of the larvae to attain required nutrition for growth, development and metamorphosis. Selected metabolites from *O. kilimandscharicum* possessed significant insecticidal activity.

Biotechnology of endophytic fungi: Nanomaterials and secondary metabolites

Publications: RSC Adv. 2014, 4, 7729; Beilstein J. Nanotech., 2014, 5, 249; Mater. Lett., 2014, 129, 159

Nanobiotechnology

Synthesis of water-dispersible, naturally protein capped, monodispersed gold nanoparticles: The extracellular biosynthesis of monodispersed gold nanoparticles from the whole cells of novel extremophilic actinomycete *Thermomonospora* species was reported. The exact mechanism of synthesis was understood by this investigation. A simple protocol was used to purify the temperature and SDS resistant sulfite reductase enzyme and organic capping molecule which were required for the synthesis and stabilization of gold nanoparticles respectively. The purified enzyme was employed for the synthesis of gold nanoparticles along with the capping molecule, which rendered gold nanoparticles monodispersed in the solution.

Biological synthesis of silver nanoparticles using the fungus

***Humicola* species:** The biosynthesis of silver nanoparticles by the thermophilic fungus *Humicola* sp. was studied. The fungus when reacted with Ag⁺ ions reduced the precursor solution and led to the formation of extracellular nanoparticles as monitored by ultra violet visible spectroscopy. The morphology of nanoparticles was found to be spherical with good dispersity as revealed by transmission electron microscopy. Cell viability assays were carried out to assess the cytotoxicity of silver nanoparticles on NIH3T3 mouse embryonic fibroblast cell line and MDA-MB-231 human breast carcinoma cell line.

Biological synthesis of cationic gold nanoparticles and

binding of plasmid DNA: A biosynthesis methodology was developed for the functionalization of gold nanoparticles to cationic nature. The synthesis of C-GNPs was done by using peanut leaf extract in the presence of cysteamine. Thus formed C-GNPs were characterized by using UVvisible spectroscopy, the particle's sizes and shapes were confirmed by a transmission electron microscope (TEM) and crystallinity of C-GNPs was characterized by diffraction. The binding of plasmid DNA on the C-GNPs was confirmed by agarose gel electrophoresis.

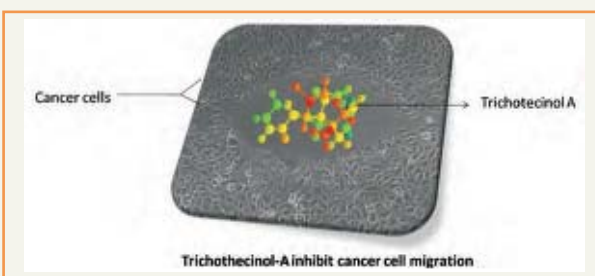
Conjugation of drugs to nanoparticles for targeted drug delivery applications

Extracellular biosynthesis of Gd₂O₃ nanoparticles and their biodistribution and bioconjugation: Extracellular, protein capped, highly stable and well-dispersed gadolinium oxide (Gd₂O₃) nanoparticles were synthesized by using thermophilic fungus *Humicola* sp. The biodistribution of the nanoparticles in rats was checked by radiolabeling with Tc-99m. These nanoparticles were bioconjugated with the chemically modified anticancer drug taxol with the aim of

characterizing the role of this bioconjugate in the treatment of cancer. The Gd₂O₃taxol bioconjugate was confirmed by UVvis spectroscopy and fluorescence microscopy, and was purified by using high performance liquid chromatography.

Secondary metabolites

Isolation, purification and characterization of trichothecinol- A: A total of 30 endophytic fungi (AAP-PS 130) were isolated from the medicinal herb *Phyllanthus amarus* and screened for the production of Trichothecinol-A. Trichothecinol-A was purified, quantified and completely characterized by different standard chromatographic and spectroscopic techniques. The endophyte producing Trichothecinol-A was identified as *Trichothecium* sp. It exhibited antifungal activity against *Cryptococcus albidus* (NCIM 3372) up to 20 µg/ml. Inhibition of wound migration assay performed on MDA-MB-231 cells revealed that 500 nM of Trichothecinol-A was able to inhibit wound migration by 50% indicating its remarkable antimetastatic property. It showed that it inhibited cancer cell migration and can thus be developed as a new class of anti-metastatic drug. The anti-metastatic as well as anti-fungal activity exhibited by Trichothecinol-A isolated from the endophytic fungus *Trichothecium* sp. of medicinal plant *Phyllanthus amarus*. Trichothecinol-A also exhibited apoptotic activity.



Biotransformations

Trichothecin from endophytic fungus *Trichothecium* sp.:

Endophytic fungi were isolated from the leaves of medicinal herb *Phyllanthus* sp. and screened for *Trichothecin*. AAP-PS-1 was found to produce Trichothecin extracellularly in appreciable amount which was identified as *Trichothecium* sp. One liter of *Trichothecium* sp. yielded 4.25 mg of Trichothecin. Trichothecin inhibited MDA-MB-231 cell migration and arrested B16F10 cells at G2/M phase indicating its potential as antimetastatic and antiproliferative compound. It was not cytotoxic in the given concentration range of Tricothecin that was used against cancer cell lines. Assessment of toxicity towards human RBC revealed only less than 0.1% hemolysis as compared to Triton X-100 that suggested safe nature of Tricothecin.

Structure-function studies of selected proteins

The structure of plant defense proteins such as lectins, hemagglutinins and protease inhibitors was studied to understand their role in plant defense. The structural changes caused by pathological mutations were investigated to understand the mechanism of genetic diseases.

Structural studies of plant defense proteins

Two lectins showing complex sugar specificity were characterized from plants belonging to Cucurbitaceae family and Solanaceae family. Genes coding Kunitz-type protease inhibitors in *Cicer arietinum* genome were identified and the selected ones were cloned for structural study and protein engineering.

Studies of Ntn-hydrolase enzymes

The biological role and enzyme applications of penicillin G acylase (PGA), penicillin V acylase (PVA) and Conjugated Bile

Publications: Biochim. Biophys. Acta, 2013, 1830, 5087; Biochimie, 2013, 95, 2392; Enzyme Microb. Tech., 2014, 56, 1; Microbiology, 2014, 160, 1162

Salt Hydrolase (BSH) were understood. The role of *K. citrophila* PGA in quorum quenching was understood and biological role of PVA was also addressed. The BSH enzymes from gut organisms were investigated for using their de-conjugation activity in treating hypercholesterolemia. The evolutionary relation and structural role in substrate specificities of PVA and BSH were studied.

Pathogenic mutations of human mitochondrial complex-I proteins

A molecular model of mitochondrial Complex-I Q module constituting of four protein subunits was generated. Various molecular changes caused by pathogenic mutations were modeled. The structural changes of two subunits NDUFS3 and NDUFS7 were determined and compared with their respective pathogenic mutant proteins experimentally with molecular modeling studies.

Quorum sensing and quorum quenching

A novel species of *Bacillus* capable of producing an enzyme with the ability to cleave gram negative quorum sensing signal molecules namely Acyl-homoserine lactone was identified. The enzyme produced by the isolated culture was identified as an AHL Lactonase. Purification and kinetic characterization of the enzyme from wild type bacterium was completed and the enzyme was also cloned and overproduced in BL21DE3 expression system. AHL Lactonase from this novel species of *Bacillus* was proved to be potent quorum quenching enzyme using CV026 based bioassay. A simple qualitative method was devised for detection of AHL Lactonases.

A new class of molecules was synthesized that exhibited remarkable potential of quorum sensing inhibition. An important part of traditional medicine was formed using the essential oils and alternative healing practices were addressed. Very few essential oils were reported to exhibit the ability to act as quorum sensing inhibitors on their own. A few essential oils, which never inhibited quorum sensing on their own, were converted into their glyco forms and these molecules showed tremendous ability to inhibit quorum sensing mediated phenotypes in different gram negative systems. These glycol-derivatives of the essential oils were potent biofilm disrupting agents.

Making quantum dots biocompatible using sophorolipids

An interesting application of oleic acid sophorolipid was reported that entails functionalization of cadmium telluride (CdTe) quantum dots (QDs) using sophorolipids (SL) as a surface-modifying agent. The final SL coated photoluminescent CdTe QDs showed the properties that made them potentially useful for biomedical applications. The biomedical application of CdTe quantum dots was explored, that enabled the Glucose sensing by glucose oxidase enzyme conjugated H_2O_2 sensitive CdTe QD system. A very elegant photoluminescence (PL) detection based assay demonstrated the use of this system in estimating glucose in blood. The glucose detection was enabled by surface functionalizing the 3-mercaptopropanoic acid (MPA) capped CdTe QDs with glucose oxidase (GOx), the enzyme specific to beta-D-glucose. The fluorescence of the GOx-functionalized CdTe QDs was quenched on the interaction with glucose in any given sample that made detection very easy.

Synthesis of novel sophorolipids using cetyl alcohol and its characterization

Sophorolipids were aimed to report as it showed biodegradability and low eco-toxicity. Novel sophorolipids

derived from cetyl alcohol, SLCA were synthesized by supplementing non-pathogenic yeast *Candida bombicola* (ATCC 22214) with glucose and cetyl alcohol as hydrophilic and hydrophobic source respectively. Physico-chemical characterization was performed to ascertain the effectiveness of SLCA by determining their surface tension lowering ability, which was found to be 31.349 mN/m with CMC value of 104 mg/L. Primary analytical characterization of SLCA was carried out using thin layer chromatography and Fourier transform infrared spectroscopy. Characterization and structure identification was confirmed that showed the incorporation of hydroxylated lipidic carbon source cetyl alcohol in sophorolipid molecule. Techniques like thin layer chromatography, Fourier transform infrared spectroscopy and liquid chromatography high resolution mass spectrometry (LC-HRMS) were used in this step. The mixture comprised of the two major forms, which possessed terminal methyl and CH_2OH group respectively. The role of cytochrome P450 monooxygenase enzyme was ruled out partially.

Synthesis of xylolipid biosurfactant with enhanced functionality

New yeast isolate *Pichia caribbica* was provided with xylose and oleic acid that resulted in synthesis of glycolipidic molecule different from typical sophorolipid synthesized by *Candida bombicola*. Xylose was incorporated as head group, i.e. hydrophilic moiety in place of glucose. The variation in structure imparted better surface tension lowering activity thus showed low CMC value and antibacterial activity was also enhanced.

Isolation of *Acinetobacter* sp. as a novel source of penicillin V acylase

A novel bacterial isolate namely *Acinetobacter* sp. was isolated that produced penicillin V acylase. It was the first experimental report of PVA activity of this genus. The PVA production from *Acinetobacter* sp. was intracellular and constitutive. The production was enhanced in yeast malt medium with sodium glutamate. Maximum enzyme activity (40 IU/L) was obtained after 30 h fermentation at 27°C and pH 7 with shaking at 180 rpm. The enzyme exhibited maximum activity at pH 7 and temp 40°C with a subunit molecular weight of 34 KDa on SDS-PAGE and MALDI-TOF/TOF analysis.

Publications: RSC Adv., 2013, 3, 22319; World J. Pharm. Pharm. Sci., 2013, 2, 6, 6062, 2014, 3, 1, 1126; 3, 3, 993; Eur. J. Lipid Sci. Tech., 2014, doi:10.1002/ejlt.201300363

Neurodegenerative diseases: Causes and corrections

Publication: PLoS One, 2014, 9, 8

The objective was to understand the molecular mechanism leading to the pathology of the neurodegenerative disorders for the treatment and management of such diseases.

Targeting Alzheimer's disease

The molecular bases of Alzheimer's disease (AD) pathogenesis remained incompletely elucidated. The disease was recognized as a multifactorial syndrome involving various molecular and cellular processes such as protein aggregation, oxidative stress, cell cycle deregulation and neuroinflammation. Acetylcholinesterase (AChE), b-secretase (BACE-1), and amyloid b (Ab) aggregation were considered as major drug targets in AD. The discovery of drug molecules capable of targeting multiple factors involved in AD pathogenesis would greatly facilitate in improving therapeutic strategies. The repositioning of existing non-toxic drugs could dramatically reduce the time and costs involved in developmental and clinical trial stages.

Protriptyline as a multi-target directed ligand in Alzheimer's disease

The preliminary screening of 140 FDA approved the nervous system drugs by docking suggested the viability of

the tricyclic group of antidepressants against three major AD targets, viz. Acetylcholinesterase (AChE), b-secretase (BACE-1) and amyloid b (Ab) aggregation, with one member, protriptyline that showed the highest inhibitory activity. Protriptyline was able to inhibit AChE and b-secretase by binding to the active site and causing conformational changes. It prevented the self-assembly of Ab and glycosylated Ab. Detailed biophysical assays, together with isothermal calorimetry, fluorescence quenching experiments, kinetic studies and atomic force microscopy established the strong inhibitory activity of protriptyline against all three major targets. The molecular basis of inhibition was supported with comprehensive molecular dynamics simulations. It was approved by FDA for the treatment of depression, narcolepsy, Attention Deficit Hyperactivity Disorder (ADHD) and headaches and its ability to cross blood brain barrier (BBB). High prevalence rate (30-50%) of AD and depression co-morbidity was observed so the use of antidepressants was rational complementary therapy for its treatment. The results strongly ratified protriptyline as a promising candidate for AD therapy and its further evaluation in animal and clinical studies.

Fungal biotechnology

Publications: J. Biol. Control., 2013, 27, 3, 194; Tetrahedron, 2013, 69, 11155; Nat. Prod. Res., 2013, 28, 4, 245; J. Biol. Control., 2013, 27, 3, 194; Kavaka, 2013, 41, 33

Mycoinsecticide development and the mission mode collections of entomopathogens and mycopathogens

Entomopathogenic and mycoparasitic fungi were developed as biocontrol agents that required a selection schedule of species and strains adapted to specific pests, environmental conditions and crops. Different biochemical and molecular aspects of fungus-host interaction, importance of minimum sub-culturing and regular passage through host, collection centre and maintenance and many issues were tackled for the development of commercially viable biocontrol agents. The mission-based culture collection provided a wide range of strains with different host specificities, virulent nature and different mechanisms for host interaction.

Larvae and adult females of *Aedes aegypti* L. were exposed to fungal suspensions of three virulent strains of *Metarhizium anisopliae* viz., M34412, M34311 and M81123. The strains resulted in 7 to 37% survival of mosquito as a result of fungal infection over the 8 days test period in case of adults and 2 to 90% survival for larvae. Mean survival period was varied between 3 and 4 days for treated adults, whilst control survival exceeded 28 days. Values of LC_{50} varied from 5.92×10^3 conidia/ml for M34412, 3.49×10^4 conidia/ml for M34311 and 5.12×10^5 conidia/ml for M81123. Exposure time of only 4 hours was necessary to cause 50% mortality to obtain the best strain *M. anisopliae* M34412.

Dimorphism and alkane degradation by *Yarrowia lipolytica* var. *indica*

The dimorphic characteristics of a variant designated as *Y. lipolytica* var. *indica* was isolated from petroleum contaminated sea water and the effect of cell morphology on hydrocarbon metabolism was studied. The variant behaved as a yeast monomorphic strain under conditions at which terrestrial *Y. lipolytica* strain W29 and its derived strains grew as almost uniform populations of mycelial cells. Organic nitrogen and N-acetyl glucosamine as carbon source were used by var. *indica* to form mycelial cells; the proportion was increased due to the incubation under semi-anaerobic conditions. Only var. *indica* was able to use it as a carbon source in all the tested strains metabolize hydrocarbons. Yeast cells of var. *indica* metabolized hexadecane with higher efficiency than the mycelial form.

Development of new antifungal agents

Dimeric chalcone named kamalachalcone E along with the known compounds rottlerin and 40- hydroxyrottlerin were isolated from the acetone extract of the fresh whole uncrushed fruits of *Mallotus philippinensis*. Kamalachalcone E exhibited IC_{50} of 8, 4 and 16 mg/mL against *Cryptococcus neoformans* PRL 518, *C. neoformans* ATCC 32045 and *Aspergillus fumigatus*, respectively. Chemically diverse oxysterols and their synthetic manipulations were carried out from a variety of D8 (9)-lanosterol derivatives and evaluated for their *in vitro* antifungal activities. Most of the synthesized oxysterols exhibited significant antifungal activity against *Candida albicans*, *C. neoformans*, and *Fusarium oxysporum*. A new dipeptide cyclo (-Ile-homoVal) along with known Phenazine-1-carboxamide and Phenazine-1- carboxylic acid methyl ester were isolated from *Pseudomonas* sp. MCC 2142. All of them were evaluated for their antifungal activities against seven wine spoilage yeasts, *Metchnikowia pulcherrima*, *Zygosaccharomyces rouxii*, *Schizosaccharomyces pombe*, *Torulaspora delbrueckii*, *Debaryomyces* sp., *Kluveromyces marxianus* and *Dekkera bruxellensis*. Dipeptide cyclo (-Ile-homoVal) was found to be most active against *Torulaspora delbrueckii* and *Zygosaccharomyces rouxii* with MIC 16 and 32 μ g/ml respectively, while Phenazine-1-carboxamide was toxic to *Torulaspora delbrueckii* and *Kluveromyces marxianus* with MIC 64 μ g/ml. Phenazine-1- carboxylic acid methyl ester exhibited antifungal activity with MIC 32 μ g/ml against all tested organisms except *Debaryomyces hansenii* for which MIC was 64 μ g/ml.

Antimicrobial activity of carvacrol and thymol was examined against natural yeast flora of the grapes and yeasts causing the wine spoilage. Carvacrol and thymol exhibited comparable or better antifungal activity than commercially used wine preservative potassium metabisulphite. The antifungal activity for both the compounds was better at pH 3.5 than pH 6.5. Addition of carvacrol and thymol (64 μ g/mL) in red wine resulted in inhibition of growth of the spoilage yeasts. Carvacrol and thymol exerted their antimicrobial action through membrane damage, leakage of cytoplasmic content and ergosterol depletion. Carvacrol and thymol proved to be a promising natural preservative with good potential to control the wine spoilage.

Fungal phytases

The objective was to produce cost effective phytase with fast and economic downstream processing. Conventional procedures, including precipitation and chromatography were employed for phytase purification.

Cumulative effect of disulfide bonds on conformational stability and active site integrity of AnigAP

Atom molecular dynamics simulations were performed to study the effect of temperature on the unfolding process and active site of disulfide intact acid phosphatase monomer (DIAP) from *A. niger* and its reduced counterpart (DRAP). The results confirmed that there was a considerable contribution of disulfide bonds towards thermo-stability in DIAP. Disulfide bond containing regions from the Cys197, Cys206, N and C-terminus were primarily responsible for the blockage of active site accessibility to substrate. Catalytically important residue distances and dihedrals change after the breakage of the disulfide bonds indicated the change in the shape of active site. The results showed that reduced 'HAP Phytases' loose the conformational stability and activity due to the flexibility rise in the absence of disulfide bonds and active site blockage.

Biochemical characterization of phytase isozymes from *Aspergillus niger* and correlation with phytases

Several dissimilar phytases were produced Phy I, II (SmF), Phy III, IV (SSF) under different fermentation conditions from *Aspergillus niger* (NCIM 563) produced. SSF phytases showed higher metabolic potential as compared to SmF. Phy I is tetramer whereas Phy II, III and IV are monomers. Phy I

Publications: Bioinformation, 2014, 9, 963; Process. Biochem. 2013, 48, 1618; J. Food Biochem., 2014, 38, 18

and IV showed pH optima of 2.5 and for Phy II and III pH optima were of 5.0 and 5.6. Phy I, III and IV exhibited very broad substrate specificity while Phy II was more specific for sodium phytate. SSF phytase was less thermostable as compared to SmF phytase. Based on the MALDILCMS/MS identified amino acid sequences of the peptides, Phy I and II showed homology with other known phytases while Phy III and IV showed no homology with SmF phytases and any other known phytases from the literature suggesting their unique nature. This study provided basis for explanation of the stability and catalytic differences observed for the enzymes.

Yeast phytase for improved mineralization and dephytization

Several isolates were screened for phytase production and five were selected as potential phytase producers such as *Zygosaccharomyces bisporus* (NCIM 3265 and 3296), *Williopsis saturnus* NCIM 3298, *Zygosaccharomyces priorionus* (NCIM 3299), and *Schizosaccharomyces octosporus* (NCIM 3297). Phytase activity was found to be cell wall associated with temperature and pH optima of 50°C and 4.0, respectively. Highest phytase production (10-28 folds) was attained in cane juice medium as compared to other media used. Addition of phytase to chickpea flour (CPF) enhanced the mineral mobilization bioavailability. It was enhanced approximately by 20-28%, 26-37%, and 24-42% for Zn²⁺, Fe²⁺ and Ca²⁺, respectively and decreased PA content by about 75-88%.

Biotic stress resistance and development of genomic resources in crop plants

Publications: *Planta*, 2014, 237; *Genome*, 2013, 56, 91

The research was focused on molecular analysis of plant-pathogen interactions, genetic analysis of gene families and development of genomic resources in crop plants.

Molecular analysis of chickpea-fusarium interactions:

High-throughput SAGE, LC-MS and NMR technologies were employed to analyze the chickpea-Fusarium interactions. Four SAGE libraries were sequenced and their preliminary analysis revealed several important genes like glycosyl transferases, ATP carrier proteins, 14-3-3-like proteins, superoxide dismutase etc. Proteomics and metabolomics analyses demonstrated that disease resistance was characterized by intense lignification, generation of phytoalexins, rapid alternation in the Yang cycle, and unfolded protein response. Many metabolic processes producing nitrogen- and carbon-rich compounds were also altered. The fungal pathogen was transformed with eGFP gene and microscopically monitored *in planta* using fluorescence microscope.

Molecular analysis of wheat-Bipolaris interactions:

Knowledge of genes underlying pathogenesis and host defense aided the disease management strategies and developed SB resistant varieties. Ten pathogenic BS races were obtained and their pure cultures were established. The pathogen races were characterized at phenotypic and genetic levels by sequencing the ITS region and their gene expression profiles yet to be determined and seedling inoculation method for green house experiments to be standardized.

Identification and characterization of microRNA genes and their targets:

Identification of 116 conserved miRNAs from linseed was done using computational approaches. Promoter region analysis of the miRNA genes indicated prevalence of MYB transcription factor binding sites. Further, 142 target genes were predicted for these miRNAs and most of these represented transcriptional regulators. The miRNA encoding genes as well as their targets expressed in diverse tissues were determined by digital expression analysis as well as real time PCR.

Identification and characterization of NBS-LRR genes in linseed:

The linseed genome sequence was analyzed and identified for 147 nucleotide binding site-leucine rich repeat (NBS-LRR) genes. The NBS domain was used for phylogeny construction and these genes were classified like non-TIR (CNL) and TIR (TNL). An unusual domain arrangement was observed in the TNL family members, predominantly in the TNL-5 clade members belonging to class D. About 12% linseed specific genes were observed. Quantitative expression analysis confirmed their inducible expression.

Development of genetic resources in linseed:

The genotyping-by-sequencing approach was employed to develop a large number of genome-wide single nucleotide polymorphism (SNP) markers for association mapping of agronomic traits in linseed. A core collection of 222 linseed accessions was developed from the entire germplasm collection comprising 2239 accessions and analyzed its genetic diversity and population structure.

Biochemical and molecular approaches for improvement of quality and yield of plants

Publications: Phytochemistry, 2014, 98, 41; Genome, 2013, 56, 91; Springer Plus, 2013, 2, 494; Plant Physiol. Bioch., 2013, 71, 121; Int. J. Biodiv., 2014, 296, 891

The objective was to understand and decipher economically important traits in agriculturally important plants by using omics based approaches.

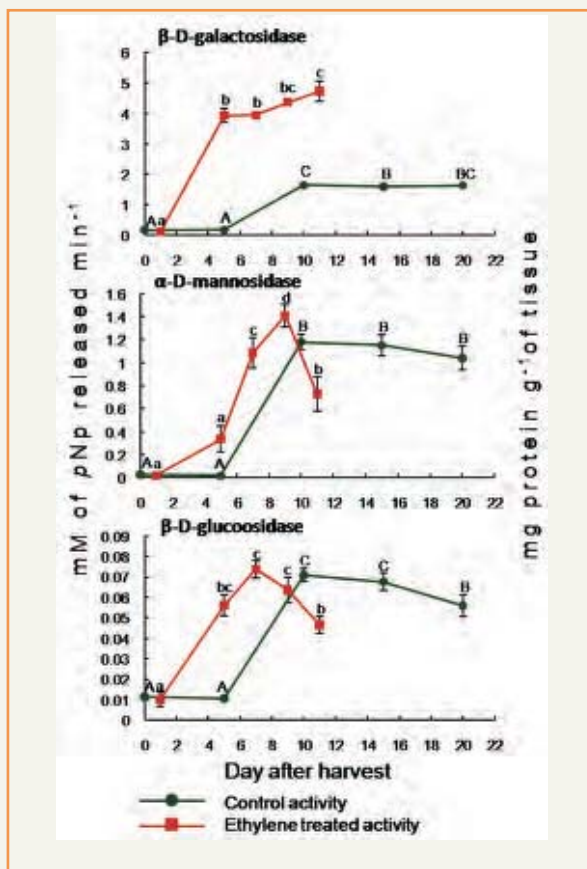
Haplotype analysis of Indian linseed varieties based on desaturase gene sequences

The desaturase gene sequences such as *SAD* (*SAD1* & *SAD2*), *FAD2* (*FAD2* & *FAD2-2*) and *FAD3* (*FAD3A* & *FAD3B*) were determined from ten linseed varieties. The haplotype determination was undergone with the help of DnaSP v5. Sequence variation measurements like number of variable sites, haplotype number, haplotype diversity (H_d) etc. were also determined. The analysis of these six genes from ten linseed varieties revealed varied number of haplotypes. A total of 2-9 alleles and 1-4 protein isoforms were identified for each of the six genes. A variation was observed in the allelic frequency for these varieties. *SAD* and *FAD2* genes showed no variation as compared to *FAD3* genes in ten varieties. Most of the observed variations were in the intronic regions and the exonic variations were synonymous or silent mutations. The number of protein isoforms detected was low except for *FAD3* genes. The various haplotypes obtained were further compared with the fatty acid (FA) composition of the ten linseed varieties. It was suggested that there was no specific haplotype that could be correlated with variation in the FA composition; so it is not responsible for the high and low ALA accumulation in the groups except in varieties TL23, NL260 and Padmini. Such correlation of haplotype to variable ALA content was masked by the variable sequential expression of all the three classes of the genes, *in vivo* in the linseed varieties studied. Recombinant enzymatic assays were established with individual haplotypes for the confirmation.

Pre-climacteric ethylene treatment and ripening related softening of alphonso mango

An assessment of the enzyme activity was carried out to identify the role of three glycosyl hydrolases viz. β -D-galactosidase, α -D-mannosidase and β -D-glucosidase in fruit softening. Crude enzyme extract was obtained from all the ripening stages of ethylene treated fruits viz. 1, 5, 7, 9, 11 days after harvest (DAH) and of control fruits viz. 0, 5, 10, 15, 20 DAH. In each stage 1g mesocarp tissue was ground to a fine power in liquid N_2 and was extracted with 5ml of extraction buffer containing 50mM HEPES-NaOH (pH 7.4), 5mM $MgCl_2$, 2% (v/v) glycerol and 2% (w/v) polyvinyl-

pyrrolidone. The homogenate was centrifuged at 15,000g for 30min at 4°C. The supernatant obtained was used as a crude enzyme preparation and assayed against P-nitrophenyl- β -D-glucopyranoside and p-nitrophenyl- α -D-mannopyranoside, p-nitrophenyl- β -D-galactopyranoside. Enzyme activities of all the three enzymes showed significant increase from 5DAH to 10 DAH stage of controlled ripening, which is the time point of ethylene burst and initiation of softening. β -D-galactosidase showed sudden and significant increase in the ethylene treated fruits compared to control fruits. α -D-mannosidase and β -D-glucosidase showed early increased activity in ethylene treated fruits but did not show significant difference from control fruits. It confirmed the involvement of β -D-galactosidase, α -D-mannosidase and β -D-glucosidase in the fruit softening. Exogenous ethylene treatment triggered expression of β -D-galactosidase which in turn involved in fruit softening.



Apicomplexan parasite metabolism and drug discovery

The metabolic functions in parasites like *Plasmodium falciparum* and *Toxoplasma gondii* were studied using a combination of genetic, biochemical and genomic approaches. The research was aimed to identify the novel metabolic functions as targets to develop the next generation of anti-parasitic agents.

Parasite metabolomics

Mass spectrometry and NMR spectroscopy based metabolic studies were carried out to understand steady state and perturbed metabolic functions in *P. falciparum* and *T. gondii*. $^{13}\text{C}/^{15}\text{N}$ enriched nutrients like glucose and glutamine were used as metabolic precursors to label targeted metabolic pathways. A combination of extraction, separation and analysis techniques and hundreds of distinct metabolites were used to monitor in mass spectrometry. Methods were developed for real time metabolite profiling by using live cells by NMR spectroscopy.

Mitochondrial energy metabolism in parasites

The subunit composition, functional relevance, and essentiality of mitochondrial ATP synthase in fast and slow growing forms of the parasite were identified to investigate. The transgenic parasite lines were generated expressing fluorescent protein YFP or mCherry tagged genomic copies of different F_1 subunits of ATP synthase to facilitate complex purification and further characterization.

Phenotypic screens to dissect action of anti-parasitic compounds

A phenotype screening approach was adopted to address this issue by using *Toxoplasma* as a model. Transgenic

parasite lines were generated that expressed the organelle specific fluorescent proteins for monitoring organelle Dynamics during cell division with or without inhibitor treatment. An image based high-content screening approach was developed in 96 well formats to facilitate this study. The first set of molecules to be screened by the approach was a collection of 400 molecules called the malaria box.

Anti-malarial and anti-toxoplasma screening

A screening facility was established to identify the potential inhibitors of parasite growth using whole cell assays on both *Plasmodium* and *Toxoplasma*. The DNA binding dye SybrGreen was used to strain and quantify parasite growth at 60 hours following inhibitor treatment for *Plasmodium* and luciferase expressing strain was used to monitor parasite growth in case of *Toxoplasma*. The small molecules were used in the screens, which were obtained from an in-house repository of synthetic and natural molecules.

Comparative genomics of parasites

Complete genome sequence was available for *Plasmodium*, *Toxoplasma* and other related parasite species, along with closely related free-living species like chromerids and host species such as humans. The information resource was leveraged to understand the biology of the parasite as well as to identify new targets for drug discovery. A semi-automatic *in silico* approach was developed for mapping enzymes from genome data and comparing metabolic functions across species. It was aimed to identify critical pathways, which were necessary for parasite survival and was targeted for drug development.

Elucidation of structure-function relationship and transitions of proteins

Publications: British Biotech. J., 2014, 4, 215; Int. J. Biol. Macromol., 2014, 64, 30; Biochimie., 2013, 95, 2392, Biochem. Physiol., 2013, doi: 10.4172/2168-9652.S2-002

Solution and *in silico* ligand binding studies of *Cicer arietinum* lectin

The recombinant lectin from *Cicer arietinum* (rCAL) showed complex sugar specificity and could bind only the asialo triantennary glycan from Fetuin. The thermodynamic study of binding to this glycan indicated the process to be spontaneous and exothermic. The presence of four hemopexin-binding domains in the gene sequence indicated possible binding to hemin. The lectin also bound spermine and thiamine with association. *In silico* investigation was carried out by protein-ligand docking using AutoDock Vina software. Binding energies were calculated for each ligand and the amino acids involved in the interaction of these ligands with the rCAL homology model were identified. ASN-8 residue was found to be important in binding of hemin and spermine to rCAL.

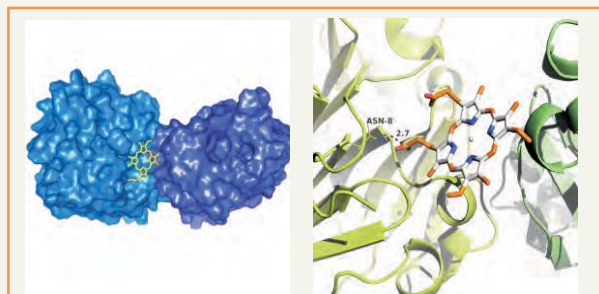


Fig. 1: Docking of Hemin on the rCAL homology model

Ficus religiosa L.: Lectin activity in fruits and *in vitro* regenerated tissues

Lectin/hemagglutinin activity was detected in fruits and fruit callus extracts. Both *In vivo* fruits (figs) and *In vitro* fig callus were used to assay the hemagglutinin activity using pronase treated and untreated rabbit blood erythrocytes. Fruit extract showed 4-8 times more hemagglutination activity in presence of pronase treated erythrocytes. The first report of callus and suspension culture with detection of thermostable (up to 70°C) hemagglutinin and lectin from fruits in this species was addressed.

Conformational transitions of cinnamoyl CoA reductase

Regulatory enzyme in lignin biosynthesis, from *Leucaena leucocephala* (LI-CCR1) was studied using fluorescence and circular dichroism spectroscopy. The native protein possessed four trp residues exposed on the surface. 66% of helical structure undergone rapid structural transitions at and above 45°C. It started forming aggregates at 55°C. LI-CCR1 was transformed into acid induced (pH 2.0) molten globule like structure that exhibited altered secondary structure, diminished tertiary structure and exposed

hydrophobic residues. The molten globule like structure was examined for the thermal and chemical stability. The altered secondary structure of LI-CCR1 at pH 2.0 was stable up to 90°C.

In presence of 0.25 M guanidine hydrochloride (GdnHCl), it got transformed into different structure which was stable in the vicinity of 2 M GdnHCl as seen in far UV-CD spectra. The structural transition of LI-CCR1 at pH 2.0 followed another transition after readjusting the pH to 8.0, forming a structure with hardly any similarity to that of native protein.

Human mitochondrial NDUFS3 protein bearing Leigh syndrome

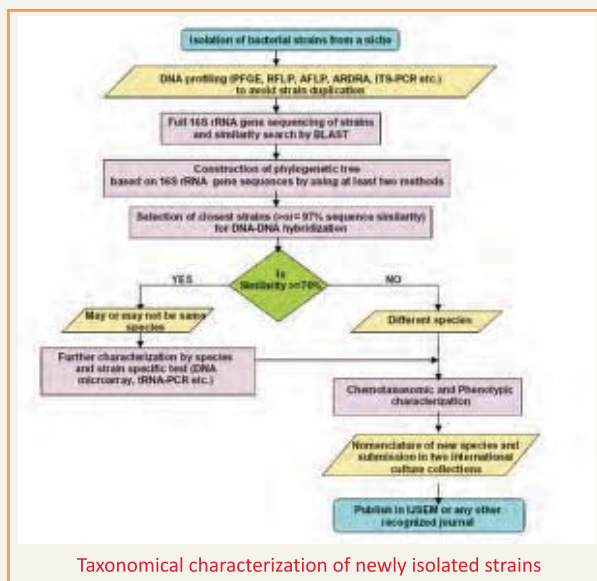
The combined mutation (T145I þ R199W) in the subunit was reported to cause optic atrophy and Leigh syndrome accompanied by severe Complex-I deficiency. The human NDUFS3 subunit and its double mutant were cloned and overexpressed in a soluble form in *E. coli*. The mutant protein showed altered polarity around tryptophan residues that changed quenching parameters and also noticeably altered secondary and tertiary structure compared to the w-t protein. Mutant also exhibited a higher tendency than the w-t protein for aggregation which was examined using fluorescent (Thioflavin-T) and spectroscopic (Congo red) dye binding techniques. The pH stability of the w-t and mutant proteins varied at extreme acidic pH and the molten globule like structure of w-t at pH1 was absent in case of the mutant protein. Both the w-t and mutant proteins showed multi-step thermal and Gdn-HCl induced unfolding. The results provided insight into the alterations of NDUFS3 protein structure caused by the mutations, affecting the overall integrity of the protein and finally led to disruption of Complex-I assembly.

Microbial systematic-polyphasic approach

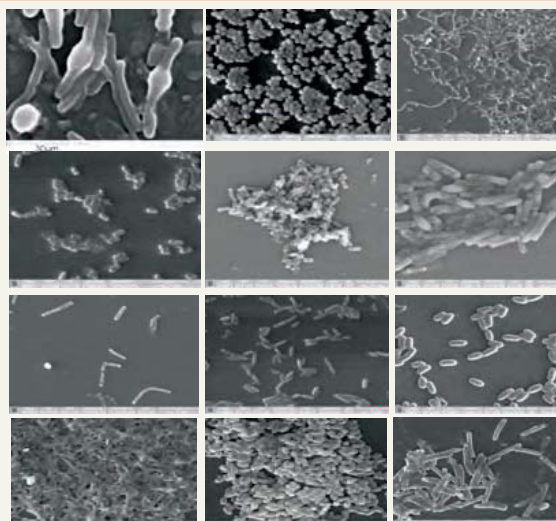
The objective was to characterize taxonomically unassigned strains using several approaches to obtain a broad range of informative data from the genetic and epigenetic level including morphology, physiology, chemistry, DNA patterns, gene sequences and whole genome hybridization. Many novel bacterial species were identified by using this polyphasic approach such as *Bacillus enclensis* sp. nov., *Fictibacillus enclensis* sp. nov., *Rhodococcus enclensis* sp. nov., *Domibacillus enclensis* sp. nov.

Potential secondary metabolites from *Streptomyces* and their biosynthetic gene

The research was focused on the systematics of *Streptomyces* available at NCIM resource center and their potential biological activity and preservation of new microorganisms. *Streptomyces* considered as the most fruitful source of microorganisms for all types of bioactive metabolites, as evidenced by a strain which showed 85% inhibition activity at 3.125 µg in MIC, further some other metabolites showed important antifungal activity against plant pathogens. These compounds may lead to anti-infectious, anti-viral and anti-cancer compounds. It also played important role as herbicides, insecticides in the agricultural fields.



Publications: Curr. Sci., 2014, 106, 58; Antonie van Leeuwenhoek, 2014, 105, 105, 461, 571; Indian J. Marine Sci., 2014, 43, 340; Int. J. Syst. Evol. Microbiol., 2014, 64, 869, 2693



Different cell arrangements in novel bacterial species by scanning electron microscopy

The revalidation of more than 200 bacterial strains of NCIM collection was done for its authentication and the molecular systematic facility was developed in the NCIM resource center.

OMICS of human gut bacteria

Publication: Gut Pathog., 2013, 5, 7

The objective was to gain whole genome based insights into the putative gene determinants of *O. intermedium* to survive in the highly acidic stomach lumen environment.

Genome characteristics

The unclosed draft genome sequence of strain M86 was of

5,188,688 bps and 5043 predicted coding DNA sequences (CDSs) and 66 RNA genes with mean G + C content of 57.9%. RAST server based annotation of the whole genome showed the presence of 437 subsystems.

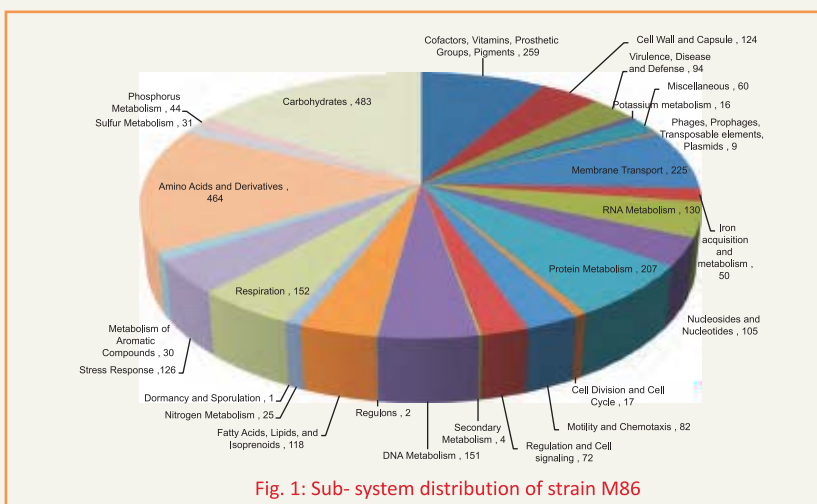


Fig. 1: Sub- system distribution of strain M86

Putative gene clusters needed for acidic environment survival

Genome of strain M86 contained urease gene cluster out of which UreA was a beta sub-unit, UreB was gamma sub unit, UreC was alpha subunit; all were part of core Urease enzyme. Four accessory proteins like UreD, UreE, UreF and UreG played an important role in Ni²⁺ uptake and insertion into active site of apo-enzyme.

The genomic properties of *O. intermedium* are poorly characterized, hence its role in human health and disease remained unclear. Elucidation of the physiological

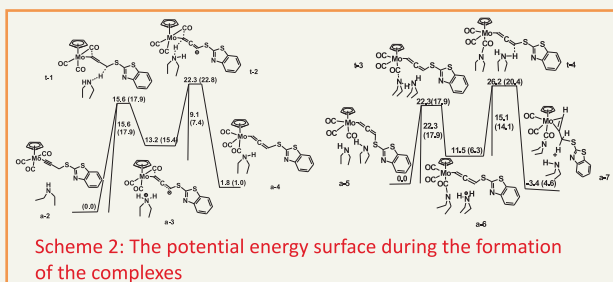
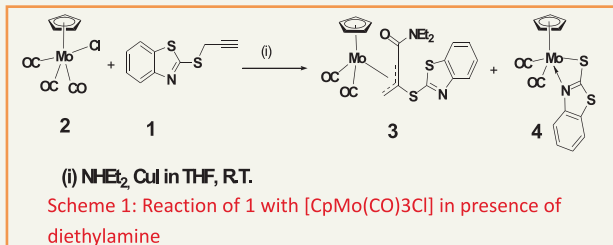
properties and identification of genes putatively involved in the various metabolic pathways may lead to a better understanding of the survival of *O. intermedium* in acidic condition. Further studies involving large scale genome sequencing and comparison of the *O. intermedium* strains isolated from several other non- ulcer dyspeptic individuals proved to help to recognize the genomic features of its survival in the acidic condition of the stomach. Comparative genomic analyses of *O. intermedium* strain M86 and other environmental isolates of genus *Ochrobactrum* will permit to understand its mechanisms for adaptation to new environments.

Development of catalyst for organic transformations and environmental applications

Publications: Appl. Catal. B, 2014, 144, 408; 2015, 162, 11; J. Mater. Chem. A, 2014, 2, 19060; ChemCatChem. 2014, 6, 3182; RSC Adv., 2014, 4, 33319

Formation of molybdenum propargyl and mercapto-benzothiazole carbonyl complexes and catalytic activity

Highly selective S-propargylation of various heterocycles was achieved (96% yield) using Cs_2CO_3 or $\text{Ba}(\text{OH})_2$ as base and further the product was coupled with $[\text{CpMo}(\text{CO})_3\text{Cl}]$ in basic medium. The propargyl complex was found to undergo the rearrangement to allylic complex with incorporation of the solvent (amine) molecule in the final rearranged product. Depending on the amine used only secondary amines led to the rearranged products. The structure of the rearranged allyl complex was unambiguously elucidated by single crystal X-ray diffraction analysis. Mechanism of the rearrangement of propargyl complex to allyl complex was studied by DFT calculations and the results indicated initial nucleophilic attack of diethylamine at the propargyl group resulting into allenyl intermediate followed by rearrangement to 3 -allyl system. The catalytic application of molybdenum carbonyl propargyl and allyl complexes was evaluated for cyclohexene oxidation as model substrate using TBHP as an oxidant.



Calcium pyrophosphate as efficient catalyst for dehydration of lactic acid to acrylic acid

Stable nonstoichiometric calcium pyrophosphate catalyst was prepared with Ca/P ratio 0.76 by modifying synthetic procedure using mixture of diammonium hydrogen phosphate and sodium phosphates as phosphate precursors. The catalyst showed very high efficiency for vapour phase dehydration of lactic acid to acrylic acid with 74% acrylic acid yield at 375°C with WHSV of 3 h^{-1} using 50% lactic acid concentration. The acrylic acid yield was further improved to 78% with 25% lactic acid concentration. The higher selectivity for acrylic acid was attributed to acid base balance

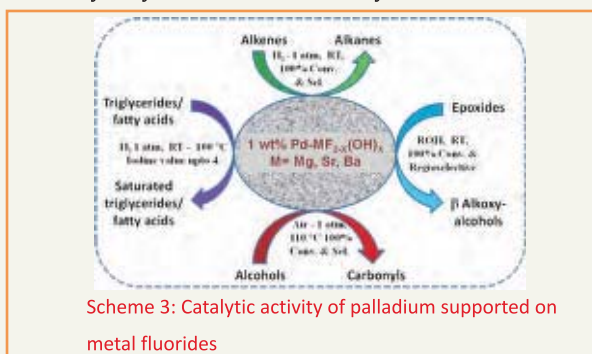
at lower Ca/P ratio leading to formation of higher amount of calcium lactate as an intermediate compared to other stoichiometric calcium pyrophosphates as evidenced by in situ FTIR studies.

Deoxygenation of lactic acid to propionic acid using supported molybdena catalyst

Molybdenum oxide supported on SiO_2 , Al_2O_3 and calcium pyrophosphate (CP) catalysts were used for deoxygenation of lactic acid to propionic acid. Decarboxylation of lactic acid to acetaldehyde with maximum selectivity was observed on acidic supports whereas on weak acidic support like CP acrylic acid was the major product. However after addition of MoO_3 on these supports, deoxygenation of lactic acid to propionic acid was observed with maximum deoxygenation on MoO_3/CP catalysts.

Palladium supported on metal fluorides as efficient catalysts

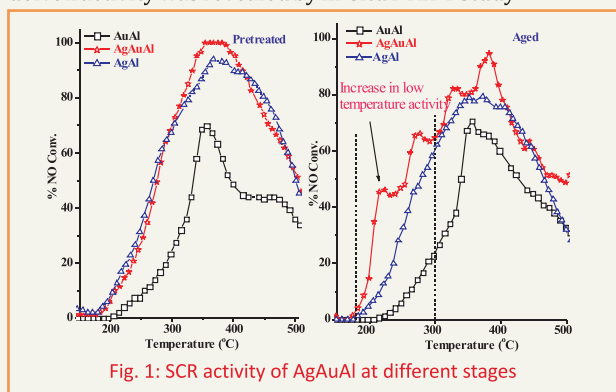
Palladium supported on metal fluorides showed high catalytic activity for hydrogenation of olefins, aerobic oxidation of alcohols and alcoholysis of epoxide. The catalysts were prepared by one pot fluorolytic sol-gel method. The acid base properties of the support played important role to tune the activity of the palladium catalyzed reactions. Pd supported on MgF_2 led to the room temperature, atmospheric hydrogenation of olefins including oils. Pd supported on BaF_2 showed high activity for aerobic oxidation of benzylic alcohols under base free conditions. Pd supported on SrF_2 showed high activity for alcoholysis of epoxide with formation of exclusive -alkoxy alcohols. The fluorolytic sol gel method was used for the formation of high surface area supports with high dispersion of palladium nanoparticles leading to high activity. All the catalysts were recycled efficiently without palladium leaching in hydrogenation, aerobic oxidation as well as epoxide alcoholysis reactions due to the strong metal-support interaction. The mechanism of the catalytic reaction and the exact role of palladium and metal fluoride support in the catalytic cycle were understood by in situ FTIR studies.



Development of catalyst for organic transformations and environmental applications

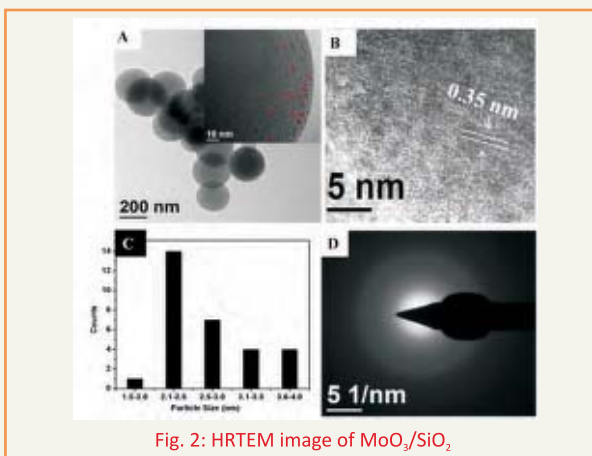
Development of catalyst for removal of NO_x from automobile exhaust engines

Bimetallic Ag-Au/Al₂O₃ catalysts were prepared by successive impregnation method for selective catalytic reduction of NO_x using hydrocarbon as reductant (HC-SCR) with 1wt% Ag and 1wt% Au loading on in house prepared high surface area alumina (450 m²/g). It was aimed to widen the temperature window for SCR activity. The effect of method of preparation, order of metal loading and various pretreatments on SCR activity and N₂ selectivity was studied with specific interest to improve the low temperature activity. Ag-Au/Al₂O₃ catalyst showed the improved low temperature as well as high temperature SCR activity. Aging of the Ag-Au/Al₂O₃ catalyst in the reaction feed at 500°C for 12 h found considerably improved low temperature activity with ~40% NO conversion at 200°C (Fig. 1). Presence of Au contributed for improved high temperature activity as well as 100% selectivity for nitrogen in entire temperature range of study. Formation of well dispersed metallic Au and Ag_n⁺ clusters during pre-treatment and aging were responsible for improved SCR activity of bimetallic catalyst compared to corresponding monometallic catalysts. The formation of monodentate nitrate species and consequent formation of isocyanate and cyanide species at lower temperature on aged catalyst compared to pre-treated catalyst leading to higher deNO_x activity was revealed by in-situ DRIFT study.



Ultrasmall MoO₃ nanoparticles supported silica nanospheres as efficient recyclable epoxidation catalyst

Ultrasmall molybdenum oxide (MoO₃) nanoparticles supported on various (SiO₂, TiO₂ or ZrO₂) nanospheres were synthesized in one pot using reverse micelle method. The prepared catalysts were characterized by physico-chemical methods. TEM images showed uniform dispersion of MoO₃ nanoparticles (1.5-4 nm) onto silica (~275 nm). No separate MoO₃ particles were identified from TEM for MoO₃/TiO₂ (~10.5 nm) and MoO₃/ZrO₂ (~6.5 nm) due to formation of solid solution by reaction of AHM with titanium and zirconium hydroxides. Among the prepared catalysts MoO₃/SiO₂ showed excellent catalytic activity up to 90% conversion and 100% epoxide selectivity for olefine epoxidation. The catalyst was successfully recycled up to five cycles without losing much activity and selectivity.



Polycarbonates and dimethyl carbonate through CO₂ utilization

Publications: J. Chem. Sci., 2014, 2, 126, 499; Appl. Catal. A Gen., 2014, 482, 300; RSC Adv., 2013, 3, 46, 23993

The research was aimed to develop solid catalysts for activating and utilizing CO₂ in the production of these carbonate chemicals.

Aliphatic polycarbonates

The systematic studies were conducted on the influence of method of preparation on the catalytic activity of Co-Zn catalysts to produce polycyclohexene and polypropylene carbonates. A highly active catalyst with no induction period in polycarbonates synthesis was prepared without using a co-complexing agent. Method used for the preparation influenced the molecular and crystal structure, and the crystallinity of Co-Zn catalysts. Density and strength of acid

sites, low-crystal symmetry like rhombohedral and monoclinic, moderate crystallinity, coordinated tert-butanol as a complexing agent and dispersed Cl⁻ ions in the structure were the critical parameters for high activity of Co-Zn catalysts. The coordinated tert-butanol activated the Zn²⁺ ions. CO₂ adsorption studies proved that high guest-host interaction in the catalyst results into high catalytic activity. Chloride in the structure avoided induction period by increasing acidity of the catalyst that improved the guest-host interactions. Polycarbonates of average molecular weight 20900 with polydispersity index of 1.8 were synthesized.

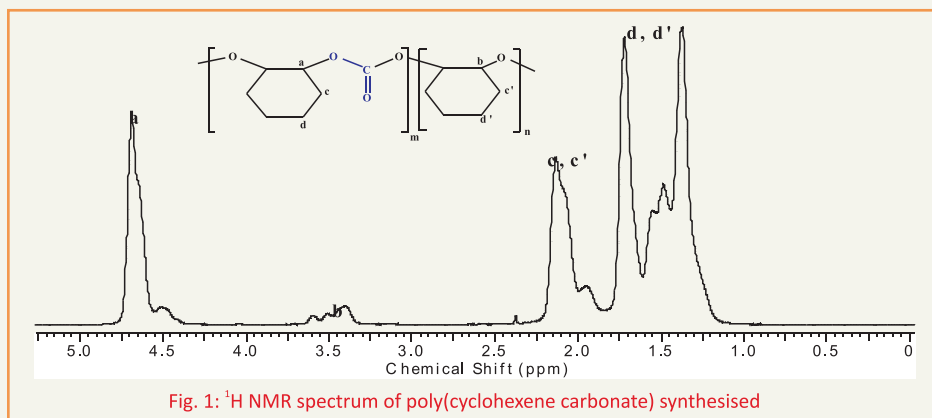


Fig. 1: ¹H NMR spectrum of poly(cyclohexene carbonate) synthesised

Dimethyl carbonate (DMC)

A novel, solid catalyst-calcined zirconium phenylphosphonate phosphite (ZrPP) was identified to produce DMC in high selectivity and yields at moderate conditions. Controlled calcination resulted in zirconium pyrophosphate (ZrP₂O₇) type interesting phosphor material. DMC yield of 26.06 mmol/g catalyst was achieved using ZrPP catalyst and N,N-dimethyl formamide as solvent medium and 3A - mole-

cular sieves water trap. CO₂ pressure at 4 MPa was also maintained. The highest DMC yield was reported with methanol conversion of 31.8 mol % over solid catalysts. The higher activity of ZrPP was attributed to its hydrophobic nature which resisted the backward reaction to occur and acid-base bifunctionality. The yield of DMC increased linearly with the density of both acid and base sites on ZrPP catalysts that indicated its involvement in the reaction.

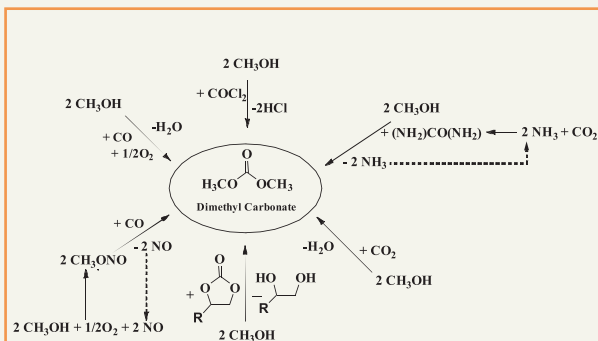


Fig. 2: Methods for DMC synthesis

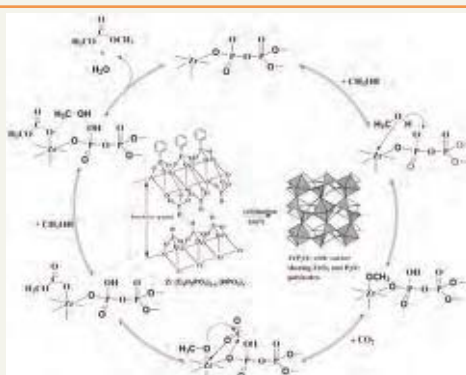


Fig. 3: Tentative mechanism for DMC synthesis over ZrPP-HF-C

Engineering Materials for better catalysis

The aim was to prepare the polyolefin from MgCl_2 based molecular adducts with different alcohols that provided an excellent route to vary the porosity, surface and electronic structure.

Rational design aspects of catalyst for water-gas shift reaction

The iron based catalyst was employed for the high temperature water gas shift (HT-WGS) reaction as it was required for the redox couple between $\text{Fe}^{2+/3+}$ in the octahedral site of the spinel structure. A rational design with relevant structural parameters of the active promoter was used essentially to increase the efficacy of the HT-WGS. CuFe_2O_4 with inverse spinel structure $([\text{Fe}]_A[\text{CuFe}]_B\text{O}_4)$, where A and B refers to T_d and O_h sites, respectively, fulfilled the balanced requirements. CuFe_2O_4 @ mesoporous alumina was integrated in an effective way and evaluated for WGS reaction; it showed sustainable activity for ten days. A spatial separation of CuFe_2O_4 crystallites at microstructural level and surrounded by hexagonal mesoporous γ -alumina (Fig. 1) ensured the long-term stability of the catalyst.

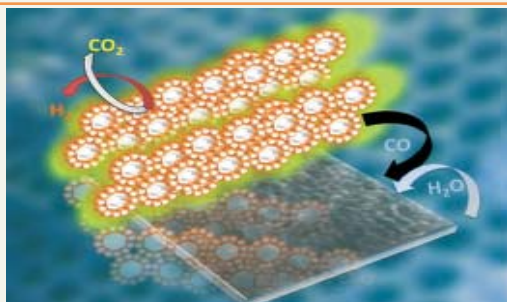


Fig. 1: Demonstration of HT-WGS reaction on CuFe_2O_4

Visible light driven water splitting with nanogold loaded titania

The goal was to produce a clean fuel such as hydrogen from water and sunlight using overall water splitting reaction (OWSR). It was observed that the OWSR by visible light driven photocatalysis did not produce a breakthrough in terms of minimum bench mark of quantum efficiency. Although the generation of H_2 using visible light driven photocatalysis by electronically integrating nano-Au particles with multifunctional, disordered mesoporous $\text{TiO}_{2-x}\text{N}_x$ (Au-NT) nanocomposites was reported. Solar H_2 generation ($1.5 \text{ mmol h}^{-1}\text{g}^{-1}$) from aqueous methanol was demonstrated with Au-NT nanocomposites. Water splitting activity of Au-NT was attributed to the single factor of 21.1 ps lifetime of charge carriers was observed from fluorescence lifetime measurements. It indicated high electron injection efficiency from nano Au to conduction band of titania, led to undergo the charge separation and utilization.

Publications: Chem. Commun., 2013, 49, 11257; ChemCatChem 2014, 6, 522; Dalton T., 2014, 43, 9143; J. Phys. Chem. A, 2014, 118, 1213

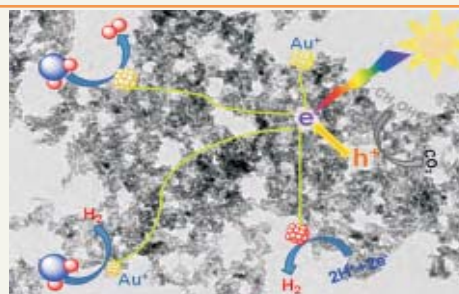


Fig. 2: Visible light absorption by nano Au clusters through surface plasmon resonance

Reversible equilibration between two phases of molecular adduct

A new molecular adduct such as $\text{MgCl}_2 \cdot n\text{FM} \cdot x\text{EtOH}$, with 9-fluorene-methanol (9FM) as an internal electron donor (IED) was synthesized and used as a support for polyolefin catalyst. Two different procedures of TiCl_4 loading led to different facets of MgCl_2 with different amounts of IED and hence different activity and polymer properties. Present catalyst system was fine-tuned towards the desired activity and polymer properties. The structural property of $\text{MgCl}_2 \cdot 4(\text{CH}_3)_2\text{CHCH}_2\text{OH}$ ($\text{Mg}(\text{iBuOH})$) molecular adducts prepared under different conditions were investigated thoroughly by solid-state NMR and non-ambient XRD. Formation of two phases was confirmed and in situ variable temperature solid-state NMR measurements confirmed the co-existence of two phases as well as its oscillation between one to another phase. It was expected that such molecular adducts show a significant role in organic transformation reactions due to oscillating structural component.

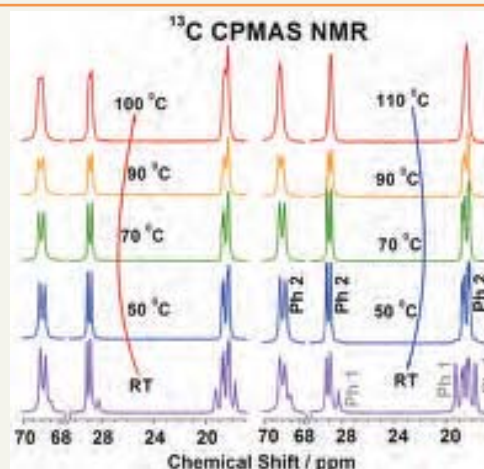


Fig. 3: Reversible equilibrium

Oxidative dehydrogenation of hydrocarbons and selective hydrogenation of biomass feedstock

Publication: Green Chem., 2013, 15, 3259

The development of the processes to convert lignocellulosic biomass to fuels and value-added chemicals was aimed as it showed rich oxygenation and high functions. Hemicellulosic fractions of biomass were used as feedstock to produce many important chemicals like furfuryl alcohol, furan, and THF.

Oxidative dehydrogenation of ethyl benzene to styrene on cerium

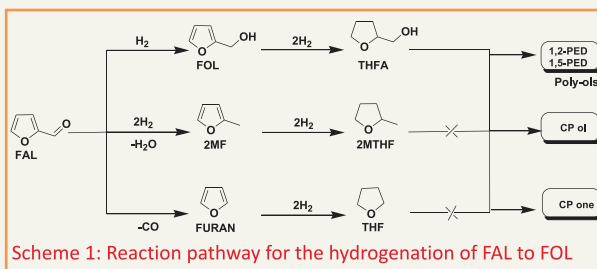
The factors incorporated successfully that favored EB to ST, such as basicity, dispersion of CeO_2 , high surface area and long term catalyst stability during the reaction. The activity of the cerium containing mixed oxides remained more or less same for longer time on stream (TOS) with maximum 49.4% conversion and 97% selectivity towards styrene. It was observed that the catalytic activity remained more or less stable with only ~3% decrease in conversion even after 72 hours.

Fluorite $\text{CeZrO}_{4.5}$ oxide catalyst for the eco-benign synthesis of styrene

$\text{CeZrO}_{4.5}$ was studied for oxidative dehydrogenation of EB to ST. $\text{CeZrO}_{4.5}$ was prepared with fluorite structure, CeO_2 and ZrO_2 by gel-combustion method, while $\text{PH-CeO}_2/\text{ZrO}_2$ was prepared using physical mixture method. The $\text{CeZrO}_{4.5}$ catalyst showed maximum conversion and selectivity of 50% and 93%. The time on stream of 72 hours reaction was done to check the stability of the $\text{CeZrO}_{4.5}$ catalyst and it showed approximately 1-2% decrease in conversion and selectivity. The catalytic activity showed that $\text{CeZrO}_{4.5}$ catalyst was stable up to 72 hours and there was no change in morphology and phase which was proved in HRTEM and XRD. The influence of different oxidants in the ODH of EB was studied by demonstrating the reaction without oxidant and with different oxidants at optimized reaction conditions.

Selective noble metal free catalysts for selective hydrogenation of biomass feedstock

A series of Mg, Al and Ni containing mixed metal oxide catalysts were derived from hydrotalcite like precursors and investigation was carried out to understand the catalytic performances in the vapor phase selective hydrogenation of FAL to FOL. The maximum activity was observed at 450°C reduction temperature and the partial reduction of nickel was confirmed by XPS analysis. The better activity was observed over 2 mol% nickel containing catalyst as compared to all other compositions prepared.



Production of aldehydes and ketones from alcohols over mixed oxides

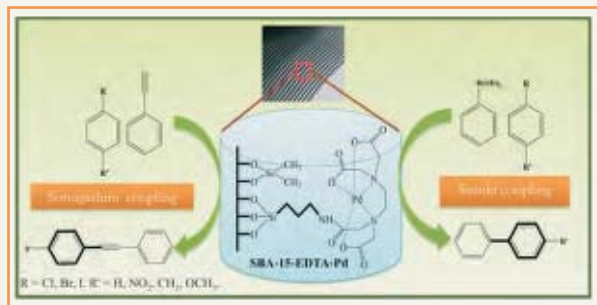
Stoichiometric oxidants like dichromate and permanganate were used for typical oxidation of alcohols in non-catalytic method. These methods resulted in generation of large amount of metal salts. Catalytic methods of alcohols oxidation were studied to overcome such disadvantage. Selective oxidation of 2-butanol to butanone was carried out over $\text{Mn}/\text{Al}_2\text{O}_3$ and $\text{Co}/\text{Al}_2\text{O}_3$. Maximum conversion was obtained at 300°C with $\text{Mn}/\text{Al}_2\text{O}_3$ with 50% conversion and 85% selectivity towards methyl ethyl ketone.

Heterogenization of Pd and Mo complexes

Development of the heterogeneous solid acid catalysts by covalent anchoring of neat metal complexes was aimed. The phosphine free SBA-15-EDTA-Pd(II) and (L)Mo(VI)O₂@SBA-15 catalysts were synthesized, characterized and evaluated in C-C coupling and epoxidation reactions.

Phosphine free SBA-15-EDTA-Pd(II) catalyst for C-C coupling

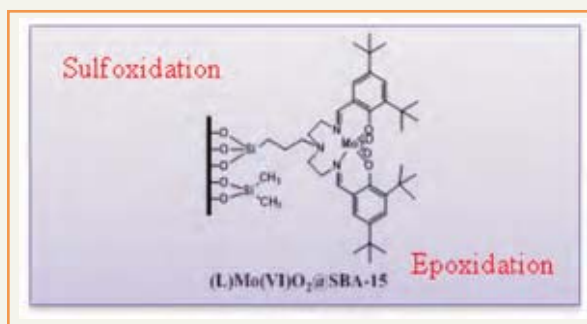
Phosphine obstructed highly efficient and reusable SBA-15-EDTA-Pd(II) catalyst was synthesized by anchoring Pd-EDTA complex over the surface of organo-functionalized SBA-15. The physicochemical properties of the organo-functionalized catalyst were analyzed by elemental analysis, ICP-OES, XRD, N₂ sorption analysis, TGA & DTA, solid state ¹³C, ²⁹Si NMR spectra FT-IR, XPS DRS UV-Visible, SEM and TEM. The synthesized catalyst SBA-15-EDTA-Pd(II) was screened in Suzuki and Sonogoshira coupling reactions showed higher catalytic activity with higher TON. The anchored solid catalyst was recycled efficiently and reused several five times without major loss in reactivity.



Publications: Catal. Sci. Technol., 2014, 4, 2978; RSC Adv., 2014, 4, 14063

Highly active catalyst for epoxidation and sulfoxidation

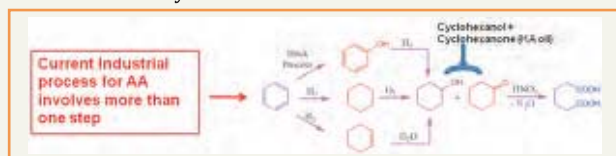
The efficient and reusable oxidation catalyst (L)Mo(VI)O₂@SBA-15 was synthesized by the anchoring of the 3-[N,N-bis-3-(salicylidenamino)ethyl]triamine ligand on the inner surfaces of organo-functionalized SBA-15 and subsequent complexation with Mo(VI)O₂ (acac)₂. The physico-chemical properties of the functionalized catalysts were analyzed by elemental analysis, ICP-OES, XRD, N₂-sorption measurements, TG & DTA, solid state ¹³C, ²⁹Si NMR, FT-IR, Raman, XPS, DRS UV-Vis, SEM and TEM. The synthesized catalysts were evaluated in epoxidation and sulfoxidation reactions and the results showed that (L)Mo(VI)O₂@SBA-15 exhibited high conversion and selectivity. The synthesized catalyst was recycled several times and Sheldon's hot filtration test was also carried out.



Novel single step green processes to produce adipic acid

The objective was to encourage industries to adopt green and eco-friendly catalytic processes for the organic syntheses to get various important chemical intermediates and platform chemicals.

The need of eco-friendly processes brought the importance to develop a single step green process for adipic acid. It started from cyclohexane that preferably involved molecular oxygen as the oxidant. The catalysts used were inexpensive and the use of any transition metals was avoided.



A single step process was developed to convert cyclohexane to adipic acid that converted nearly 70% of cyclohexane with 73% selectivity to adipic acid. The process used O_2 as oxidant and the catalyst was metal free. No corrosive solvents like acetic acid were used in the process. It used only non-corrosive solvents like acetonitrile. Though this was a batch process at the moment, efforts were made to convert it into a continuous process. Since, no metals were present in the catalyst; it was devoid of any metal leaching problems. The catalyst was recyclable.

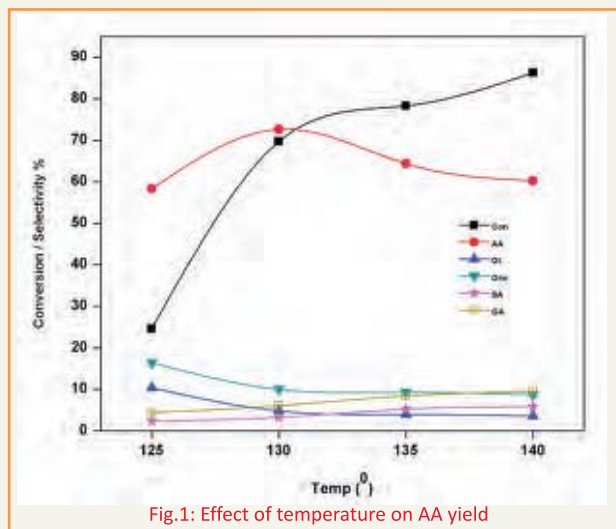


Fig.1: Effect of temperature on AA yield

The developed green catalytic process was superior to the reported catalytic process so far as it uses a metal free catalyst to drive selective oxidation of hydrocarbons using molecular oxygen to give desired products in high yields.

Preparation of acetophenone from ethylbenzene

The described catalyst was used for many other selective oxidation reactions. One such reaction was conversion of ethylbenzene (EB) to acetophenone. The catalyst converted EB to acetophenone gave good yields at low temperatures (130°C). After 8 h of reaction time, 56.2 wt % of EB conversion and 65.3 % selectivity for acetophenone were observed. The major by-product 1-phenylethyl alcohol (1-PEA) was reduced by controlling the reaction time. Other by-products like benzaldehyde and benzoic acids were also very useful industrial chemicals.

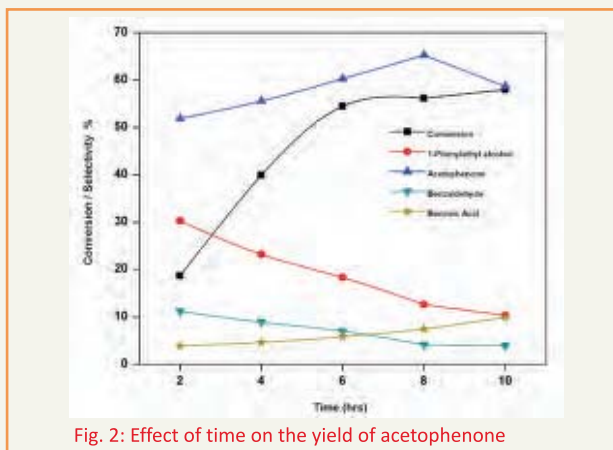


Fig. 2: Effect of time on the yield of acetophenone

Catalytic transformation of biomass derived platform molecules for Biorefinery application

The aim was to design multifunctional catalyst systems for hydrogenation of glycerol dehydration to acetol; levulinic acid to γ -valerolactone (GVL) with and without external hydrogen and furfural to tetrahydrofurfuryl alcohol. Multifunctional catalysts were also developed for liquid phase oxidation of lignin model compounds such as veratryl, vanillyl, sinapyl and coumaryl alcohols.

Copper catalysts for selective liquid phase dehydration of aqueous glycerol to acetol

The extent of different copper species was formed and the alteration in acid sites in various copper catalysts was modified with Ba, Mg, Zr, Zn, Al, and Cr. The role of active species in selective glycerol dehydration to acetol was understood.



EXAFS of the Cu-Al and Cu-Zr catalysts were used to observe the Cu-Cu metal bond formation. The active catalysts exhibited moderate and strong acidity and presence of only Brønsted sites responsible for enhancing its glycerol dehydration efficiency. Glycerol dehydration to acetol was found to be catalyzed not only by Brønsted acid sites but also by the metallic Cu. The variation in the acetol selectivity for these catalysts was Cu-Al > Cu-Zr > Cu-Mg. Two catalytic pathways involving Lewis and Brønsted acid sites were proposed for glycerol dehydration. Tautomerization of the enol gave acetol through an abstraction of a proton by the metallic Cu and CuO with simultaneous protonation of the secondary carbon in both the pathways.

Single pot conversion of furfuryl alcohol to levulinic esters and γ -valerolactone

The direct conversion of furfuryl alcohol to GVL via alcoholysis or hydrogenation sequence using sulfonic acid-functionalized ionic liquid (SO₃H-ILs) and 5% Ru/C catalyst

Publications: RSC Adv., 2013, 3, 37, 16499; Green Chem., 2013, 15, 2540; ChemPlusChem, 2013, DOI: 10.1002/cplu. 201300024; ACS Sust. Chem. & Eng., 2013, DOI: 10.1021/sc400302b

system was achieved with a novel approach (Fig. 1). Increase in Ru loading from 5 to 10% enhanced the GVL selectivity dramatically from 68 to 94%. Available active metal sites were more significant in the tandem reactions of alcoholysis and hydrogenation of methyl levulinate. Recycling of 5% Ru/C in combination with IL was achieved for three times.

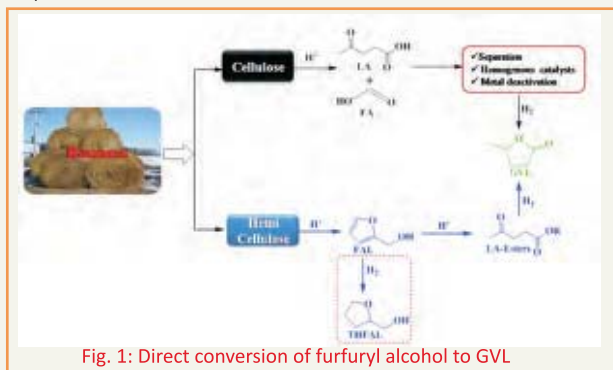


Fig. 1: Direct conversion of furfuryl alcohol to GVL

Surface synergism of Ag-Ni-ZrO₂ nanocomposite for catalytic transfer hydrogenation

An efficient bimetallic and magnetically separable Ag-Ni/ZrO₂ catalyst was developed for transfer hydrogenation of LA with complete conversion and selectivity to GVL. The synergism of both the metals was responsible for H₂ generation from formic acid and also for the in-situ hydrogenation of LA. Hydrogenation proceeded smoothly to GVL confirmed the bifunctional role of the catalyst in cyclization of 4-hydroxy LA esters. One pot hydrogenation of biomass derived C3 to C6 molecules was demonstrated to variety of useful molecules with almost complete conversion and > 80% selectivity. The recovery of the catalyst was easy due to its magnetic nature. It was recycled up to five times without losing its activity and metal leaching.

Selective aerobic oxidation of vanillyl alcohol to vanillin in base free conditions

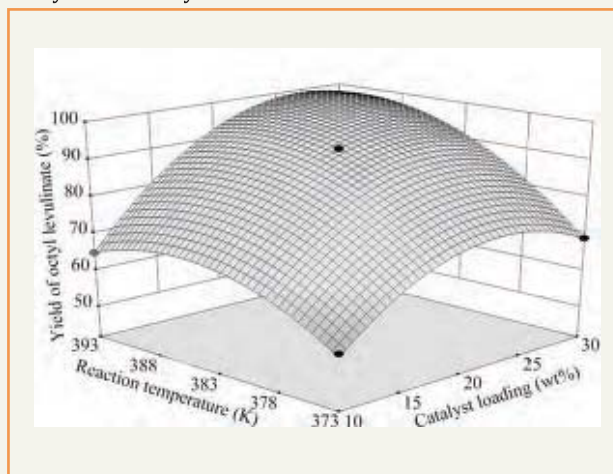
Metal hydroperoxo complex was formed readily by Mn in the mixed MnCo. It gave the phenolate ion of vanillyl alcohol under base free conditions, which undergone smooth air oxidation to give vanillin with > 83% selectivity. The high catalytic activity of the mixed oxide MnCo-MO was because of the synergic effect of the two metal oxide phases in contact which was absent in single Mn or Co metal oxide.

Catalytic process development for sustainable chemicals

The development of catalytic processes for the utilization of renewable feedstock such as levulinic acid, cellulose and glycerol to valuable chemicals and fuels using potential heterogeneous catalysts was mainly focused.

Octyl levulinate biolubricant additives over meso-HZ5

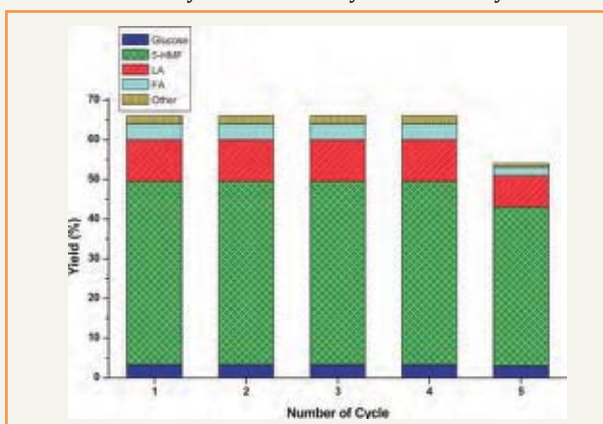
The use of modified HZSM-5 (Meso-HZ-5) as heterogeneous catalyst was highlighted specially for the synthesis of octyl levulinate biolubricant additives by catalytic esterification of biomass derived renewable levulinic acid with n-octanol. The process parameters were optimized through Response Surface Methodology (RSM) using Box-Behnken model. RSM indicated that catalyst loading and reaction temperature were most significant parameters in the reaction. The developed quadratic model was found to be adequate and statically accurate with correlation value (R^2) of 0.9971 to predict the yield of octyl levulinate. The yield of octyl levulinate was obtained to be 99%. The study was extended for validation of theoretical and experimental data including catalyst reusability.



Publications: J. Ener. Chem., 2014, 23, 4, 535; ACS Sustain. Chem. Eng., 2014, 2, 1928; Energ. Technol., 2014, 2, 5, 446

One pot synthesis of 5-hydroxymethylfurfural (5-HMF) over bimodel HZ-5 zeolite

Direct synthesis of 5-HMF was systematically studied by hydrolysis of microcrystalline cellulose over Bimodel HZ-5 Zeolite. Bimodel HZ-5 zeolite obtained by post-synthesis modification of HZSM-5 was found to be a potential heterogeneous catalyst with 67% cellulose conversion and 46% yield of 5-HMF. The catalyst was observed to be reusable for four cycles without any loss in activity.



Glycerol etherification to biofuel oxygenated additives over H-Beta zeolite

The catalytic etherification of glycerol was studied systematically in batch process using n-butanol to produce biofuel oxygenated additives over H-beta zeolite. The H-beta zeolite was found to be the most promising catalyst with 55% glycerol conversion and 98% selectivity towards mono-butyl-glycerol ether (ME). The catalyst was observed to be active and stable up to 4 cycles. The reaction was performed at milder operating conditions than reported. The optimized results were also used to develop kinetic model.

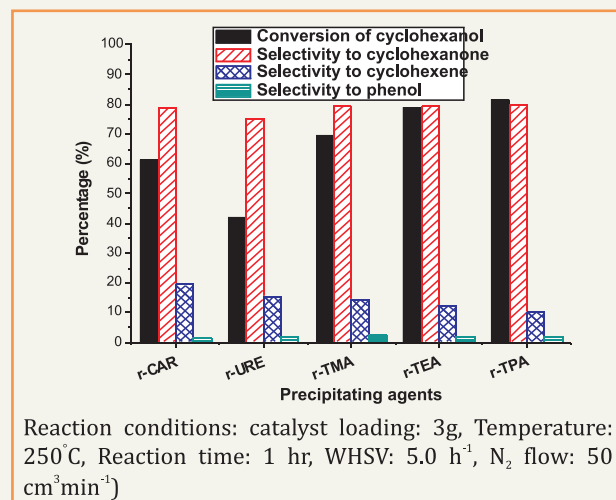
Environmentally benign catalysts: Synthesis, characterization and performance

Publications: Appl. Catal. A-Gen., 2013, 467, 421; Micropor. Mesopor. Mat., 2013, 182, 73; Catal. Commun., 2014, 43, 188

The research was focused on the optimization of the parameters and routes for the preparation of the catalysts to maximize its performance.

Cu/Al₂O₃ catalysts for dehydrogenation of cyclohexanol

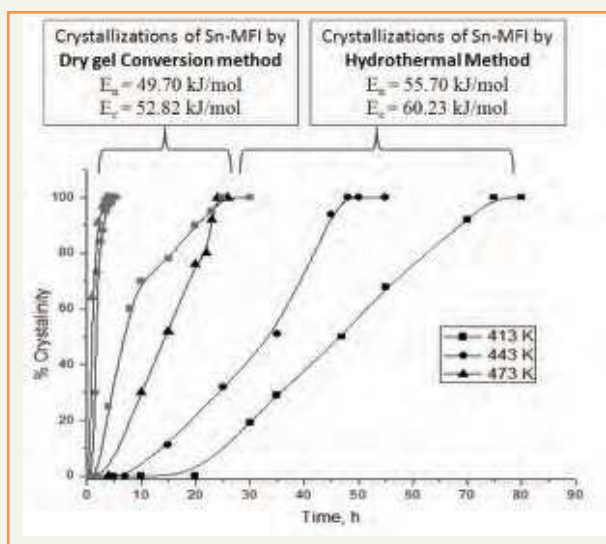
Cu/Al₂O₃ catalysts (molar Cu: Al = 1:1) were prepared using potassium carbonate (CAR), urea (URE), and tetraalkyl ammonium hydroxides (TMA, TEA and TPA) with different alkyl chain lengths as precipitating agents and evaluated for their catalytic performance in the dehydrogenation of cyclohexanol to cyclohexanone reaction at low temperature. The increase in the alkyl chain length was found to yield the catalyst with enhanced catalytic performance in terms of cyclohexanol conversion (r-TMA < r-TEA < r-TPA) with similar selectivity to cyclohexanone. On account of high Cu⁺/Cu⁰ ratio well dispersion of copper with higher surface area and lower acidity with higher population of moderate acidic sites was achieved. It was synthesized using tetrapropyl ammonium hydroxide as precipitating agent that showed 81.5 % cyclohexanol conversion and 79.57 % selectivity to cyclohexanone.



Sn-MFI molecular sieves: Crystallization kinetics by dry gel conversion method

Crystallization kinetics of Sn-MFI molecular sieve by Dry Gel Conversion (DGC) method was compared with conventional hydrothermal method. Both the E_n (49.70 kJ/mol) and E_c (52.82 kJ/mol) values for DGC method were found to be lower than that of the E_n (55.70 kJ/mol) and E_c (60.23 kJ/mol)

(kJ/mol) for hydrothermal method. Kinetic parameters *K* and *q* were derived using kinetic expression. DGC method showed higher value of *K* and lower value of *q* at identical temperature as compared to hydrothermal crystallization method. The values of E_n, E_c, lnA_n and lnA_c were found to decrease with increase in water at the bottom of autoclave in the range of 0.66-3.33 ml. The E_n and E_c values were found to decrease with increase in SiO₂/SnO₂ molar ratio that indicated ease of nuclei formation and crystallization with lower Sn content in the dry gel.



Bimodal micromesoporous H/BEA zeolite for synthesis of ethyl levulinate

A series of bimodal micromesoporous H/BEA zeolite derivatives were prepared by the post-synthesis modification of H/BEA zeolite by NaOH (0.05M/1.2M) treatment. Samples were characterized by powder XRD, low temperature nitrogen adsorption or desorption, temperature programmed desorption of ammonia and ICP. The mesopore formation was found to play a crucial role in liquid phase esterification of levulinic acid with ethanol. The enhanced catalytic activity of a bimodal micromesoporous H/BEA zeolite derivative prepared by treatment with 0.1M NaOH was attributed to the high mesoporosity coupled with better preserved crystallinity and acidic properties. This recyclable and optimum catalyst exhibited 40% LA conversion with 98% EL selectivity using LA.

Novel heterogeneous catalysts for sustainable chemistry

Heterogeneous catalysts were focused to improve the efficiency by increasing the selectivity of reactions and reducing the energy consumption. It was aimed to develop novel catalysts with certain targeted properties. Study was done to correlate the relation between the structure and properties of the catalysts and its synthesis method.

Multifunctional catalyst

Several reactions were carried out in multiple steps. It was possible that each step might need a different type of a catalyst. Deacetalization-Henry condensation reaction is a two-step reaction that required acidic and basic active sites. This industrially relevant reaction was shown to have many possible products. Selective catalysts that formed one of the products were involved in separation and purification. These were also highly desirable as it saved the energy. The spatial location of acidic and basic sites was crucial to maintain the selectivity of the catalysts. Inorganic metastable phases such as metal oxohydroxides were developed and demonstrated.

It was shown for the first time FeOOH to bi-functionally active and different polymorphs of FeOOH show difference in selectivity. Similar effects were also observed in other metastable oxohydroxides such as CrOOH, CoOOH and AlOOH.

Hierarchically porous materials

Hierarchy in porosity was identified crucial to minimize the limitations in mass and heat transfer that causes undesirable side reactions and rapid catalyst deactivation. A new and inexpensive method was developed to produce hierarchically porous materials and control the textural properties. The method was tested on silica and silica based materials. The method carried kinetically trapped in situ generated gas bubbles by rapidly polymerizing the silane precursors. Production of multi-scale porous silica was done successfully by controlling the kinetics of in situ gas bubble generation and the rate of polymerization of silane precursors.

Development of greener methods for the conversion of biomass into chemicals

Publications: Catal. Sci. Technol., 2014, 4, 2904; RSC Adv., 2014, 4, 12625; React. Kinet. Mech. Cat., 2014, 112, 173; ChemPlusChem, DOI: 10.1002/cplu.201402145

The research was desired to utilize the biomass in the form of agriculture waste for the synthesis of chemicals using the heterogeneous catalysts. It was also desired to evaluate its activity in biomass conversion.

C5 sugars and furfural from hemicellulose

Hemicellulose upon hydrolysis supposed to produce C5 sugars and furfural. It was desired to develop a one-pot method using solid acid catalysts for the same purpose. Metal oxide catalysts with acidic properties were identified for the efficient one-pot synthesis of furfural (max 61%) from hemicellulose. Sol-gel synthesized WO_3/SiO_2 and $\text{Ga}_2\text{O}_3/\text{SiO}_2$ were stable under reaction conditions and exhibited similar activity in minimum eight runs. The effects of synthesis procedure, support material and metal oxide on catalytic activity were investigated. The preparation of catalysts by the sol-gel method showed the higher acid amount without any metal leaching.

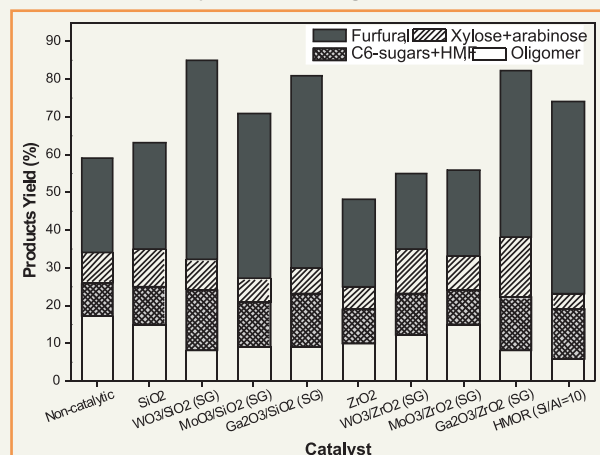


Fig. 1 Solid acid catalyzed one-pot conversion of hemicellulose (xylan). Reaction condition: hemicellulose (0.3 g), catalyst (0.075 g), water+toluene=60 mL (1:1 v/v), 0.2 MPa N_2 , 443 K, 8 h.

Aromatic monomers from lignin

A demonstration was performed to convert lignin below 250°C to aromatic monomers using bare solid acid catalysts. The well characterized dealkaline lignin with high degree of polymerization and molecular weight of 60kDa was depolymerized into value-added aromatic monomers with high yields (60 %) using solid acid catalysts under inert atmosphere. A variety of catalysts like crystalline to amorphous sizes were used to investigate. It was observed that catalysts with well defined structure were prone to undergo alterations in their structures. It was shown that $\text{SiO}_2\text{-Al}_2\text{O}_3$ recycled effectively although with slight decrease in the activity after each catalytic run. Catalyst morphology was studied using different physico-chemical techniques

before and after the reaction, which explained the reasons for catalyst deactivation for dealkaline lignin substrate.

Hydrodeoxygenation of phenols

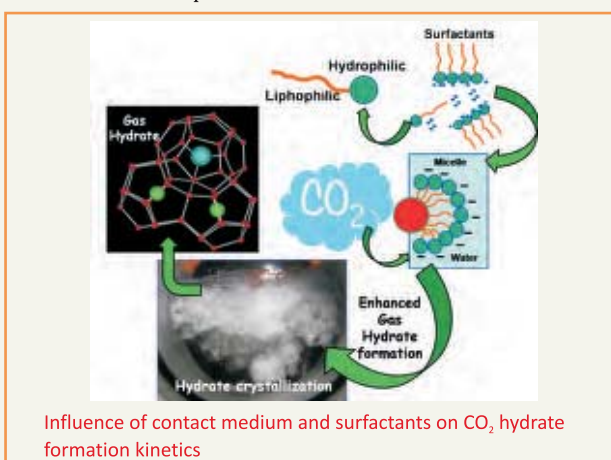
A systematic study was performed to check the effects of supports like acidic, neutral and basic, and the noble metals like Pd, Pt, and Ru on HDO of phenol, guaiacol and eugenol. The combinations of metals and supports were evaluated under the similar reaction conditions. It was found that the metals supported on highly acidic support ($\text{SiO}_2\text{-Al}_2\text{O}_3$) showed complete hydrogenation products with a possibility of C-O bond cleavage to achieve a real HDO activity. A complicated product distribution was achieved on a mildly acidic support ($\gamma\text{-Al}_2\text{O}_3$), neutral (C) and basic (HT) supports gave restricted hydrogenation activity but yielded the products with very high selectivity. Reaction pathways were suggested and deliberated on the basis of the results. Catalysts showed reproducible activity in recycle runs and were characterized by various (XRD, TEM, TPD, ICP-OES) techniques to establish catalyst activity-property relationship.

Supported metal catalyzed oxidation of HMF into FDCA

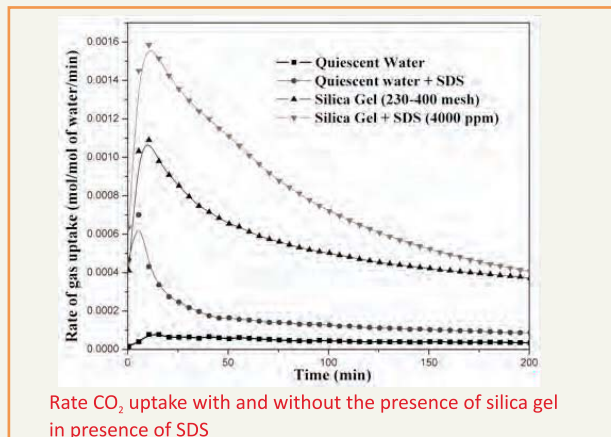
Supported Pt catalysts were synthesized, characterized and were used in the liquid phase air oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA). A stepwise increase in the reaction temperature (75 and 140°C for 12 h each) under the optimum reaction condition was seen. The method achieved the 96% FDCA yield in presence of 1 bar oxygen pressure over Pt/g- Al_2O_3 . It was shown that with increasing oxygen pressure (1-10 bar) the FDCA yields decreases since at higher partial pressure of oxygen over oxidation reactions of substrates and products are possible. The effects of weak or strong base, its equimolar or excess concentration were studied in detail. It was important to increase the reaction temperature in stepwise manner to achieve higher yields of FDCA since at higher temperatures HMF undergone self degradation and thus yielded less FDCA. The self degradation of HMF was also proved by undertaking the reaction under nitrogen environment. The effect of reducible and non-reducible supports and their oxygen storage capacity (OSC) was addressed and was supposed to be one of the factors to change the course of reaction. It was also shown that FDCA formed in the reaction was successfully isolated (91%, isolated yield) in the pure form and its purity was confirmed by NMR, melting point, and elemental analysis. The catalysts were characterized with XRD, TEM and ICP-OES techniques.

Gas hydrate research

Hydrate based gas separation process for CO₂ separation from its mixture was studied. A commercially viable process demanded a rapid hydrate formation rate at reasonable operating pressure. Higher solubility of hydrate forming guest in the water phase and large contact area between the hydrate formers and water were the two very important parameters to reduce the mass transfer resistance, which resulted the fast hydrate formation rate necessary for large scale continuous operation.



Carbon dioxide hydrate formation kinetics was investigated in a fixed bed crystallizer at constant pressure and temperature. Water dispersed three different silica gels having different surface area were used to enhance the hydrate formation kinetics and water was used to hydrate conversion ratio compared to a stirred tank reactor. It was observed that silica gel with larger surface area leads to higher gas consumption as well as reduced the induction time for hydrate crystallization. Different additives enhanced the gas dissolution by reducing the interfacial surface tension; it showed that sodium dodecyl sulphate (SDS) was most effective and enhanced the rate of hydrate formation as well as reduced the induction time.



Publications: Fuel, 2013, 105, 664; J. Phys. Chem. C, 2013, 117, 23, 12172

Final water to hydrate conversion ratio suggested that surfactants affected on total amount of water converted to hydrate which was very important for fuel gas separation through hydrate formation and decomposition process. Certain surfactants showed hydrate inhibition phenomena which were detrimental for this process. It was concluded that in presence of silica gel the rate of gas uptake enhanced considerably and anionic surfactant used as a kinetic promoter. It proved that bigger pores and higher surface area were the two important parameters while selecting a fixed bed packing for such a hydrate forming reactor. A fixed bed reactor was more economical compared with a stirred tank reactor for a commercial hydrate formation process.

Heat transfer calculations for decomposition of structure I methane hydrates

Microcanonical ensemble molecular dynamics simulations of methane hydrate were demonstrated to study the endothermic decomposition process. The mechanism of decomposition of methane hydrate as a function of time was explored at the molecular level. The initial temperature and pressure of the simulation were chosen so as to depict the natural gas hydrate in conditions of oceanic sediments. A strategy was developed to perform the microcanonical ensemble simulation of solid-liquid interface of hydrate and amorphous water. Adiabatic heat transfer calculations were performed and an attempt was made to fit the MD simulation results; to the heat balance equations derived from the heat transfer calculations. The properties like equilibrium temperature of methane hydrate and rate of supply of hot water for sustained release of methane from solid hydrate phase were determined at the macroscopic scale.

The temperature drop and pressure rise was observed during the methane hydrate decomposition process by performing NVE simulations. The decomposition was started from the hydrate-bulk water interface; however the decomposition of second and subsequent layers of unit cell was not instantaneous. It was dissociated only once 30-50 percent of the interface unit cell. The results were obtained from the MD simulations were fitted to heat transfer equations with assumptions of constant supply of heat and thus rate of supply of hot water for a constant decomposition rate was calculated.

Industrial wastewater treatment, recycle and reuse

Publications: J. Environ. Res. Dev., 2014, 8, 697; PCT Int. Appl., 2013, WO 2013054362 A2 20130418

The objective was to address the issues pertaining to pollution control and industrial wastewater intensively to treat it up to an extent that reclaimed water can be recycled and reused.

Industrial wastewater treatment

The research was aimed to work on industrial wastewater treatment, water recycle and its reuse. Newer separation processes and combinations of finer aspects of existing physico-chemical and biological methods were developed. Specific aspects related to methodologies like ion exchange, coagulation, cavitation, solvent extraction, membrane separations and cavitations were investigated independently and also in combination for effective separations. A workshop entitled 'Indus Water' was also conducted. The focus was on the different aspects to realize environmentally benign and globally competitive processes and technologies through the research and industrial work.

Cavitation technology

A technology based on hydrodynamic cavitation for the treatment of industrial waste water was developed. Cavitation technology was used for the treatment of any industrial effluent for removal of COD and colors. The technology can be implemented alone or in combination

with other processes such as biological treatment process oxidation, adsorption, ion exchange or coagulation. The technology showed the potential to remove COD effectively and significantly at low cost of operation. When combined with anaerobic process, it enhanced the profitability through increased gas yield along with digester stabilization.

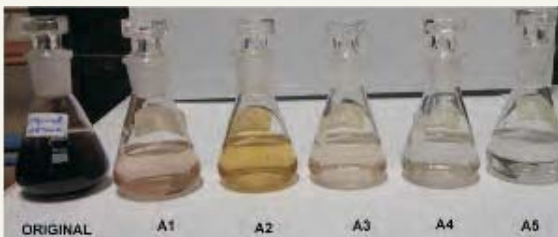
Coagulation technology

Coagulation technology was used to treat any industrial effluent to remove the COD and color. The technology needed implementations combined with other processes to optimize distribution of pollutant removal load in different treatment stages. It showed the potential to remove COD significantly at low cost of operation. It enhanced the performance and reduced the cost of operation when used in the form of coagulant formulations. A newer form of inorganic polymeric coagulant being developed by the group with high molecular weight and basicity expected to offer substantial improvement comparatively.

The adsorption technology was also developed which proved to be a good alternative for the wastewater treatment.



Cavitation pilot plant (Capacity: 1 m³/h)



Industrial wastewater treatment results on industrial wastewater

Desulfurization of transportation fuels

The objective was to address the issues pertaining to pollution control and deep desulfurization of transportation fuels -below 15 ppm S.

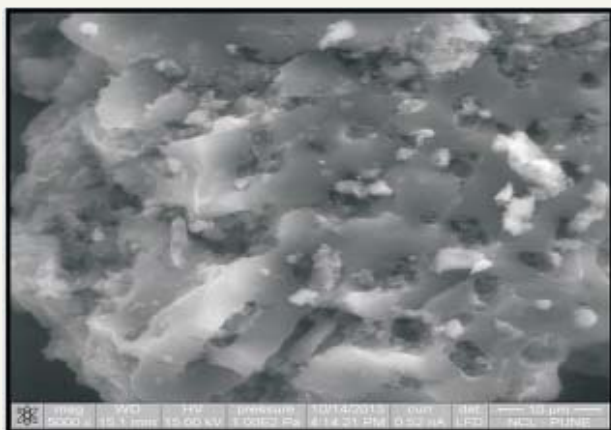
Deep desulfurization of fuels

Reduction in the sulfur levels of transportation fuels, maximum of 15 and 30 ppm in diesel and gasoline respectively from the existing levels as high as 10 times of these values is mandatory. Sulfur in the transportation fuels has been a major concern from environment point of view as well as from the viewpoint of application in Fuel Cells. The fuel cells required much more stringent conditions on sulfur levels which are of the order of 1 ppm, and preferably 0.1 to 0.2 ppm, to avoid poisoning of the catalyst due to sulfur.

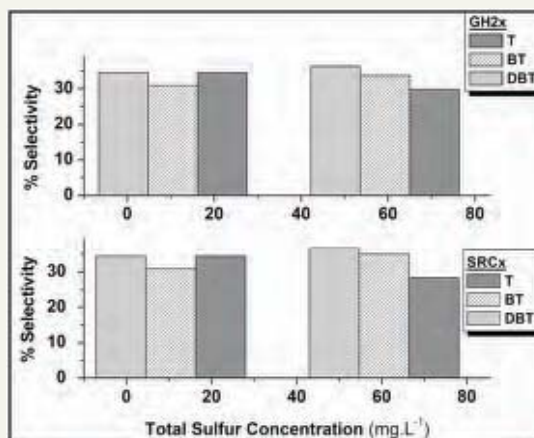
The sorption process believed to offer an economically viable option to the existing processes and hence research on sorption and sorbents is the key to new technology development.

Adsorption technology

Adsorption technology, an attractive alternative to achieve the deep desulfurization for removal of refractory sulfur compounds from organics. The application was to be useful specifically in petroleum industry for transportation fuels and industries that used organic feed where sulfur was a problem e.g. Camphor industry. The newer and modified adsorbents were developed for increased sulfur removal capacity with ease of regeneration.



SEM image of Ni-GH2x



Selectivity of sulfur compounds over model fuel

Genetic programming to develop the soft sensors

Publications: Bioenerg. Res., 2014, 7, 681; Biochem. Eng. J., 2014, 85, 89; Chem. Eng. Res. Des., 2014, 92, 6, 1119

Accurate prediction of higher heating value of solid biomass fuels

Predominant linear correlations were proposed to predict the HHV of biomass fuels. The scrutiny of the relationships between the constituents of the proximate and ultimate analyses and the corresponding HHVs suggested that all relationships were not linear. The nonlinear models were more appropriate. Artificial novel intelligence formalism, namely genetic programming was employed for the first time that developed two biomass HHV prediction models. The constituents of the proximate and ultimate analyses were utilized as the model inputs. The prediction and generalization performance of these models were compared with the corresponding multilayer perceptron (MLP) neural network based high-performing linear and nonlinear HHV models. This comparison of the HHV prediction performance of the GP and MLP models was consistently better than that of existing linear and nonlinear counterparts. The models developed were proved to be the most accurate models for the prediction of the higher heating value of solid biomass fuels.

Soft-sensor development for biochemical systems using genetic programming

The genetic programming was introduced as an artificial intelligence based data-driven modeling formalism for the development of soft-sensors for biochemical processes. The example input-output data was searched and optimized for both form and parameters of appropriate linear or nonlinear data-fitting model. GP based soft-sensors were developed for two bioprocesses, namely extracellular

production of lipase enzyme and bacterial production of poly(3-hydroxybutyrate-co-3-hydroxyvalerate) copolymer.

The soft-sensor predicted the time-dependent lipase activity (U/ml) in case study I; in case study-II it predicted the amount of accumulated polyhydroxyalkanoates (% dcw). The prediction and generalization performance of the GP-based soft-sensors were compared with the corresponding multi-layer perceptron (MLP) neural network and support vector regression (SVR) based soft-sensors. The comparison indicated that the GP-based soft-sensor was clearly outperformed the two other soft-sensors in the first case study. In case study-II involving bacterial copolymer production, the GP and SVR based soft-sensors were performed equally.

Biodegradable iron chelate for H₂S abatement

A batch reactor process for the abatement of a common pollutant, namely H₂S using Fe³⁺-malic acid chelate (Fe³⁺-MA) catalyst was developed. Process modelling and optimization was conducted in three stages with a view to maximize the H₂S conversion. Sensitivity analysis of process inputs was performed to select the most influential process operating variables and parameters, an artificial neural network (ANN)-based data-driven process model was developed by using influential process variables and parameters as model inputs, and H₂S conversion (%) as the model output, and the input space of the ANN model was optimised using the artificial immune systems (AIS) formalism.

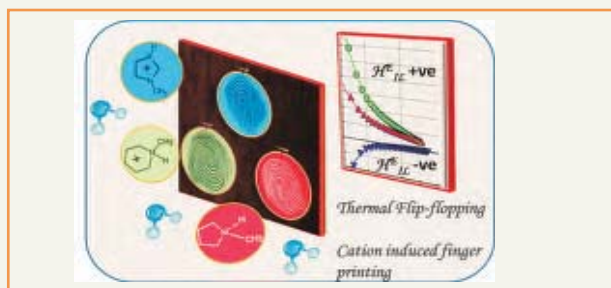
Physical chemistry of organic reactions in unusual media

Publications: J. Phys. Chem. B, 2014, 118, 2487, 4160, 10704;
Chem. Phys. Chem., 2014, DOI:10.1002/cphc.201402338

The objective was to study the nonbonding interactions of ionic liquids to reveal the molecular origin of the effect in different chemical reactions and investigate the structure-property relationship in ionic liquid systems involving microemulsions. Hydrophobicity and enthalpies in non-reactive and biologically active molecules, liquid-liquid equilibrium and reaction mechanism were also investigated.

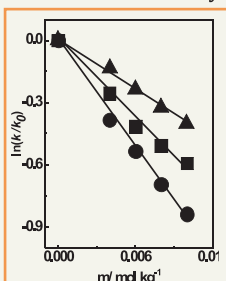
Elucidation of ionic interactions in the PIL solutions by isothermal titration calorimeters

The Protic Ionic Liquids (PIL) such as 1-methylimidazolium tetrafluoroborate, 2-methylpyridinium tetrafluoroborate, and N-methylpyrrolodinium tetrafluoroborate in comparison to 1-butyl-3-methylimidazolium tetrafluoroborate were used. The excess partial molar enthalpy, H^E_{IL} was obtained from isothermal calorimetric titrations at 298.15 K which was used to probe the nature of interactions of the PIL cations with solvent molecules against those present in APIL-solvent systems.



Delineation of pairwise interactions upon using ionic liquids as co-solvents

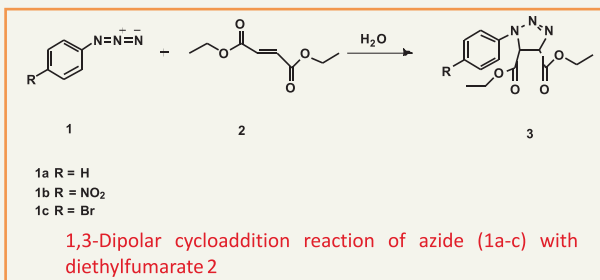
Ionic liquids were introduced as co-solvents during Diels-Alder reactions promoted by water to increase the solubility window of solvent water. The dependence of the second order rate constants for Diels-Alder reaction between anthracene-9-carbinol and N-ethylmaleimide on the molality of added co-solvent was analyzed in terms of pair-wise Gibbs function interaction parameters. Additivity of pairwise group interaction parameters (SWAG procedure) was applied to examine the validity of additivity during the analysis. Pairwise Gibbs functions were calculated for a variety of ionic liquids to comprehend the efficacy of ionic liquids as co-solvents. A comparative kinetic and thermodynamic study was presented to guide the tailorability of ionic liquids as co-solvents during cycloaddition reaction in water.



$\ln(k/k_0)$ plotted vs concentrations for ■ [Bmim]I, ● [Bmim]NO₃, ▲ [Bmim]SCN at very low concentration region

Click chemistry at 'on water conditions'

Investigation of 1,3-dipolar cycloaddition reaction under heterogenous conditions was carried out in order to inspect the hydrophobic contribution towards rate enhancement at the interface on addition of prohydrophobic salts. The influence of different substituents on the reactivity of 1,3-dipole was explored. Kinetic studies divulged a conspicuous role of prohydrophobic salts under these conditions. No rate enhancement was observed at higher salt concentration. Role of 'active' interfacial area was found to be crucial for the desired enhancement in heterogenous reaction conditions, which showed implications in determining the optimum salt concentration and conditions required for such reactions.



Elucidating polarity parameter of binary mixtures of ionic liquids

A thorough analysis of polarity parameters in both hydrophilic as well as hydrophobic ionic liquids was carried out using different solvents of varying polarities to elucidate the mechanism causing the hyperpolarities in ionic liquid-alcohol mixtures, the application of a model for the description of E_T^N values for all the binary mixtures and the interrelation of the polarity parameters in binary mixtures. A strong correlation was observed in the values and hydrophobicities of pure ionic liquids suggesting the role of the values for describing hyperpolarity.

Eutectic mixture and ionic liquids directed kinetics

An experiment to identify the role of eutectic mixture of carbohydrate and urea as a potential green solvent in promoting organic bimolecular reaction was performed. Further investigations were made which will help to discover the new realm of the green solvents. The catalytic and mechanistic roles of the ionic liquids during several C-C bond formation reactions are under investigations.

Applications of NMR spectroscopy

The objective was to apply methodologies based on solid and solution state NMR spectroscopy to address various structural problems in the area of chemical and material science for structure-property correlation.

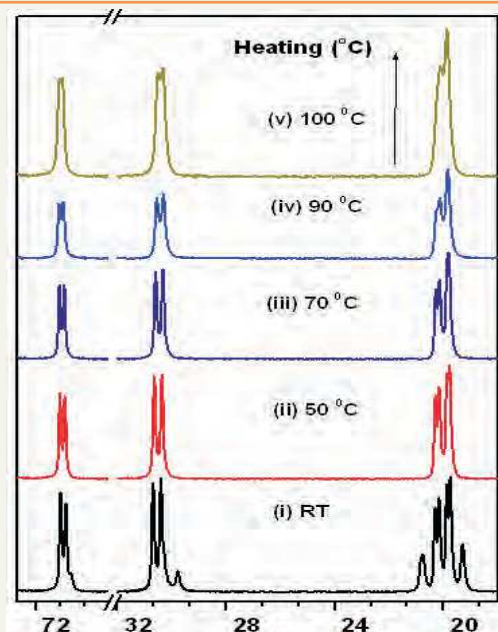
Structural chemistry

Structural features of a number of synthetic peptide oligomers mimicking bio molecular structural architectures resulting from non bonding interactions were investigated by modern NMR spectroscopic techniques. The focus was on building blocks containing proline, anthranilic acid, orthanilic acid, 2-aminobenzenesulfonic acid moieties. Oligomers of these systems showed to possess different back bone conformations driven by the change in their hydrogen bond patterns.

Publications: Eur. J. Org. Chem., 2013, 3529; Org. Lett., 2013, 15, 1504; J. Phys. Chem. A., 2014, 1213; Chem. Commun., 2013, 2222

Catalysis and surface science

Structural features of magnesium chloride and alcohol adducts were not well understood though they were used as a support materials for Ziegler-Natta polyolefin catalysts. It was observed that the nature of adducts formed between isobutanol (iBuOH) and $MgCl_2$ is very sensitive to the preparation conditions employed. One of the formed adducts contained four molecules of isobutanol, which was found to be relatively more stable. A detailed *in situ* variable temperature solid-state NMR investigation of this system indicated co-existence of two phases which were found to be dynamic in nature.



^{13}C CPMAS NMR spectra of an $MgCl_2$ -iBuOH molecular adduct

This chapter and Scientific Computing have interrelation and for the sake of brevity, the content is not repeated. Please also refer the chapter on Scientific Computing: p. 96 - 97

Neelanjana Sengupta
n.sengupta@ncl.res.in

Assembly and interfacial behavior of disease prone proteins: Molecular insights

Publications: J. Phys. Chem. B, 2014, DOI: 10.1021/jp505629q; PLOS ONE, 2014, 9, 8, e105196; DOI:10.1371/journal.pone.0106883; Biophys.Chem; 2013, 184, 108

Competition between self-assembly and adsorption of the amyloid beta protein

Self-assembly and adsorption of the Amyloid beta (Abeta) protein on the outer surface of a single-walled carbon nanotube (SWCNT) of high curvature was achieved. It was reported that surface hindered and promoted the self-assembly depending on the critical interaction strength.

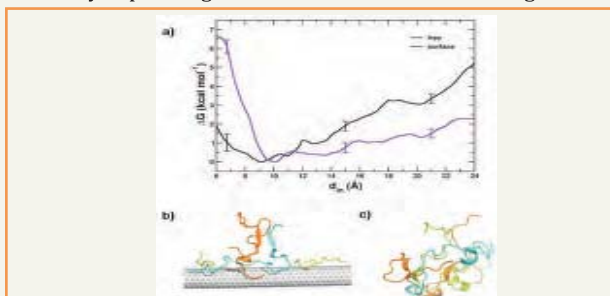


Fig. 1: a) Free energy profiles as a function of distance (d_n), snapshots corresponding to the free energy minimum for b) surface adsorbed and c) free complexes

Aqueous co-assembly of two different amyloidogenic proteins

Co-assembly of two different amyloidogenic proteins namely Abeta and alphaSynuclein or aSyn was achieved in fully aqueous environment. The two proteins with very different physico-chemical properties beyond the initial diffusive regime were demonstrated a strong propensity to interact.

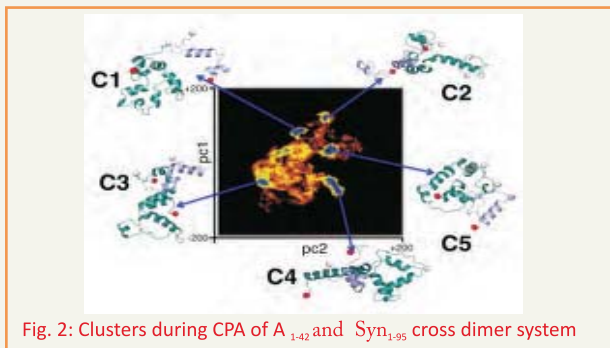


Fig. 2: Clusters during CPA of A_{1-42} and Syn_{1-95} cross dimer system

The clusters evolved during cartesian principal component analysis (PCA) of A_{1-42} and Syn_{1-95} cross dimer system. The two-dimensional representation of the distribution of density function ΔG , corresponding to the fluctuations of the Carbon atoms on the plane of the top two principal components are shown Fig. 2. The ΔG values spread in the

range of 0 to 4.2 kcal mol⁻¹ and the representative structures from five distinct clusters were reported.

Energetic and dynamic properties of the hydration layer of an amyloidogenic system

The microscopic hydration properties of Abeta were compared with that of a folded protein, namely Ubiquitin (UBQ). It was reported that while the hydration layer of both demonstrates sub-diffusive behavior, the Abeta hydration dynamics were closer to bulk water behavior compared to UBQ. Further, the conformational fluctuations in Abeta gave rise to very high degrees of dynamical and interaction heterogeneity, which were suppressed if the peptide's conformational degrees of freedom were artificially suppressed.

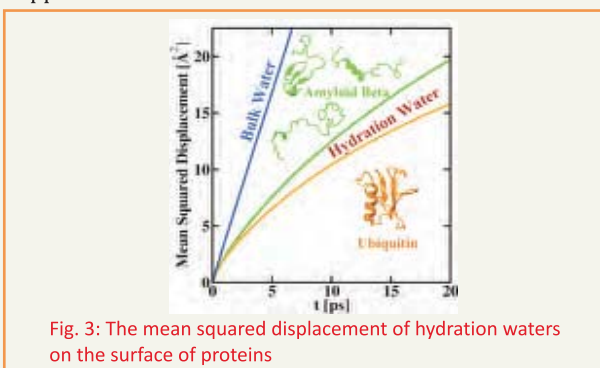


Fig. 3: The mean squared displacement of hydration waters on the surface of proteins

It was reported that mean squared displacement (MSD) of hydration water on the surface of proteins was slower than that of water in the bulk phase. The sub-diffusive behaviour was also evident from the non-linear nature of the MSD plots of the surface water. However, the water hydrating amyloidogenic Abeta was distinctly faster than hydrating the folded protein, Ubiquitin.

Active drug protriptyline against multiple pathways of Alzheimer's disease

The drug protriptyline was found active against multiple pathways of Alzheimer's disease. It was also reported that the drug protriptyline bound three distinct proteins that played important roles to trigger Alzheimer's disease. The three targets were Abeta, Acetylcholinesterase (AChE) and beta secretase, its binding with protriptyline resulted in loss of respective activities and self-assembly propensities.

Development and applications of quantum chemistry theories

Sourav Pal
s.pal@ncl.res.in

Publications: J. Chem. Theory Comput., 2013, 9, 4313; 2014, 192; J. Chem. Phys., 2013, 139, 124116; J. Phys. Chem. A, 2013, 117, 8691, 10933; 2014, 118, 1350; J. Phys. Chem. C, 2013, 117, 20982

Lower scaling approximation to Equation-of-Motion Coupled-Cluster

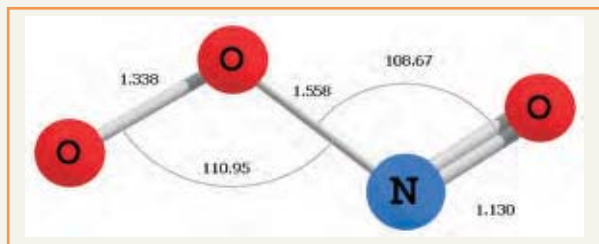
A lower scaling approximation to EOM-CCSD was formulated using a perturbative truncation of the coupled cluster similarity transformed Hamiltonian. The method was implemented for IP, EA and SF variants of EOMCCSD.

Singlet-triplet gap of naphthyle cation

The singlet triplet gap of naphthyle cation, a radical of significant importance in interstellar chemistry was calculated. The study showed that naphthyle cation had singlet ground state that was contrary to previous reports. It was highlighted that how previous inaccurate theoretical calculation led to wrong interpretation of experimental results and consequently wrong assignment of ground state multiplicity of naphthyle cation was observed.

On potential stability of peroxy nitrate radical

A benchmark multi-reference coupled cluster study on structure, stability and energetics of transiently stable peroxy nitrate radical was done. That was an important intermediate in stratospheric ozone chemistry. The study showed that peroxy nitrate radical with a bound structure and trans form of it gave rise to the experimental IR spectra at 1840 cm^{-1} . On contrary to previous single reference studies which claimed peroxy nitrate radical to be unstable.



Orientation of water molecules around the phosphate

The adsorption of water molecules around a polar region particularly around the phosphate moiety in the phospholipid molecules was studied. The adsorption sites for water molecules were validated by density functional theory based reactivity descriptors, viz. Fukui functions in the phosphatidyl ethanolamine (PE) model system.

Calculation of interaction energy using the local hard-soft, acid base principle

The second order approximation on ad hoc charge transfer parameter (ΔN) was introduced to calculate interaction energies of multiple site based interactions using local hard soft acid base principle. Interaction energies of some prototype molecules studied to validate the approach and discussed the advantages and limitations of the approach.

Site selectivity in small - sized neutral and charged Al_n ($4 \leq n \leq 7$) clusters

Potential sites for adsorption on the small sized aluminum clusters were identified using density functional theory (DFT) based reactivity descriptors. Susceptibility of various types of reactive sites within a cluster toward an impending electrophilic or nucleophilic attack was predicted using the reactivity descriptors depending on the symmetry. The study devised general rules to understand how the size, shape, and charge of the cluster influence the number of available sites for an electrophilic and nucleophilic attack. The predictions by reactivity descriptors were validated by performing an explicit adsorption of water molecule on Al clusters.

Dinitrogen activation by silicon and phosphorus doped aluminum clusters

Activation of molecular nitrogen on doped aluminum clusters in the framework of density functional theory was studied. Calculations on silicon and phosphorus doped aluminum clusters demonstrated an enhancement of N_2 activation with respect to their pristine ground state and high energy counterparts. Ab initio molecular dynamics simulations established the consequential efficiency of doped clusters toward dinitrogen activation at finite temperature. The study highlighted the critical role of doping foreign impurities for future endeavors in the design of cost effective and efficient catalysts for N_2 activation at ambient temperatures.

Effect of charge and ligand on the finite temperature behavior of gold clusters

Born Oppenheimer molecular dynamics calculations were carried out to study the effect of charge and ligand on the finite temperature of gold cluster, Au_6 . It was found from the results that neutral Au_6 cluster was significantly stable to be compared with the charged clusters. It was observed that ligation of the cluster with a small ligand was used to tune its thermal stability.

Effect of silicon doping on the reactivity and catalytic activity of gold clusters

The effect of silicon doping on the reactivity and catalytic activity of gold clusters was studied. Silicon doping did not alter the reactivity and catalytic activity of the odd atom gold clusters which were known to be reactive and catalytically active. Silicon doping resulted in the enhancement in reactivity and catalytic activity of gold clusters with even number of atoms which were found catalytically inert.

Molecular simulation studies of solvation effects: From simple hydrophobic solutes to polypeptides

Publications: J. Chem. Phys., 2013, 139, 104501; Proc. Nat. Acad. Sci. USA, 2014, 11358

The objective was to obtain the free energy profile of complex biophysical and chemical processes to develop a molecular picture based on computational modelling.

Structure and dynamics of water molecules in the hydration layer

The focus was to understand the structure and dynamics of water molecules in the hydration layer around a range of

Hydrophobic solutes starting from small molecules to large polymers with various size, shape and topology. The dependence of the tetrahedral order parameter of water molecules in bulk water as a function of temperature and in the hydration layer of hydrophobic solutes as a function of the size of the solute was understood (Fig. 1). The structural ordering of surface water was reduced with the increasing size of the solutes.

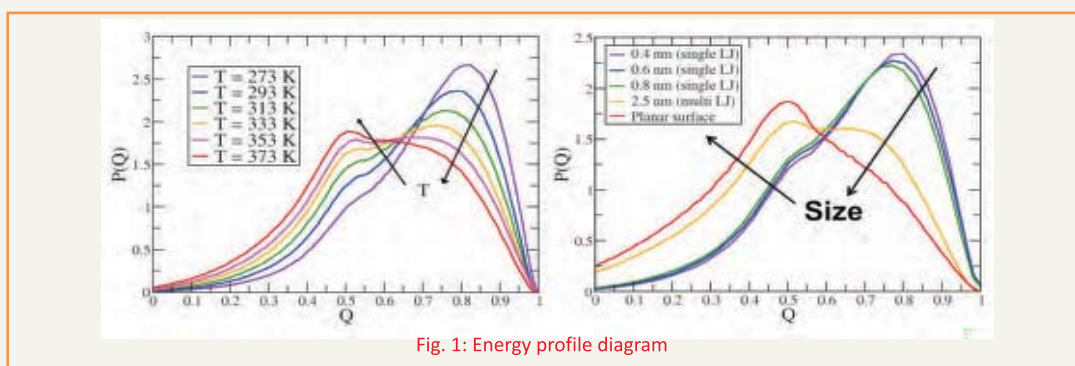


Fig. 1: Energy profile diagram

pH dependence and pH induced aggregation behaviour in prion proteins

It was aimed to understand the pH dependence of the effective size of polypeptides and induced aggregation behaviour in Prion proteins. The balance between the electrostatics and hydrophobic interactions was captured. Extensive Replica Exchange Molecular Dynamics simulation

technique was used to capture the dimerization process in Prion proteins. Some representative metastable beta-sheet rich conformational states were isolated successfully. The electrostatic free energy profile of proton translocation in the enzyme Cytochrome *c* Oxidase for multiple point mutations was obtained. The conformational signatures of the switching behaviour in RhoA GTPases were understood.

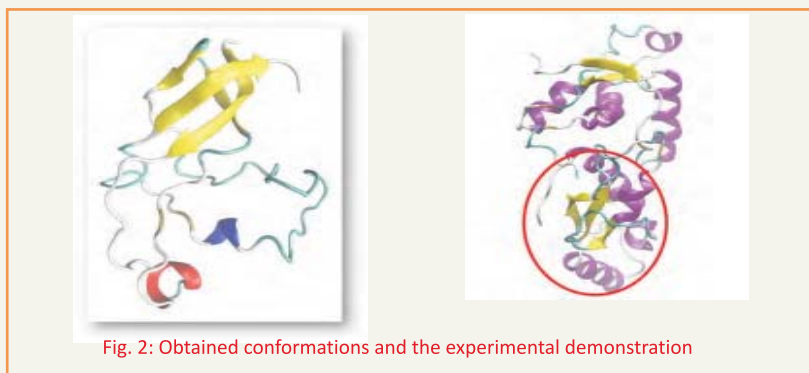


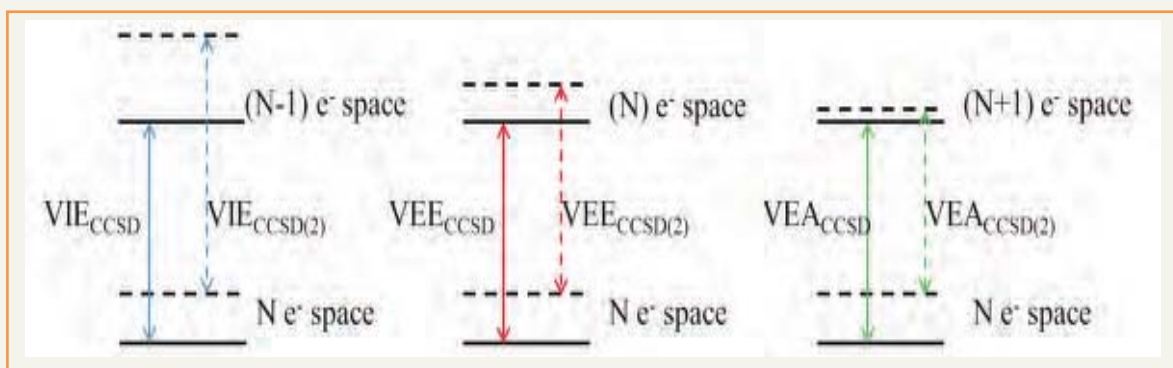
Fig. 2: Obtained conformations and the experimental demonstration

Development and implementation of hybrid quantum mechanical methods to molecular structures

Publications: J. Chem. Phys., 2014, 140, 94101; J. Phys. Chem.A., 2014, 118, 28, 5323

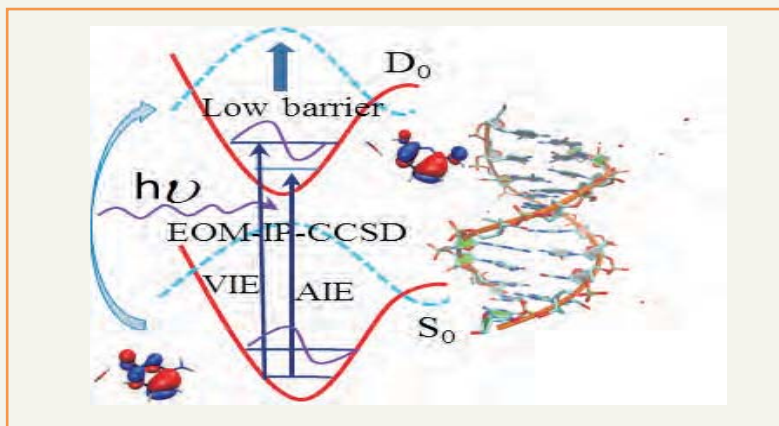
The objective was to formulate and implement a hybrid QM/EFP method with perturbatively approximated EOM-CCSD(2) which was achieved successfully. This formulation reduced the cost of ground state calculation of the QM part from iterative N^6 scaling CCSD to non-iterative N^5 scaling MP2 or CCSD(2). The performance of EOM-IP-CCSD(2)/EFP,

EOM-EE-CCSD(2)/EFP, and EOM-EA-CCSD(2)/EFP with respect to more accurate and computationally expensive EOM-CCSD and EOM-CCSD/EFP methods were tested. EOM-CCSD(2)/EFP found to be superior to methods like EOM-CIS(D)/EFP and EOM-CISD/EFP and computationally cheaper than EOM-CCSD/EFP.



The relative stabilities of the stable tautomers of cytosine in gas phase and under microsolvation were calculated. The enol tautomer was found to be most stable in the gas phase. The stabilities of the tautomers dramatically changed upon monohydration and the keto tautomer having higher dipole became more stable. The computations of the VIEs and AIEs of the microsolvated tautomers were done; and it was noticed that the solvatochromic shifts were consistent with the amount of differential charge-dipole interactions between the cation and neutral states; both red and blue

solvatochromic shifts were noticed unlike the case of thymine. Different ionization channels were probed for keto-enol and keto-ketoimine tautomerizations. It was reported that first ionized state provided a lower-barrier tautomerization except in the case of gas-phase keto-ketoimine tautomerization. The effect of ionization on the tautomerization in the microsolvated structures was further probed by charge-dipole interactions. It was found that changes in the barriers were consistent with the amount of charge-dipole interactions.



Understanding growth pattern and melting in finite size systems

Publications: J. Chem. Phys., 2014, 141, 54308; 140, 154307; Proc. of SPIE, 2014, 8985, 89850P1

Rationalizing role of structural motif and underlying electronic structure on the finite temperature behavior of clusters:

Finite temperature behavior of 36 atom Al and Ga cluster was simulated to understand the influence of the structural motif of the ground state on the melting transition in the small clusters. A case was reported with clusters of aluminium and gallium which have same number of atoms, valence electrons, and similar structural motif of the ground state but drastically different melting temperatures. It was observed that for both the clusters, isomers accessible before cluster melts had striking similarities and strong influence of the structural motif of the ground state. Further, the shape of the heat capacity curve was similar in both the cases but the transition was more spread over for Al_{36} which was consistent with the observed isomerization pattern. The simulations executed suggested a way to characterize transition region on the basis of accessibility of the ground state at a specific temperature.

Scaling up the shape: Novel growth pattern of Gallium clusters

The Kohn-Sham formulation of the density functional theory was employed to find the putative global minima for GaN clusters with size N ranging from 49 to 70. A unique growth pattern in the clusters was discovered, all of which were hollow core-shell structures. It was evolved with size from one spherical core-shell to the next spherical core-shell structure mediated by prolate geometries, with an increase in overall diameter of the core, as well as the shell, without putting on new layers of atoms. A complete picture of bonding in gallium clusters was presented by critically

analyzing the molecular orbitals, the electron localization function and Bader charges. Bonding in these clusters was a mixture of metallic and covalent type that was leant towards covalency, accompanied by marginal charge transfer from the surface to the core. Most molecular orbitals of Ga clusters were non-jellium type. Covalency of bonding was supported by a wide localization window of electron localization function, and joining of its basins along the bonds.

Origine of Terahertz (THz) resonances in organic molecular crystals

Molecules with strong resonances in the terahertz frequency range are ideal to realize "Terahertz tags" which can be easily incorporated into various materials. THz spectroscopy of molecules, especially at frequencies below 10 THz, provided valuable information on the low frequency vibrational modes, viz. intermolecular vibrational modes, hydrogen bond stretching, torsional vibrations in several chemical and biological compounds. Very few attempts are made to engineer molecules that can demonstrate customizable resonances in the THz frequency region. Diamidopyridine (DAP) based molecules were used as a model system to demonstrate engineering of THz resonances (<10 THz) by fine-tuning the molecular mass and bond strengths. Density Functional Theory (DFT) simulations were carried out that explained the origin of THz resonances and factors contributing to the shift in resonances due to the addition of various functional groups. The design approach presented was easily extended to engineer various organic molecules suitable for THz tags application.

Scientific Computing

This chapter and Theory and Computational Science have interrelation and for the sake of brevity, the content is not repeated. Please also refer the chapter on Theory and Computational Science : p. 91 - 95

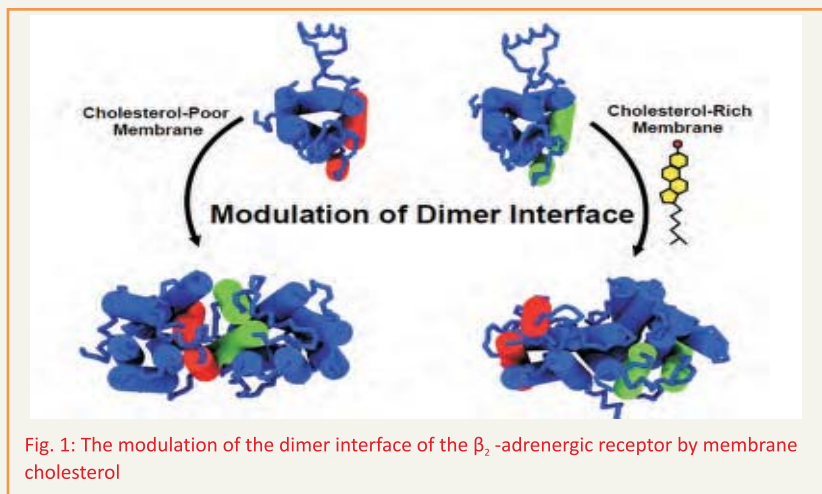
Durba Sengupta
d.sengupta@ncl.res.in

Publications: Biophys. J., 2014, 106, 1290; Phys. Chem. Chem. Phys., 2013, 15, 1904

Different aspects of membrane proteins, in particular the β_2 -adrenergic receptor were investigated. The recent high-resolution crystal structure of the β_2 -adrenergic receptor revealed the presence of possible cholesterol-binding sites in the receptor.

The dimerization of the β_2 -adrenergic receptor in lipid bilayers containing cholesterol was explored by using MARTINI coarse-grained molecular-dynamics simulations. A novel aspect of these results was that receptor dimerization was modulated by membrane cholesterol. It was showed that cholesterol can bind to transmembrane helix IV, and cholesterol occupancy at this site may restrict its involvement at the dimer interface (Fig. 1). It was observed that with increased concentration of cholesterol, the presence of transmembrane helices I and II was also

increased, but presence of transmembrane helix IV at the dimer interface was reduced. The correlation between cholesterol occupancy and GPCR organization was explored; the results indicated that dimer plasticity is relevant not just as an organisational principle but also as a subtle regulatory principle for GPCR function. The results constituted an important step towards designing better drugs for GPCR dimer targets. The coarse-grain molecular dynamics simulations were used to study the association of ErbB2 transmembrane helices and three "oncogenic mutants". Self-assembly simulations and the dimerisation free-energy profiles confirmed the energetically-favorable dimerized state for both the wild type and the mutants. The dissociation free energy of all three mutants was calculated to be larger than the wild type peptide.



Along with favourable protein-protein interactions, non-specific environmental effects were observed to contribute to the association. Local bilayer thinning along with membrane perturbations were seen around the mutants. The membrane perturbations were reduced upon helix

association; it suggested that lipid chain packing is an important driving force for helix dimerization. The results highlighted the importance of both specific as well as non-specific driving forces in the association of transmembrane helices.

Scientific Computing

Kumar Vanka
K.vanka@ncl.res.in

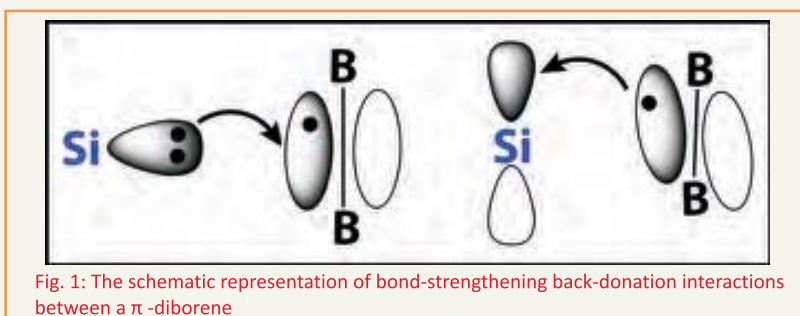
Selected Publications: Organometallics, 2014, 33, 17, 4357; Chem. Commun., 2014, 50, 62, 8522; Dalton T., 2014, 43, 5, 2194; J. Phys. Chem. C, 2014, 118, 2, 784

The objective was to design and develop the transition metal and main group based new systems for the activation of small molecules. Concepts such as frustrated Lewis pairs (FLPs), metal-ligand cooperation and the exploitation of silylenes were also investigated and understood computationally.

Bond strengthening back donation with silylenes

Novel ideas were explored in the field of small molecule activation. Full quantum chemical calculations were carried

out with density functional theory (DFT) that showed the bond-strengthening back-donation to a π -diborene discovered for transition metal systems. These systems proved to be favored for main group silylene complexes. The result showed the range and applicability of the bond-strengthening back-bonding interaction. It also showcased the potential of silylene complexes towards new chemistry such as the cooperative activation of carbon monoxide and carbon dioxide.



Nayana Vaval
np.vaval@ncl.res.in

Publications: Mole. Phys., 2014, 112, 669; Phys. Rev. A, 2014, 89, 42510; Phys. Rev. A, 2014, 90, 10501

The potential energy surface of the single, double and triple bonded systems was studied by using extended coupled cluster method. The objective was to investigate the interatomic coulombic decay for HF clusters and to study the ionization potential of different alkaline-earth metals.

Study of potential energy surface using extended coupled cluster method

The potential energy surface (PES) was studied for HF, N₂ and C₂ molecules using extended coupled cluster (ECC) method. Decoupled approximation was used along with the normal ECC for the study. Double and triple bonded N₂ and C₂ were the interesting systems for PES study. Decoupled approach within ECC framework showed good convergence for all the molecules.

Relativistic equation-of-motion coupled-cluster for IP and DIP of atoms

Relativistic equation of motion coupled cluster (EOMCC) method was used for the ionization potential of He-like ions, Be-like ions along with Na⁺, Al⁺, K⁺, Be, and Mg. This method was employed to calculate the principal valence double-ionization potential values of He and alkaline earth metal (Be, Mg, Ca, Sr, and Ba) atoms. Four component Dirac spinors were used for the calculations.

Inter atomic coulombic decay: Equation of motion coupled cluster

The equation of motion coupled-cluster method (EOM-CC) was used for the study of the decay in (HF)_n (n=2,3). Inter atomic coulombic decay was non-radiative decay mode of excited or ionised molecules in an environment. Equation of motion coupled cluster was used along with the complex absorbing potential for study of life time.

Sustainable Polymer Industry through Research Innovation and Training

Publications: Rheo. Acta, 2014, 53, 85; J. Polym. Sci. Part A Polym. Chem., 2013, 52, 1; 2014, 52, 1; J. Rheo., 2013, 5, 559, Macromolecules, 2013, 46, 3631

Research and scientific services programs

Research was conducted on molecular modeling of polymerization catalysts, understanding the role of macromolecular architecture of polymers on industrial Extrusion Film Casting (EFC) operation, high melt strength biodegradable polylactic acid (PLA) and polymers in hydrogen PEM fuel cells.

Learning and sharing programs

Several training workshops were conducted as part of the LSP of the CoE-SPIRIT (Sustainable Polymer Industry through Research Innovation and Training) for industrial personnel, students and faculty from academia. Then training involved the thermal analysis of polymeric materials; GPC of macromolecular materials; DLS techniques for particle size analysis and colloidal stability; rheology of paints and emulsions and DFT techniques for molecular modeling of catalytic systems. The training programs were co-organized with the entre-preneurship development centre. Participants from all corners of India attended the training workshops.

EFC and thermoforming of PLA regarded as a globally emerging area and likely to grow in India. PLA showed low melt strength which limited its applicability in film forming and thermoforming processes that is typically used in manufacturing packaging materials. The aim of the research was to develop a long chain of branched PLA with control on molecular architecture in order to improve its melt strength. This was achieved by either reacting linear PLA with certain peroxides in presence of suitable additives or by reacting

end functional groups of PLA using multifunctional branching agents and clickable groups. An alternative method was experimented to improve the melt strength of PLA; which involve the preparation of ionomers of PLA (Fig. 2). Electrostatic interactions of the ionic groups in an ionomer imparted hindrance to the chain movement in the melt state. It made drastic difference in the properties of ionomer melt to be superior to polymer melt. It showed that the PLA so prepared has increased melt elasticity. This research provided the important inputs to the practice of extrusion film coating and thermoforming of PLA and to the development of improved grades of PLA for these applications.

A special polymer membrane electrolyte was used by the PEFCs to enable the selective permeation of protons from the anode to the cathode in the fuel cell to complete the electro-chemical reaction of oxidation of hydrogen to water with simultaneous generation of an electric current. Development of such special high temperature poly-benzimidazole (PBI) based membrane was achieved.

The purpose was to guide the development of polymer membranes and electrodes with improved proton conductivity and reduced charge transfer resistance. Full 3D simulations of polarization and electrochemical impedance experiments were carried out on PEFC using COMSOL multiphysics software. The sensitivity of fuel cell performance to various parameters was examined using COMSOL.

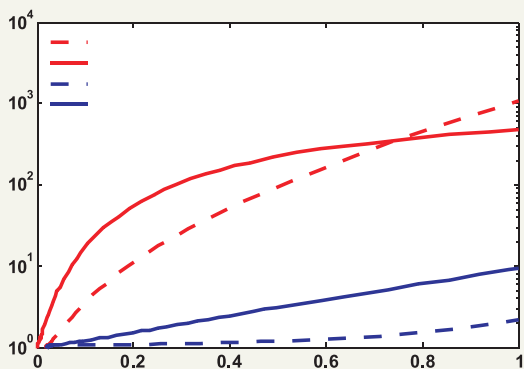


Fig. 1: Differences in the predicted values of molecular stretch in an EFC process

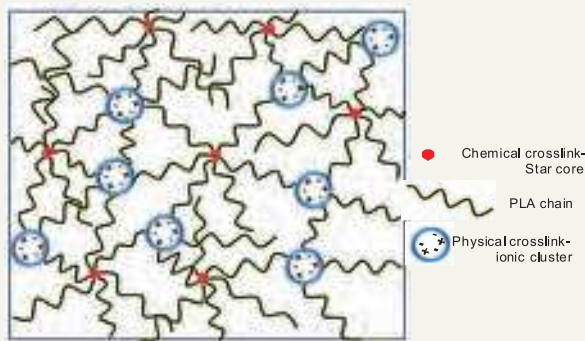


Fig. 2: Microstructure of star-PLA ionomers

Solar Energy

The objective was to find the efficient and low cost energy harvesting and storage solutions, and to employ several nano-engineering strategies to tune the optical, electronic and catalytic properties of organic and inorganic materials.

Hybrid photodiode ZnO(N)-Spiro-MeOTAD as a self-powered UV-Visible photosensor

The UV-VIS photo-detector was developed from n-type oriented ZnO nanorods and p-type Spiro-MeOTAD semiconductor that showed high sensitivity (102) and a UV/visible rejection ratio of 300. It also exhibited fast response times of τ_{rise} 200 ms and τ_{fall} 950 ms. A small modification of nitrogen incorporation in ZnO was identified that directed to a highly-sensitive self-powered visible light photo-detector with at least 1000% improvement in quality factors like photocurrent, sensitivity and response time as compared to previously reported organic-inorganic hybrid photo-detectors based on metal chalcogenides (CdSPANI or CuInSe₂P₃HT). The broadband sensitivity of such N:ZnO Spiro-MeOTAD photodiode enabled sensing of low intensity ($\sim 28 \mu\text{W cm}^{-2}$) ambient white light with a high photocurrent density of 120 nA cm^{-2} made it an efficient ambient white light detector.

3D micro-porous conducting carbon beehive by single step polymer carbonization

Porous carbon with high surface area was synthesized from polymer salt that showed excellent performance as supercapacitor electrode. The presence of the alkali metal in the selected polymer precursor resulted in a high specific surface area of $1327 \text{ m}^2 \text{ g}^{-1}$. Micropores with pore size ranging from 12 nm contributed 80% of the pore volume along with small fraction of meso and macropores made it ideal to use as an electrode for supercapacitors. The supercapacitor performance of the material was tested in both aqueous and organic electrolytes. The material delivered an energy density of 31 Wh kg^{-1} at its highest power density of 11000 W kg^{-1} in a two electrode system based on active material loading.

Sub-threshold hydrogen generation and super-threshold carbon quantum dot formation:

A conducting carbon cloth was synthesized by a simple one-step pyrolysis of cellulose fabric, that showed turbo stratic microstructure and functional groups having interesting consequences for water splitting and hydrogen generation in the alkaline electrolysis process. This work twisted the carbon-assisted electrolysis. The active sites in the carbon cloth allowed the slow oxidation of its surface during the electrolysis that transformed the surface groups from C-OH to COOH and at a voltage as low as 0.2 V in a two-electrode system along with

Publications: Nanoscale, 2014, 6, 503; Energ. Environ. Sci., 2014, 7, 728; ChemSusChem, 2014, 7, 883; Phys. Chem. Chem. Phys., 2014, 16, 4251; Electrochim. Acta, 2014, 123, 248

platinum as the cathode, instead of 1.23V (plus overpotential) which was required for platinum, steel, or even graphite anodes. Sub-threshold hydrogen evolved was $24 \text{ mL cm}^{-2} \text{ h}^{-1}$ at 1 V, at a super-threshold potential ($> 1.23 \text{ V} + \text{overpotential}$) led to remarkable phenomenon. At such conditions rapid exfoliation of the tiny nanoscale (57 nm) units of carbon quantum dots (CQDs) was reported in copious amounts due to an enhanced oxidation rate. The CQDs showed bright-blue fluorescence under UV light.

Heteroatom-doped carbon electro-catalyst for oxygen reduction reaction by pyrolysis of protein-rich pulse flour:

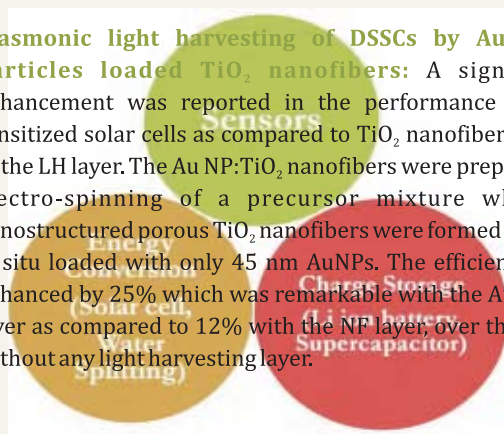
A nitrogen-doped hierarchically porous carbon-based efficient ORR electrocatalyst was developed from protein-rich pulses. The process involved 3D silica nanoparticles templating of the pulses flour followed by its double pyrolysis. The N-doped porous carbon generated exhibited remarkable electrocatalytic activity towards ORR in the alkaline medium. The oxygen reduction on this material followed the desired 4-electron transfer mechanism involving the direct reduction pathway. The synthesized carbon catalyst also showed good electrochemical stability and fuel tolerance.

Carbon cloth as a permeable and flexible counter electrode:

Electronically and catalytically functional carbon cloth obtained by one-step pyrolysis of cellulose fabric competed favorably with the commonly employed expensive platinum or FTO system as a counter electrode for dye sensitized solar cell (DSSC). High efficiency of 5.8% was achieved using such cloth as a counter electrode as against 7% with the conventional Pt/FTO system. The permeable property of the cloth eliminated a complete step of drilling hard TCO substrates for final dispensing of electrolyte into the device and the sealing process was also facile. The flexibility of the carbon cloth adapted easily to be flexible and wearable DSSC designs.

Plasmonic light harvesting of DSSCs by Au-nanoparticles loaded TiO₂ nanofibers:

A significant enhancement was reported in the performance of dye sensitized solar cells as compared to TiO₂ nanofibers (NFs) as the LH layer. The Au NP:TiO₂ nanofibers were prepared by electro-spinning of a precursor mixture whereby nanostructured porous TiO₂ nanofibers were formed and got in situ loaded with only 45 nm AuNPs. The efficiency was enhanced by 25% which was remarkable with the AuNF LH layer as compared to 12% with the NF layer, over the value without any light harvesting layer.



Surface Science

Chemical bonding information from APPES

The material changes from one form to another form and the oxidation of copper metal surfaces to copper oxides were explored in a systematic manner. It was carried out with the valence bond electrons up to 1 mbar pressures that gave the chemical bonding information. It gave the opportunity to map out the changes from copper metal to copper oxides through a series of intriguing observations. Metallic features at Fermi level disappeared along with narrow Cu 3d band at 3 eV and O 2p band appeared at 6 eV on oxygen exposure at 0.3 mbar and 500 K. On further heating to 625 K at 0.8 mbar oxygen, typical features of cupric oxide were observed with an energy overlap of Cu 3d and O 2p bands energy appeared close and hence large overlap occurred. It was expected that the method can be extended to explore the evolution of any material from its parent component and this technique would be helpful to find out the active phase of the materials that catalyses reactions.

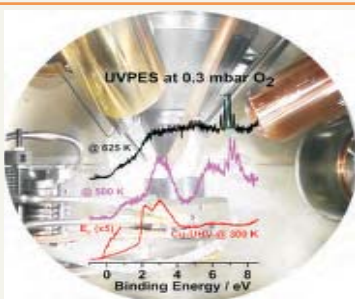


Fig. 1: Gradual oxidation of copper metal surface (red trace) to cuprous (pink trace) and cupric oxide (black trace) at 500 and 625 K at 0.3 mbar oxygen

Shifting the rigid confines of catalysis regime towards ambient conditions

An attempt was done to make changes in the confines of the catalysts in action. The surface modification of palladium was undergone by diffusing oxygen into its sub-surfaces and marginal oxidation was also done. A minor change in electron transfer capability by oxidizing the Pd-surface was expected to change the catalysis regime. Nitric oxide reduction reactions were explored with hydrogen as reductant in the presence of oxygen was explored. Catalysis studies with molecular beam instrument demonstrated a shift in NO reduction catalysis towards ambient temperatures, compared to unmodified Pd surfaces (Fig. 2). The influence of marginal oxidation was also confirmed by APPES at different partial pressures of oxygen.

Publications: Anal. Chem., 2014, 86, 3683; ChemCatChem, 2014, 6, 531; RSC Adv., 2014, 4, 10261; ACS Appl. Mater. Inter., 2014, 6,



Fig. 2: Rate of nitrogen formation for virgin and modified Pd-surfaces and the shift in NO reduction catalysis

Unravelling the structure sensitivity of reactions using morphology controlled nanoparticle surfaces

The objective was to bridge the pressure-gap between the actual working condition of materials and the ultra-high vacuum conditions employed in surface science. Ambient pressure photoelectron spectrometer (APPEs) brought down the pressure-gap from thirteen to two-three orders of magnitude. Specially designed materials were prepared and tested for environmental reactions. There is a consensus that the optimum size for gold to be catalytically active is approx 5 nm, beyond which the catalyst activity is negligible. Trisoctahedral Au nanoparticles with size ranging from 45 to 100 nm carrying several {310} defect sites were found fairly active for CO oxidation and benzyl alcohol oxidation proving the structure sensitivity and size insensitivity for the reaction.



Fig. 3: Trisoctahedral gold nanoparticles (110 nm) carrying {310} defects

RESOURCE

CENTERS



Catalyst Pilot Plant		102
Center for Materials Characterization		102
National Collection of Industrial Microorganisms		102
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Digital Information and Knowledge Resource Center		102

Catalyst Pilot Plant: Catalyst Pilot Plant (CPP) aims to translate the processes for the preparation of the solid catalysts, adsorbents, supports and the catalytic batch processes from the laboratory scale to pilot plant scale to pilot plant scale. CPP is equipped with the facilities for scale-up studies at different scale of operations. It houses the fixed bed reactors for the performance evaluation of the catalysts on laboratory scale in various reactions of academic and industrial importance like petrochemicals and petroleum reactions, reactions involving value addition to renewable feedstock such as alternative fuels and chemicals. It is also supported by an array of physico-chemical characterization facilities.

Center for Materials Characterization: Center for Materials Characterization (CMC) is equipped with various instruments such as X-ray diffractometer, Scanning electron microscope, Environmental scanning electron microscope, High resolution transmission electron microscope, Transmission electron microscope, Electron spectroscopy, Mass spectrometer etc. which are used for R & D projects of the Laboratory. During the year, more than eighteen thousand samples were analysed out of which 218 samples were from outside CSIR-NCL. It generated the ECF more than 39 Lakhs.

National Collection of Industrial Microorganisms: NCIM is dedicated to the isolation, identification, collection, preservation and distribution of authentic microbial strains of industrial and biotechnological applications.

Summary of the highlights during the year:

- ECF generation of ₹ 144 lakhs
- Around 300 microbial strains were lyophilized for long-term preservation
- 75 Microbial strains were received for deposit and 25 Samples were authenticated using molecular methods
- DNA extraction, PCR amplification, and sequencing protocols for bacteria, fungi, yeast and algae were optimized and implemented
- Sequenced 150 in-house samples as a part of sequencing services
- Authenticated 200 strains of NCIM by sequencing and analysis
- 4th Edition of NCIM Catalogue of strains was published in the form of hard copy and online version with updated deposit forms, and sequencing forms

Central NMR Facility: Central NMR facility provides NMR support to the scientific activities of the laboratory. The scientists associated with it also carry out research activities on application of solid state and solution state NMR spectroscopy in different areas of chemical, biological and materials sciences. The center maintains and operates NMR spectrometers at 200, 300, 400, 500 and 700 MHz and a JEOL ECX 400 spectrometer. Recently, a new 700 MHz spectrometer was equipped with accessories capable for solution state and solid state NMR research activities. The center plays an integral part in the basic and applied research activities of the laboratory and renders the technical support.

About 40000 samples were analyzed using this facility. It included 400 samples from industry, other R&D and academic institutes that generated the ECF of ₹ 43.2 lakhs.

Digital Information and Knowledge Resource Center: Digital Information and Knowledge Resource Centre (DIKRC) includes Network Administration Unit and the Knowledge Resource Centre.

Network Administration Unit provides the essential IT services to the lab that involve planning, installation, operation, enhancement, and maintenance of IT infrastructure of the lab. The unit takes care of MS Exchange 2010 server based E-mailing system for more than 1800 E-mail users and anti-spamming solution is also maintained. The unit has deployed a security UTM product and the IP based Surveillance system.

Knowledge Resource Centre manages the both archival print resources and contemporary digital resources. It has subscribed to various print & E resources to fulfill the objective of providing critical information support. KRC has a collection of 1.43 lakh documents including books and bound volumes of journals. During the year 140 books were purchased and access to major publisher's online journals was available through CSIR-NISCAIR consortium project. Theses were submitted by research students and the links were provided on intranet to the awarded theses. Access to various online journals was made available. During the year 57 students, 7 corporate members and 66 casual visitors availed the services of library.

S & T SUPPORT SERVICES



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Business Development

Business Development Division (BDD) plays a technology facilitation role through discussions related to research discussions related to research proposals, business negotiation, research valuation, IP ownership and contracts management of all research projects performed in CSIR-NCL,

right from its inception to its conclusion. MIS is also responsible for the budgeting of the laboratory. IT group of BDD is responsible for the development, operation and management of various IT applications.

Instrumentation and Communication

Wireless Instrumentation

The LabVIEW Real Time (RT) based development was done for 1000 Hz frequency wireless communication. It was also tested for 1000 Hz wireless transmission and reception using Zigbee protocols total system comprises of cRIO, cDAQ and adds on "C" modules for data acquisition and control, serial modules for wireless communication. Wi-Fi development was completed using MOXA and tested for more than 200 meters in laboratory area. Development of wireless control of PMDC Motors, through variable speed drives was completed with ARM7 embedded platform and LabVIEW platform. Zigbee protocols were used as wireless communication. These prototype developments were carried out for Indus Magic project.

Communication System: SIP Implementation

Session Initiation Protocol (SIP) was implemented for SIP telephones by using Alcatel Omni PCX Enterprise Communication System. Instrumentation and Communication Unit expertise was used to develop the embedded systems, embedded ethernet, embedded web browser, IP protocols, Wireless instrumentation using Zigbee, Bluetooth and Wi Fi protocols. Interfacing with Network for SIP hard phone implementation is aimed at different places in the laboratory area.

Lab Safety Management

Safety awareness and orientation courses were conducted throughout the year at least once a month. The course involved the lectures, video shows and discussions. A total of 635 students, project assistants and trainees attended the course work for the new batch. Training for emergency response was organized for all staff and students that included fire safety demonstrations and training. The hazardous waste generated in the lab was disposed off as per the standard procedures and guidelines of Maharashtra

Pollution Control Board. Approximately 50KL of waste solvents were disposed off during the year. The laboratory infrastructure was strengthened with the provision of antidotes for toxic and corrosive chemicals, fire safety cabinets. The number of accidents and incidents reported were reduced considerably, in view of the enhanced awareness and compliance as well as institutional support for up gradation of facilities.

Research Planning and Audit

Research Planning and Audit unit plans and reviews the project. It coordinates Research Council (RC) meetings. It also deals with the committee to disburse funds to scientists to attend conferences abroad. The unit organizes the task force review meetings. The progress for all on-going projects including the start-up grants and other related projects was reviewed twice a year. Two RC meetings were held during the year. The unit takes care of agenda document containing

Director's presentation and report, key presentations from other staff, reports of major projects, and other reporting items. The data of various projects was pooled together and analyzed for its output and outcomes which was presented to the RC. The unit interacted and provided detailed supporting information to different audit teams. The questions from Parliament and certain queries under RTI were responded by the unit.

Publication and Science Communication

Publication and Science Communication (PSC) Unit establishes communication between the laboratory and its stakeholders. It uses the facilities like web, print, electronic and social media. It manages the video conference facility, external and internal websites; prepares annual reports and brochures. The unit communicates the impact making work from the laboratory in the form of R&D features, prepares

and issues press releases and also prepares videos for its stakeholders. It supports to organize conferences and manages CSIR-NCL publication database. It participates in exhibitions and manages the institutional repository and open access. It organizes the press conferences with scientists for reporters.

Engineering Services

Engineering Services Unit carries activities that support the laboratory in various engineering aspects like Civil, Mechanical and Electrical. The unit fabricates the glass wares at the Glass Blowing Section as per the needs. Besides it takes care of staff quarters, guest house, community center, student's hostels, workshop, NCL Innovation Park etc.

Some of the major works carried out by the unit during the year were the extension of first floor of MBL in Biochemical

Engineering Division, remodeling of internal space for INDUS MAGIC in PP-III, construction of building for OSDD outreach center and MSM project, extension of first floor for Polymer Processing Center, procurement and installation of lab furniture and fume hoods, repairs of old scientist apartments and renovation of various quarters in NCL colony and main aerial power supply conversion into underground for staff quarters.

No.	Work Category	Percentage
1.	Lab and colony renovations	20
2.	Electrical renovations and distribution	10
3.	12th Five Year Plan works	40
4.	Setup for Scientific work	10
5.	Creation of Hostel accommodation	20

Human Resource Management

Project Training: More than 480 intern students pursuing the courses such as M.Sc., M.Pharm., B.E., M.E., B.Tech., M.Tech. at various colleges, universities and Indian institutes including IITs, IISERs, and NITs as well as foreign institutes completed their Summer/Winter Projects at CSIR-NCL.

Guest workers: Eighty three guest-workers worked at CSIR-NCL including fellows of various Indian Sciences and Engineering Academies. Three students from abroad were also trained.

Institutional visits: The Unit coordinated twenty institutional visits mainly of students pursuing professional courses in chemical sciences, medical sciences, agricultural sciences, engineering sciences, besides basic and applied sciences from postgraduate colleges located across the India.

CSIR-UGC NET Examination: The tests were conducted at Pune Centre on June 23, 2013 and Dec 22, 2013 for 20185 and 21423 registered candidates, respectively.

वित्त एवं लेखा

1.	निधि की उपयोगिता	
	सीएसआईआर अनुदान राशि	
	परियोजनाएँ	(रु. लाख में)
	नेटवर्क (सी/एफ सहित)	4114.286
	गैर नेटवर्क	10607.094
	NMITLI परियोजनाएं	396.545
	ईएमआर एवं वैज्ञानिक पूल	961.264
	प्रयोगशाला आरक्षित निधि	1127.709
	बाहरी वित्तपोषित परियोजनाएँ	1906.720
	विविध जमा राशि	102.569
	बाहरी निकायों की ओर से भुगतान	354.603
	प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	79.292
	कुल	19650.082
2.	प्रयोगशाला आरक्षित निधि का अर्जन	(रु. लाख में)
	वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर के अलावा) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	256.915
	अन्य लेखाशीर्षों से	432.214
	कुल	689.129
3.	31.3.2014 को अतिरिक्त निधि का निवेश (रु. लाख में)	801.000
4.	आपत्ति—पुस्तिका मदों का निपटारा	
	वर्ष के दौरान किए गए समायोजन	(रु. लाख में)
	निजी	3974.875
	यात्रा भत्ता/छुट्टी यात्रा खर्चा (एलटीसी)	74.354
	स्थानीय	110.265
	कुल	4159.494
	कुल मदें	664
5.	निम्न लिखित प्रकार के वाउचर तैयार किए गए	
	भुगतान	17554
	प्राप्त राशि	4522
	टी.ई.	188
	कुल	22264
6.	निपटान किए गए लेखा—परीक्षा अनुच्छेद (19 लेखा—परीक्षा अनुच्छेदों में से)	13
7.	बैंक समाधान विवरण	(रु. लाख में)
	समायोजित की गई राशि	17996.727
	मदों की संख्या	4008

अगस्त 22-23, 2013 के दौरान वित्त अधिकारियों की ईआरपी सभा आयोजित की गई।

Finance and Accounts

1.	Funds Utilization	
	CSIR Grant	
	Projects	(₹ in lakh)
	Network (including C/F)	4114.286
	Non – network	10607.094
	NMITLI Projects	396.545
	EMR & Scientist Pool	961.264
	Laboratory Reserve	1127.709
	Externally Funded Projects	1906.720
	Misc. Deposits	102.569
	Payment on behalf of outside bodies	354.603
	Deposits for Sponsored conf. / seminars	79.292
	Total	19650.082
2.	Generation of Lab Reserve	(₹ in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	256.915
	From other heads	432.214
	Total	689.129
3.	Investment of surplus funds as on 31.3.2014 (Rs. in lakh)	801.000
4.	Clearance of OB items	
	Adj. made during the year	(₹ in lakh)
	Private	3974.875
	TA/LTC	74.354
	Local	110.265
	Total	4159.494
	No. of items	664
5.	Following types of vouchers were generated	
	Payment	17554
	Receipt	4522
	TE	188
	Total	22264
6.	Audit Paras Settled (out of 19 Audit paras)	13 Nos.
7.	Bank Reconciliation	(₹ in lakh)
	Amount adjusted	17996.727
	No. of items	4008

भंडार एवं क्रय

(वस्तुओं के निपटान के फलस्वरूप प्राप्त राशि नहीं दी गई है)

संपादित किए गए कार्य/गतिविधियों के संख्यात्मक संकेतक

मद	संख्या		मूल्य (रु. करोड़ में)	
	2012-13	2013-14	2012-13	2013-14
कुल प्राप्त एवं निष्पादित मांगपत्र	1519	1207	64.22	44.50
कुल दिए गए ऑर्डर (आयातित)	290	190	34.42	16.16
कुल दिए गए ऑर्डर (स्वदेशी)	1133	950	22.31	20.71
कुल प्राप्त सामग्री (आयातित)	362	240	35.18	36.00
कुल प्राप्त सामग्री (स्वदेशी)	1952	870	14.74	57.88
ऑनलाइन मांगपत्र	1516	1033	1.68	1.29
स्थानीय खरीद (ऑनलाइन आर सी सहित)	8980	7841	13.89	17.15
भंडार से जारी की गई कुल सामग्री	6096	16771	3.08	9.31
वित्तीय वर्ष 2012-13 में समायोजित बकाया शेष			26.71	45.53
वित्तीय वर्ष 2011-12 में सीमा शुल्क से छूट प्राप्त राशि का उपयोग			24.89	34.66
वित्तीय वर्ष 2011-12 में उत्पाद शुल्क से छूट प्राप्त राशि का उपयोग			6.15	2.63

खरीदे गए प्रमुख उपकरण/अन्य वस्तुएं

क्र. सं.	मदें	मूल्य (रु. लाख में)
1	ग्लोव बॉक्स वर्क स्टेशन	58.45
2	एप्लाइड बायोसिस्टम्स 3500 गस जेनेटिक एनालाइजर	101.00
3	पावडर एक्सरे डिफ्रेक्टोमीटर	116.25
4	प्रोटीन प्यूरीफिकेशन वर्क फ्लो	41.00
5	जीसी-एचआरएमएस	209.00
6	एआरआईएस-जी 2 रोटेशनल रियोमीटर	137.00
7	स्पेक्ट्रोफ्लोरोमीटर एनआईआर डिटेक्शन रेंज सहित	39.40
8	नाइट्रोजन सेपरेटर, स्क्रोल टाइप एयर कूल्ड ऑइल फ्री साइलेंट एयर कंप्रेसर फॉर ड्राइविंग एनएमआर, एयर ड्रायर एवं एसेसरीज	66.65
9	मोड्यूलर एफपीएलसी : एनजीसी क्वेस्ट प्लस 10 क्रोमेटोग्राफी प्रणाली	39.35
10	मिनीप्लेक्स 600 डेस्कटॉप एक्सरे डिफ्रेक्टोमीटर	32.61
11	हाई कंटेंट स्क्रीनिंग सिस्टम	220.00
12	जीसीएमएस एवं एलसीएमएस प्रणाली	89.50
13	एचपीएलसी प्रणाली	35.00
14	एफटीआईआर स्पेक्ट्रोमीटर	32.00
	कुल	1217.21

Stores and Purchase

Numerical indicators of work/activities completed

Item	Numbers		Value (₹ in Crores)	
	2012-13	2013-14	2012-13	2013-14
Total Indents received and Processed	1519	1207	64.22	44.50
Total orders placed(imported)	290	190	34.42	16.16
Total order placed (indigenous)	1133	950	22.31	20.71
Total consignments received(Imported)	362	240	35.18	36.00
Total consignments received(indigenous)	1952	870	14.74	57.88
On-line indents	1516	1033	1.68	1.29
Local Purchases (Including on-line RC)	8980	7841	13.89	17.15
Total Stores Issues	6096	16771	3.08	9.31
Outstanding balance adjusted during the financial year 2012-13			26.71	45.53
Utilization of Custom Duty Exemption during Financial year 2011-12			24.89	34.66
Utilization of Excise Duty Exemption during financial year 2011-12			6.15	2.63

Major Equipments other items procured/processed

Sr. No	Item Name	Value (₹ in Lakhs)
1	Glove Box Work Station	58.45
2	Applied Biosystems 3500xl Genetic Analyzer	101.00
3	Powder X-Ray Diffractometer	116.25
4	Protein Purification Work Flow	41.00
5	GC-HRMS	209.00
6	ARES-G2 Rotational Rheometer	137.00
7	Spectrofluorimeter With NIR Detection Range	39.40
8	Nitrogen Separator, Scroll type Air Cooled Oil Free Silent Air Compressor for Driving NMR, Air Dryer and Accessories	66.65
9	Modular FPLC : NGC Quest Plus 10 Chromatography system	39.35
10	Miniflex 600 Desktop X-Ray Diffractometer	32.61
11	High Content Screening System	220.00
12	GCMS & LCMS System	89.50
13	HPLC System	35.00
14	FTIR Spectrometer	32.00
	TOTAL	1217.21

ANNEXURES



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Annual Report 2013-14 Patents Granted: Foreign

Title	Inventor(s)	Grant No.	Country/ Region
Transesterification Catalyst Process For Preparation Thereof And A Process For Transesterification Using The Catalyst	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	10-1366063	KR
Process For Producing Hydrocarbon Fuel	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	10-1320413	KR
Anti Tubercular Agents	C Mitra; Dhiman Sarkar; Sampa Sarkar; Rohit Ramesh Joshi; Vijay Murlidhar Khedkar; Raghuvir Ramakant Pissurlenkar; Evans Clifton Coutinho; Anamik Kantilal Shah	2012/09026	ZA
A Process For Fractionating Sugarcane Bagasse Into High Alpha-Cellulose Pulp, Xylan And Lignin	Anjanikumar Jyotiprasad Varma	ZL200880111416.3	CN
		8529731 B2	US
Process For Producing Fatty Acids	Srinivas Darbha; Jitendra Kumar Satyarthi; Raja Thirumalaiswamy; Shilpa Shirish Deshpande	ZL201080042209.4	CN
		2464714	DE, FR, EP, GB, ES
Process For Recovery Of Highly Pure Acrylonitrile	Purushottam B P; Madhukar G S; William S R; Yashwant G M; Narayan J C	1611087	BE, EP, FR, GB, IT, NL
A Process For The Preparation Of Highly Pure (-)-Methyl Lactate	Barve Prashant Purushottam; Kulkarni Bhaskar Dattatreya; Nene Sanjay Narayan; Shinde Ravindra William; Gupte Milind Y	1910266	BE, DE, EP, GB, NL
A Process For The Preparation Of Copolymer - 1 (Cop-I), Composed Of L-Alanine, L-Lysine, L-Glutamic Acid And L-Tyrosine-Drug For The Treatment Of Multiple Sclerosis	Garnaik Baijaya ntimala	2438080	DE, EP, GB, SE
Continuous Flow Process For The Preparation Of Sulphoxide Compounds	Amol Arvind Kulkarni; Ramesh Anna Joshi; Rohini Ramesh Joshi; Nayana Tushar Nivangune, ; Manisha Abhiman Jagtap	2451810/ B1	DE, EP, ES, FR, GB, IT
Titanium Gel Composition For The Removal Of Organic Dyes And Other Organic Contaminants From Aqueous Solution	Mohan Kerba Dongare; Shubhangi Bhalchandra Umbarkar	2459282	DE, EP, ES, GB, PL, SE
Accelerated Gelation Of Regenerated Fibroin	Shailesh Prakash Nagarkar; Ashish Kishore Lele	2459650	DE, EP, ES, FR, GB, IT
Novel Processes For The Preparation Of Pure Methyl Lactate From Alkali Metal Lactate Using Carbon Dioxide And Methanol	Prashant Purushottam Barve; Bhaskar Dattatraya Kulkarni; Milind Yashwant Gupte; Sanjay Narayan Nene; Ravindra William Shinde	2470494 B1	DE, EP, ES, FR, NL
Method For The Preparation Of Biofuels From Glycerol	Dharbha Srinivas; Lakshmi Saikia; Paul Ratnasamy	2478091	RU
		2008352536 B2	AU

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Patents Granted: Foreign

Title	Inventor(s)	Grant No.	Country/Region
Taste Masked Pharmaceutical Compositions Comprising A Ph Sensitive Polymer Providing Enhanced Bioavailability Of Polymorphic Bitter Drugs	Mohan Gopalkrishna Kulkarni; Anupa Ramesh Menjoge	2549539	CA
Water-Soluble Macromonomers Containing Terminal Unsaturation And The Process For Preparation Thereof	Kulkarni Mohan Gopalakrishna; Patil Prerana Maruti	5388841	JP
Sulfonic Acid Functionalized SWCNTS, A Key To Increase The Conductivity Of Nafion Membranes For PEMFCS Applications	Vijayamohanan K Pillai; R Kannan; Bhalchandra A Kakade	5398744	JP
		8399149	US
A Shortest Process For The Enantioselective Synthesis Of (S)-N-(5-Chlorothiophene-2-Sulphonyl)-B,B-Diethylalanol (7.B.2) A Drug On Alzheimer's Disease (Ad)	Varun Rawat; Pandurang V Chouthaiwale; Gurunath Suryavanshi; Arumugam Sudalai; Vilas Bhiku Chavan	8440844	US
A Process For Fractionating Sugarcane Bagasse Into High Alpha-Cellulose Pulp, Xylan And Lignin	Anjanikumar Jyotiprasad Varma	8529731 B2	US
Aziridination Of Olefins	Pratibha Uttam Karbal; Pandurang Vilasrao; Tanveer Mahamadali; Gurunath Mallappa Suryavanshi; Arumugam Sudalai; Gurunath Suryavanshi	8558010 B2	US
A Novel Dicarboxylic Initiator And Its Application For The Synthesis Of Alpha, Gamma Difunctional Polydienes, Polystyrenes And SBS Or Sis Triblock Copolymers In Non-Polar Solvent Without Additives	Suvarnapathaki Rupali Kedar; Kulkarni Mohan Gopal Krishna; Gnanou Vyes; Matmour Rachid; More Arvind Sudhakar; Wadgaonkar Prakash Purushottam	2007219101	AU
Method For The Preparation Of Biofuels From Glycerol	Dharbha Srinivas; Lakshmi Saikia; Paul Ratnasamy	2008352536 B2	AU

Annual Report 2013-14 Patents Granted: Indian

Title	Inventor(s)	Grant No.
Novel Dicarbanic Initiator, A Process For The Preparation And Use Thereof	Gnanou Vyes; Matmour Rachid; More Arvind Sudhakar; Wadgaonkar Prakash Purushottam	254971
Thieno[2 3 - D] - Pyrimidine-4 (3H) – One Compounds With Antifungal Properties And Process Thereof	Borate Hanumant Bapurao; Maujan Suleman Riyajsaheb; Sawargave Sangmeshwer Prabhakar; Joshi Shreerang Vidhyadhar; Vaiude Sharangi; Chandavarkar Mohan Anand	255029
A Process For The Production Of Dialkyl Carbonates	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	255654
A Process For The Preparation Of Polymeric Composition Useful For The Conversion Of Esters And Amides To Corresponding Alcohols And Amines	Mashelkar R. A.; Kulkarni M. G.; Karmalkar R. N.	255713
Pharmaceutical Composition For Improving Palatability Of Drugs And Process For Preparation Thereof	Anupa Ramesh Menjoge; Mohan Gopalkrishna Kulkarni	256010
An Improved Process For The Production Of Phenyl Ketones	Chidambaram M.; Venkatesan C.; Singh A. P.; Ramaswamy A. V.	256055
High Selectivity Process For The Preparation Of Diphenyl Oxalate	Umbarkar Shubhangi Bhalchandra; Biradar Ankush Venkatrao; Dongare Mohan Keraba	256642
A Novel Oligomeric Lactide Macromer Based Copolymer And Process For The Preparation Thereof	Suvarnapathaki Rupali Kedar; Kulkarni Mohan Gopalkrishna	256915
Polymer Exfoliated Phyllosilicate Nanocomposite Compositions And A Process For The Preparation Thereof	Shroff Rama Mallikarjuna; Swaminathan Sivaram	257549
An Improved Process For The Liquid Phase Oxidation Of Toluene To Benzaldehyde	Chaudhari Raghunath Vitthal; Rajurkar Kalpendra Baburao; Tonde Sunil Sopana; Rane Vilas Hari	257910

University of Pune

Author	Title	Guide
Adate P.	Novel organocatalytic asymmetric approach towards prismatic Iridoid class of terpenes	Pandey G.
Barvkar V. T.	Genomics and proteomics approaches to study flax seed	Gupta V. S.
Beena K. B.	Carbon nanofiber based Hybrid materials for PEMFC applications	Kurungot S.
Bhattacharya S.	Study of Response Properties using Coupled cluster Method	Pal S.
Bhise A. D.	Studies directed towards the synthesis of naturally occurring lactones, amino alcohols and polyols	Pradeep Kumar
Bhogeswararao S.	Selective Hydrogenation of alpha, Beta- Unsaturated Aldehydes and Biomass Products over Supported Noble Metal Catalyst	Srinivas D.
Bhongale S. S.	Analytical Methodologies for the Estimation of Polymer Precursors	Ponrathnam S.
Bhure M. H.	Synthetic Studies towards 1-Deoxythionojirimycin, 1,4-anhydro-4-thio-D-Arabinol and related thiosugars and development of ionic liquid mediated organic transformations	Daniel T.
Biswal M.	Novel synthesis and applications of functional carbon, transition metal oxides and their Nanocomposites	Rode C. V. & Ogale S. B.
Cherian S. K.	Synthetic strategies towards (+) -L-733060, Bruguiers and Natural synthetic lactones and DDQ mediated Deprotection	Pradeep Kumar
Chowdhury P. S.	Studies directed towards enantioselective total synthesis of some naturally occurring Lactones and Hydrolytic Kinetic Resolutions (HKR) of terminal Mono and Bis-Epoxides	Pradeep Kumar
Darbha V. R. K.	Evaluation of batch processes for continuous flow synthesis of metal & metal oxide nanomaterials	Prasad B. L. V.
Deo M. S.	Quasi 1 D metal oxide Nanostructures for Electronic and Opto-Electronic Applications	Jog J. P.
Deore P. S.	Selective carbon-carbon bond forming reactions with maleic anhydrides and maleimides: facile synthesis of bioactive natural and unnatural products	Argade N. P.
Deshpande S. H.	Synthesis of Chiral Ligands and their applications to asymmetric hydrogenation using transition metal complexes	Kelkar A. A.
Dey D.	Exploiting Chiral 7-Azabicyclo[2.2.1] Heptane Skeleton as a Template for the Stereoselective synthesis of Biologically active Alkaloids	Pandey G.
Dixit M.	Ab-Initio and DFT Investigations of Hydrogen Storage	Pal S.
Dumare N.	Synthetic studies towards Mitralactonine, Pipecolic acid and Piperidine alkaloids	Chavan S. P.
Dushing M. P.	Target cum Flexibility : towards the synthesis of Spirocyclic Nucleosides, Carbapenems and Tri-/Tetracyclic Tetrahydroisoquinoline Alkaloids	Ramana C. V.

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Ph.D. Theses

Author	Title	Guide
Erande N.	Novel chemical modifications in NonGenetic nucleic acids for selective targeting of DNA or RNA	Vaijayanti Kumar
Ganai A. K.	Synthesis functionalization and catalytic applications of Silica, mesoporous Silica Nanoparticles adn their 3-D Scaffolds.	Prasad B. L. V.
Garai S.	Synthetic Studies Towards Heritol,(-)-Venlafaxine, 7-Deoxypancratistatin and Development of Important Synthetic Methodologies.	Chavan S. P.
Gnanakumar S. E.	Synthesis and molecular properties of new MgCl ₂ based molecular adducts towards catalytic polyolefin production	C. S. Gopinath
Gokhale S. A.	Mathematical modeling of gene expression system in Eukaryotes: form gene induction to protein synthesis	Gadgil C.
Gunjal A. D.	Synthesis and biophysical studies of 2'-5' isoDNA analogies locked in N-type or S-type sugar ring conformations	Vaijayanti Kumar
Gupta J.	Intermediate Hamiltonian Fock Space molecular response properties	Pal S.
Gupta N.	Molecular studies on withanolides Biosynthetic pathway Gene (s) (Squalene synthase) from Withania Somnifera	Khan B. M.
Gupta N. R.	Design and Synthesis of Novel Associating Polymers	Badiger M. V.
Harbindu A.	Studies Directed Towards the Synthesis of Naturally Occurring Spiroacetals, Lactones and Biologically active [1,2,4]triazino derivatives	Pradeep Kumar
Hengne A. M.	Catalytic transformations of bio-derived Cs/C6 platform molecules to monomers and fuel additives	Rode C. V.
Inamdar S. M.	Asymmetric Synthesis Towards Bioactive Molecules: Linezolid, Eperezolid, Moprolol, Toliprolol, Bunitrolol Via Nitroaldol Reaction and Organic Transformations Over Copper Fluorapatite	Mulla S. A. R.
Jha A.	Development of Heterogeneous Catalyst for Liquid Phase Hydroxy	Rode C. V.
Jha V.	Synthetic studies towards biologically active compunds containing 1,2-/1,3-aminoalcohols and 1,3-diamines employing asymmetric dihydroxylation and proline catalysed reactions	Pradeep Kumar
Joshi-Navare K.	Biosynthesis of novel glycolipids: basic and applied aspects	Prabhune A.
Kale S. S.	Hybrid Strategy In Structural Design: Generation Of Conformationally Ordered Ant-Pro Oligomers, Tubulin Binding Agents And Hydroxyethylamine Isosteres.	Sanjayan G. J.
Kaur T.	Synthesis of antibacterial Natural Products: Primin, Centrolobine, Oenostacin and Studies on the synthesis of Alpha-aminophosphonates and Metallopnas	Ganesh K. N & Bhattacharya A. K.
Kayastha A. K.	Armed disarmed effect for oligosaccharide synthesis via gold catalyzed alkyne activation	Hotha S.

Author	Title	Guide
Khandelwal H. B.	Production, purification and characterization of fungal alkaline protease and its applications	Laxman R. S.
Kolet S. P.	Microbial Hydroxylation of Steroids: Characterization of Steroid Hydroxylase	Thulasiram H. V.
Kotbagi T. V. K.	Synthesis of Fine Chemicals From Renewables Using Supported Metal Oxides as Catalysts	Dongare M. K. & Umbarkar S. B.
Kotikam V.	Synthesis and evaluation of designed (S)-Polycarbamate Nucleic acids, Erythrulose- based- and 2'- Functionalized-Oligonucleotide Analogs for RNA targeting	Vaijayanti Kumar
Kumar A.	Synthesis, Characterization and Catalytic Applications of Transition Metal Incorporated Mesoporous SBA Molecular Sieves	Srinivas D.
Kumar K.	Fluorescence as a probe to study self-organization in methacrylate polymers and the design of Novel Hierarchical architectures	Asha S. K.
Kumari S.	Designing of Chitosan and metal/metal oxide nanoparticle based nanocomposites for tissue engineering and drug delivery applications	Singh R. P.
Kumari S.	High performance polymers: synthesis, characterization and chemical modifications	Wadgaonkar P. P.
Lasonkar S. P.	Synthetic studies towards D-(+)- Biotin, Olapatadine, alpha-Cuparenone and development of important synthetic methodologies	Chavan S. P.
Mandal L.	High performance photodetectors and field effect Transistors based on low temperature solution processing Routes	Jog J. P. & Ogale S. B.
Mane R. B.	Studies on Structure activity correlation in catalytic hydrogenolysis of renewable Glycerol	Rode C. V.
Mate V. R.	Solid catalysts with modified REDOX properties for developing green processes for Fragrance chemicals	Rode C. V.
Mhamane D. S.	Novel synthesis of Graphene and related Nanocomposites for Energy applications	Rode C. V. & Ogale S. B.
Mohaideen K. K.	Studies on Microstructural and Magnetostrictive Properties of Sintered Cobalt Ferrite Derived From Nanocrystalline Materials	Joy P. A.
Mujahid M.	Asymmetric synthesis of Pharmaceutically important compounds employing hydrolytic kinetic resolution strategy and development of novel chromone based derivatives as potent antitubercular agents	Muthukrishnan M. & Pradeep Kumar
Narayan R.	Development of novel methacrylic and supramolecular comb polymers of Rylenebisimides for applications in optoelectronics	Asha S. K.
Pal S.	Non-metallic approaches for C-H and C-Si bond activations	Pandey G.
Pati D.	Synthesis of Glycopolypeptides their self-assembly and its interactions with lectins	Sengupta S.

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Ph.D. Theses

Author	Title	Guide
Patil K. M.	Design, Synthesis and Evaluation of Amino- and Guanidino-Substituted Oligomers and Oligonucleotides for Better Cellular Uptake	Vaijayanti Kumar
Patil S. V.	Kinetics, simulation and scale-up of process for fermentative production of glycerol and arabitol using Hansenula Anomala	Kulkarni B. D.
Ramesh V. V. E.	Design, Synthesis and Conformational Investigations of Novel α -Hybrid Peptides and Hydroxyethylamine β , α Conformationally Restricted Isosteres	Sanjayan G. J.
Ramtenki V.	Synthesis of metal and metal oxide	Prasad B. L. V. & Ranana C. V.
Raut M. D.	Supramolecular assemblies of various cyclohexanecarboxylic acids	Pedireddi V. R.
Roshna V.	Synthetic Oligomers with Heterogeneous Backbones featuring α /beta-Conjugated building blocks	Sanjayan G. J.
Roy A.	Use of conformational control in the design of novel abiotic Oligomers, building blocks and biomedically potential Combretastatin analogs	Sanjayan G. J.
Sakala G. P.	Biophysical Studies of Aromatic β -aminoacid Tethered Heterogeneous Peptide Oligomers and Analogues of Ixorapeptides	Sanjayan G. J.
Shaikh A.	Gold-catalyzed Glycosidation for Glycoaminoacids and Glycopolypeptides.	Hotha S.
Shinde D. B.	Electrochemical synthesis and functionalization of carbon based nanomaterials	Vijayamohan K.
Singh S.	Cloning and Characterization of glycosyltransferase gene(s) (GTs) from Withania somnifera and establishment the structure function correlation of the GTs	Khan B. M.
Sonawane P. D.	Structural and Functional Studies of Cinnamoyl CoA Reductase (CCR) from Leucaena leucocephala	Khan B. M.
Sutar R. L.	Preparation and Evaluation of some chiral catalysis for aldol reactions in organic and aqueous Media	Joshi N. N.
Tayal R.	Hydrophilic Acrylics: Polymerisation Kinetics, Adsorption/Desorption Isotherms	Kulkarni B. D.
Varshney N. K.	Structural investigations of selected microbial penicillin G acylases and a protozoal N-myristoyltransferase	Suresh C. G.
Wakankar M.	Molecular studies on a lectin from Cicer arietinum L.	Gaikwad S. M.

Academy of Scientific and Innovative Research (AcSIR)

Author	Title	Guide
Banerjee T.	Optimizing the interfacial electron transfer rates in Ru(II)-, Os(II)-, Re(I)-polypyridyl based sensitizer-TiO ₂ ensembles	Das Amitava
Thushara K. S.	MgCl ₂ .nROH:new molecular adducts for the preparation of TiCl ₄ /MgCl ₂ catalyst for olefin polymerization (R=isopropyl, isobutyl, 2-butyl, tertiary butyl)	Gopinath C. S.

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Network Projects

Title	Project Leader
A multi-scale Simulation and Modeling Approach to Designing Smart Functional Materials for use in Energy, Electrochemistry and Bio-mimetics	Dr. S. Pal
Advanced Drug Delivery System	Dr. Sayam Sengupta
Affordable Cancer Therapeutics	Dr. S. P. Chavan
Biocatalysts for Industrial Applications & Greener Organic Synthesis	Dr. Thulasiram H. V.
Bioprospection of plant resources and other natural products	Dr. (Mrs.) Vidya Gupta
Catalysts for Specialty Chemicals	Dr. A. P. Singh
Catalysts for Sustainable Energy	Dr. D. Srinivas
Centre for BIOtherapeutic Molecule Discovery	Dr. Ashok Giri, Dr. G. J. Sanjayan
Centre for Surface and Interface Science Research	Dr. Gopinath C. S., Dr. Vinod C. P.
Clean Coal Technology	Dr. D. Srinivas
Creating Intellectual Property and capabilities for the development of improved security features and substrates for the Indian currency note	Dr. V. Premnath
CSIR-NCL OSDD Outreach Center	Dr. Ramana C. V.
CSIR-NCL-IGIB Joint Research Initiative: Interfacing Chemistry and Biology	Dr. Thulasiram H. V.
Development of Functional food and their formulations for potential health benefits of common man	Dr. (Mrs.) Vidya Gupta
Development of sustainable processes for edible oils with health benefits from traditional and new resources	Dr. N. Y. Kadoo
Development of Sustainable Waste Management Technologies for Chemical and Allied industries	Dr. S. P. Kamble, Dr. V. M. Bhandari
Emerging and re-emerging challenges in infectious disease: System based Drug design for infectious diseases	Dr. N. P. Argade
Encapsulated Microorganisms for Environmental Protection	Dr. R. V. Gadre
Energy Efficient Technologies	Dr. U. K. Kharul
Genome Dynamics in cellular organization, differentiation and enantiostasis	Dr. Moneesha Fernandes
Genomics and Informatics Solutions for Integrating Biology	Dr. M. Karthikeyan
Genomics of medicinal plants and agronomically important traits	Dr. Ashok Giri
Host Interactome analysis: Understanding the Role of Host molecules in Parasitic Infection	Dr. Ram Rup Sarkar
Hydrogen Energy: Overcoming materials challenges in PEMFC towards generation, separation, storage and conversion of hydrogen	Dr. U. K. Kharul
Inherently Safer Practices for Industrial Risk Reduction	Dr. M. Karthikeyan

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Network Projects

Title	Project Leader
Innovate, develop and up-scale modular, agile, intensified and continuous (Indus MAGIC) processes and plants	Dr. V. V. Ranade
Innovative solutions for Solar Energy storage	Dr. C. S. Gopinath, Dr. Manjusha Shelke
Integrated NextGen approaches in health, disease and environmental toxicity	Dr. Mahesh J. Kulkarni
Man as a Superorganism: Understanding the Human Microbiome	Dr. C. G. Suresh
Membrane and Adsorbent Technology Platform for Effective Separation of Gases and Liquid	Dr. Girish R. Desale
Metabolic profiling of human body fluids by MS and NMR	Dr. Venkat Panchagnula
Molecules to Materials to Devices	Dr. B. L. V. Prasad
Nanomaterials: Applications and impact on Safety, Health and Environment	Dr. Absar Ahmad
National Repository of Molecules	Dr. Dhiman Sarkar
Natural products as Affordable Healthcare Agents	Dr. H. V. Thulasiram
Neurodegenerative Diseases: Causes and Corrections	Dr. Mahesh J. Kulkarni
New Approaches towards Understanding of Disease Dynamics and to Accelerate Drug Discovery	Dr. Dhiman Sarkar
Non-Infringing Chemistry and Engineering for Pharmaceuticals	Dr. D. Srinivasa Reddy
Nuclear Magnetic Resonance Centre for Advanced Research	Dr. Rajamohanan P. R.
Organic reactions in generating innovative and natural scaffolds	Dr. C. V. Ramana
Plant Diversity: Studying adaptation biology and understanding/exploiting medicinally important plants for useful bioactives	Dr. (Mrs.) Vidya Gupta
Plant-Microbe and Soil Interactions	Dr. N. Y. Kadoo
Research Initiative for Low Emissions	Dr. Shubhangi Umbarkar
Screening molecules in lead exploration	Dr. Mahesh Kulkarni
Technologies and Products for Solar Energy Utilization through Networks	Dr. P. P. Wadgaonkar, Dr. Krishnamoorthy
Towards Understanding Skin Cell Homeostasis	Dr. Moneesha Fernandes
Up gradation of facilities/National Repository of molecules and National Collection of Industrial Micro Organisms Resource Center	Dr. J. M. Khire
Zero Emission Research Initiative for Solid Wastes from Leather	Dr. E. Deenadayalan

The National Chemical Laboratory Research Foundation (NCL RF) promotes excellence in Science and Technology and supports creative and innovative environment. It brings creative research, novel technologies and organizational innovations into focus and encourages the core values which CSIR-NCL considers important for the well being of the organization.

Awards and Lectures

NCL RF gives various awards on NCL Foundation Day. It organizes various lectures by distinguished personalities on the occasion of NCL Foundation Day, National Science Day

and National Technology Day and several special lectures in memory and honor of former NCL directors.

Award of merit based scholarships to the children of CSIR-NCL employees: Merit based scholarships to the children studying in IX and XII standards, of employees in group D (Non-Tech) and support staff in group I are awarded. The scholarship amount for the students who stand first is ₹4000/- and for those who stand second is ₹3500/- from each class. About fifteen scholarships are awarded every year on the occasion of CSIR Foundation Day.



Indian Customers

- Aarti Industries Ltd.
- Aceto Chem Pvt. Ltd.
- Aditya Birla Science & Tech. Co. Ltd.
- Aether Industries Ltd.
- Albert David Ltd.
- AMP Technologies
- Anupam Rasayan India Ltd.
- Asian Paints (India) Ltd.
- Battelle Science & Technology India Pvt. Ltd.
- Bayer CropScience Ltd.
- Cadbury India Ltd.
- Chemplast Sanmar Ltd.
- Clean Science & Technology Pvt. Ltd.
- CSIR-Tech Private Ltd.
- Deccan Nutraceuticals Pvt. Ltd.
- Dow Chemicals International Pvt. Ltd.
- Emcure Pharmaceuticals Ltd.
- Excel Industries Ltd.
- Galaxy Surfactants Ltd.
- GMM Pfaundler Ltd.
- Godrej Consumer Products Ltd.
- Hindustan Polyamides & Fibres Ltd.
- Kan Biosys Pvt. Ltd.
- KPIT Technologies Ltd.
- Navin Fluorine International Ltd.
- Racold Thermo Ltd.
- Rallis India Ltd.
- Reckitt Benckiser (India) Ltd.
- Reliance Industries Ltd.
- S C Johnson Products Pvt. Ltd.
- Sandoz Private Ltd.
- SeQuent Scientific Ltd.
- Shantani Proteome Analytics Pvt. Ltd.
- SRF Ltd. (Chennai)
- Syngenta India Ltd.
- Tata Chemicals Ltd.
- Technorbital Advanced Materials Pvt. Ltd.
- Torrent Pharmaceuticals Ltd.
- Transpek-Silox Industry Ltd.
- Tridiagonal Solutions Pvt. Ltd.
- Unichem Laboratories Ltd.
- United Phosphorous Ltd.

Foreign Customers

- Pfizer Ltd.
- ARKEMA FRANCE SA
- General Cable Corporation
- GlaxoSmithKline LLC
- Pfizer Ltd.
- Sherwin-Williams Company
- Solvay SA
- Solvay SolexisS.p.A.
- Solvay Speciality Polymers, Italy
- Swedish International Development Agency
- University of Liverpool

Publicly Funded Clients

- GAIL (India) Limited
- Indian Oil Corporation Ltd.
- Oil & Natural Gas Corporation Ltd.

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Dateline CSIR - NCL

06/05/2013	Prof. K. Venkataraman Memorial Lecture by Professor K. K. Balasubramanian of Sri Ramachandra University, Chennai
14/05/2013	National Technology Day Lecture by Dr. B. Gopalan, Executive Director, Orchid Pharma, Chennai
24/05/2013	Sir Shanti Swaroop Bhatnagar Distinguished Lecture on 'Celebration of Science' by Prof. C. N. R. Rao
24/07/2013- 25/07/2013	Workshop on Nanotechnology and Advanced functional Materials (NTAFM 2013)
16/09/2013	L. K. Doraiswamy Honor Lecture on 'Dynamic Modeling of Metabolic Systems : The Cybernetic Approach' by Prof. Doraiswami Ramkrishna, Purdue University, USA
23/09/2013	Symposium on 'Wonderland of Molecular Structures through the Looking-Glass of X-ray Crystallography'
26/09/2013	CSIR Foundation Day Lecture on 'Survival under starvation' by Professor Dipankar Chatterji, President, Indian Academy of Science
30/09/2013	Mini Symposium on 'Advanced Glycation - Where Chemical Biology meets Medicine'
07/10/2013- 09/10/2013	Indo Mexico Workshop on 'Biotechnology Beyond Borders'
13/12/2013 - 14/12/2013	Workshop on 'Intensification and Up-scaling of Continuous Processes'
03/01/2014	NCL Foundation Day Lecture by Prof. A. K. Sood, IISc, Bangalore on 'Driven Soft and Granular Matter'
25/01/2014	Dr. K. Anji Reddy Memorial Lecture by Prof. Goverdhan Mehta on 'A Safari in the world of Chemistry'
25/01/2014	NCL Alumni – Global Meet 2014
27/02/2014	National Science Day Lecture by Prof. Jyoti Chattopadhyaya, Uppsala University Biomedical Center, Sweden
05/03/2014	Prof. B. D. Tilak Memorial Lecture on 'Tunable Ruthenium Catalysts for Carbene Reactions, C-H Bond Functionalization as Key Steps for Green Chemistry' by Prof. Pierre H. Dixneuf, CNRS-Université de Rennes, France



Annual Report 2013-14 Awards/ Recognitions

A. J. Varma	- Lifetime Achievement Award of the Association of Carbohydrate Chemists and Technologists (ACCTI) - Professor B. D. Tilak Visiting Fellowship 2013-14 by ICT Mumbai
Akkattu Biju	Thieme Chemistry Journal Award
Amitava Das	Editorial Board member for 'RSC Advances'
Amol Kulkarni	Editor-in-Chief of the 'Journal of Flow Chemistry' as the Regional Editor for the Asia
Arvind Arbale	Member of Board of Studies in Chemistry
Ashok P. Giri	Fellow of Maharashtra Academy of Sciences
Borate Hanumant and Collaborators	Indian Drug Manufacturers Association (IDMA) Margi Memorial Best Patent Award 2012-2013
Business Development Division CSIR-NCL	CSIR Technology Award 2013
C. S. Gopinath	Dr. S. S. Deshpande National Award
C. V. Ramana	- Fellow of Indian Academy of Sciences - CRSI Bronze Medal
Darbha Srinivas	VASVIK Research Award
G. J. Sanjayan	- OPPI Scientist Award - Bhagyatara Award Punjab University, Chandigarh
Manjusha Shelke	Indo-US Research Fellowship
Neetu Singh	DBT's Innovative Young Biotechnologist Award
Pankaj Poddar	- MRSI Medal, 2014 - Fellow of Maharashtra Academy of Sciences
Pradeep Kumar	National Representative for the Chemistry and the Environment Division Committee an IUPAC Body
R. A. Mashelkar	Padma Vibhushan Award
Ram Rup Sarkar	Indo-US Research Fellowship
Satishchandra Ogale	- MRSI Special Medal - Member of the Advisory Board of Royal Society of Chemistry's international journal 'Energy & Environmental Science'
Shafeek A. R. Mulla	Fellow of Maharashtra Academy of Sciences
Sourav Pal	- Member of The International Society of Theoretical Chemical Physics (ISTCP) National Representative for India - SASTRA-CNR Rao Award - Charles A. Coulson Lecture at the Center for Computational Quantum Chemistry, University of Georgia - President of Chemical Research Society of India - Professor Sadhan Basu Memorial Lecture
Thulasiram H. V.	Fellow of Maharashtra Academy of Sciences
V. R. Patil	Best Supply Chain Management Practices in R&D Organizations

Annual Report 2013-14 Outreach Programme

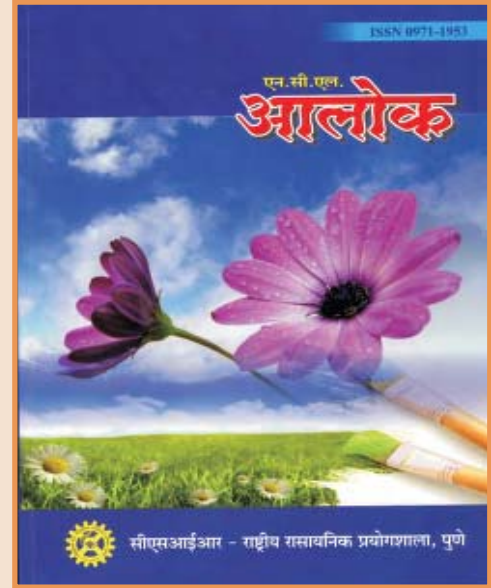
The Outreach Programme is the science activity of CSIR- National Chemical Laboratory and faculty from Indian Institute of Science, Education and Research, Pune. The objective is to boost and share the excitement of science and technology with school children. Following talks were organized during the year:

Topic	Speaker
Where Mathematics meets Biology	Dr. Leelavati Narlikar, CSIR-NCL
Why light is wonderful?	G. V. Pavan Kumar, IISER-Pune
Strange events in our Solar System	Prof. Jayant Vishnu Narlikar, IUCCA
Life in our Universe: How did it come about?	Dr. Sudha Rajamani, IISER-Pune
How computers work?	Dr. Debashree Ghosh, CSIR-NCL
Jugglology	Dr. Steven Spallone, IISER-Pune
How to experience the world beyond our senses- down to atomic level?	Dr. Pankaj Poddar, CSIR-NCL
Science of big molecules: Past, present and future	Dr. M. Jayakannan, IISER-Pune
Information transfer via vesicles in cells	Dr. Thomas Pucadyil, IISER-Pune
Introduction to the practice of inquiry through Jigsaw Puzzles	Dr. Tara Mohanan
Explosions in the Universe	Dr. Poonam Chandra, NCRA, TIFR
How to stand on giant shoulders	K. P. Madhu, IISER-Pune

भारत सरकार की राजभाषा नीति तथा राजभाषा संबंधी नियमों का अनुसरण करने की दृष्टि से सीएसआईआर— राष्ट्रीय रासायनिक प्रयोगशाला में प्रत्येक स्तर पर गहन प्रयास किए जाते हैं। सीएसआईआर—एन.सी.एल. एक वैज्ञानिक प्रयोगशाला है, जहां अधिकांश कार्य वैज्ञानिक तथा तकनीकी स्वरूप का होता है तथा शेष प्रशासनिक कार्य अधिकांशतः हिन्दी भाषा में किया जाता है। इस प्रयोगशाला में किए जा रहे राजभाषा कार्यान्वयन संबंधी उल्लेखनीय प्रयास निम्नानुसार हैं।

1. **तिमाही बैठक का आयोजन** — प्रत्येक तिमाही में प्रयोगशाला की राजभाषा कार्यान्वयन समिति की तिमाही बैठक नियमित रूप से निदेशक महोदय की अध्यक्षता में आयोजित की जाती है एवं इन बैठकों में प्रयोगशाला में राजभाषा हिन्दी के प्रगामी प्रयोग तथा राजभाषा कार्यान्वयन संबंधी प्रयासों की समीक्षा की जाती है। इन बैठकों में प्रयोगशाला के प्रत्येक प्रभाग /अनुभाग प्रमुख सदस्य के रूप में तथा नगर के हिन्दी शिक्षण योजना की सहायक निदेशक बाहरी प्रेक्षक के रूप में उपस्थित रहते हैं।
2. **हिन्दी कार्यशाला का आयोजन** — प्रयोगशाला के स्टाफ को हिन्दी कार्य करने में आ रही समस्याओं का निदान करने तथा हिन्दी में कार्य करने हेतु प्रोत्साहित करने की दृष्टि से प्रत्येक तिमाही में नियमित रूप से हिन्दी कार्यशाला का आयोजन किया जाता है। इन कार्यशालाओं में स्टाफ को भारत सरकार की राजभाषा नीति की जानकारी देने के साथ-साथ अपना दैनंदिन सरकारी कार्य हिन्दी में करने तथा कंप्यूटर पर यूनिकोड प्रणाली के माध्यम से हिन्दी में काम करने का प्रशिक्षण दिया जाता है।
3. **हिन्दी संगोष्ठी का आयोजन** — वैज्ञानिक कार्यों में राजभाषा के प्रयोग को बढ़ावा देने हेतु तथा राजभाषा हिन्दी के प्रचार प्रसार की दृष्टि से यहाँ समय-समय पर वैज्ञानिक संगोष्ठी का आयोजन हिन्दी भाषा में किया जाता है। इसी क्रम में प्रयोगशाला में दिनांक 07 मई, 2013 को “कार्बनिक रूपान्तरण में उत्प्रेरक का प्रयोग” नामक विषय पर एकदिवसीय राष्ट्रीय विज्ञान संगोष्ठी का आयोजन किया गया।
4. **गृहपत्रिका का प्रकाशन** — प्रयोगशाला में प्रतिवर्ष हिन्दी गृहपत्रिका “एनसीएल— आलोक” का प्रकाशन नियमित रूप से किया जाता है। गृहपत्रिका प्रकाशन का मूल उद्देश्य हिन्दी भाषा में लिखे गए वैज्ञानिक लेखों का प्रचार प्रसार तथा कर्मचारियों की हिन्दी में लेखन और अभिव्यक्ति क्षमता को प्रोत्साहित करना है।

5. **हिन्दी पखवाड़ा समारोह का आयोजन** — प्रयोगशाला में प्रतिवर्ष हिन्दी पखवाड़ा समारोह का भव्य आयोजन किया जाता है। इस अवसर पर स्टाफ के लिए विभिन्न हिन्दी प्रतियोगिताओं तथा सांस्कृतिक कार्यक्रमों का आयोजन किया जाता है। हिन्दी पखवाड़ा के आरंभ में हिन्दी दिवस के अवसर पर प्रतिवर्ष प्रयोगशाला की वार्षिक गृहपत्रिका “एनसीएलआलोक” का विमोचन किया जाता है।



6. **हिन्दी सुविचार तथा अंग्रेजी शब्दों के हिन्दी अर्थ का ईमेल द्वारा प्रेषण** — प्रयोगशाला के हिन्दी कक्ष द्वारा प्रतिदिन हिन्दी सुविचार तथा अंग्रेजी शब्द के अर्थ का प्रेषण मेल द्वारा सभी कर्मचारियों को किया जाता है, ताकि कर्मचारियों में हिन्दी भाषा के प्रति रुचि उत्पन्न हो सकें।
7. **राजभाषा संबंधी नियमों का अनुपालन** — इस प्रयोगशाला में राजभाषा अधिनियम की धारा 3(3) के अंतर्गत जारी होनेवाले सभी दस्तावेज अनिवार्य रूप से द्विभाषी जारी किए जाते हैं। तथा राजभाषा विभाग द्वारा जारी वार्षिक कार्यक्रम में निर्धारित किए गए लक्ष्यों की प्राप्ति की ओर विशेष ध्यान दिया जाता है। प्रयोगशाला से जारी होने वाली सभी निविदा सूचनाएँ तथा विज्ञापन इत्यादि द्विभाषी रूप में प्रकाशित किए जाते हैं।

राजभाषा नियमों का अनुपालन करते हुए प्रयोगशाला में सभी मानक प्रपत्र, फार्म, आवेदन पत्र, साइनबोर्ड, नाम-पट्ट तथा रबर की मोहरें इत्यादि द्विभाषी रूप में तैयार किए गए हैं। प्रयोगशाला की वेबसाइट को द्विभाषी रूप में प्रदर्शित किया गया है तथा यहां उपलब्ध

सभी कम्प्यूटरों में द्विभाषी रूप से कार्य करने की सुविधा उपलब्ध है। प्रयोगशाला में प्राप्त हिन्दी पत्रों के उत्तर अनिवार्य रूप से हिन्दी में ही दिये जाते हैं तथा क तथा ख क्षेत्रों को जाने वाले अधिकांश पत्रों के लिफाफों पर पते हिन्दी भाषा में लिखे जाते हैं।

प्रयोगशाला में हिन्दी काम-काज को बढ़ावा देने तथा राजभाषा नीति के अनुपालन हेतु 3 अनुभागों को हिन्दी में कार्य करने के लिए निर्दिष्ट किया गया है।

8. **हिन्दी प्रशिक्षण** — केंद्र सरकार, राजभाषा नियम 1976 (संघ के सरकारी प्रयोजनों के लिए प्रयोग) के नियम 10 (4) के अंतर्गत इस प्रयोगशाला को ऐसे कार्यालयों के रूप में, जिसके 80 प्रतिशत से अधिक कर्मचारी वृंद ने हिन्दी का कार्यसाधक ज्ञान प्राप्त कर लिया है, राजपत्र में अधिसूचित किया गया है। इस प्रयोगशाला के 98 प्रतिशत कर्मचारियों को हिन्दी, हिन्दी टंकण एवं आशुलिपि का प्रशिक्षण दिया जा चुका है। इसके अलावा प्रशासन अनुभाग के कुछ अधिकारियों / कर्मचारियों तथा वैज्ञानिक स्टाफ को कंप्यूटर पर हिन्दी में कार्य करने हेतु प्रशिक्षित किया गया है तथा शेष स्टाफ को प्रशिक्षित करने की प्रक्रिया जारी है।

9. **नगर राजभाषा कार्यान्वयन समिति की बैठकों में सहभागिता** — प्रयोगशाला के निदेशक एवं हिन्दी अधिकारी नगर राजभाषा कार्यान्वयन समिति की बैठकों में नियमित रूप से भाग लेते हैं साथ ही नगर स्तर पर आयोजित विभिन्न हिन्दी गतिविधियों में एनसीएल द्वारा सक्रिय प्रतिभागिता की जाती है।

10. **प्रोत्साहन योजनाएं**— प्रयोगशाला के स्टाफ को हिन्दी में कार्य करने हेतु प्रोत्साहित करने की दृष्टि से यहाँ विभिन्न राजभाषा प्रोत्साहन योजनाएँ लागू हैं। इसके अलावा सीएसआईआर मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिंतन लेखमाला आदि योजनाएँ इस प्रयोगशाला में लागू हैं। इन सभी योजनाओं में प्रयोगशाला के वैज्ञानिक और कर्मचारी उत्साहपूर्वक भाग लेते हैं।

11. **हिन्दी पुस्तकों की खरीद** — राजभाषा हिन्दी के प्रचार-प्रसार हेतु प्रयोगशाला के पुस्तकालय हेतु प्रतिवर्ष हिन्दी पुस्तकें खरीदी जाती हैं।

12. **एनसीएल के वैज्ञानिक तथा तकनीकी क्षेत्रों में हिन्दी का प्रचार-प्रसार** — प्रयोगशाला के वैज्ञानिक तथा तकनीकी क्षेत्रों में राजभाषा हिन्दी का प्रचार-प्रसार करने के

उद्देश्य से यहां आयोजित होने वाले होने वाले विभिन्न वैज्ञानिक कार्यक्रमों तथा अन्य समारोहों का संचालन अंग्रेजी के साथ साथ हिन्दी माध्यम से भी किया जाता है। साथ ही इन समारोहों, व्याख्यानो एवं संगोष्ठियों की रिपोर्ट हिन्दी एवं अंग्रेजी दोनों भाषाओं में सीएसआईआर-समाचार में प्रकाशनार्थ राष्ट्रीय विज्ञान संचार एवं सूचना स्रोत संस्थान (निसकेयर), नई दिल्ली को नियमित रूप से भेजी जाती है। इसके अतिरिक्त इस प्रयोगशाला के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाली संगोष्ठियों तथा विज्ञान सम्मेलनों में भाग लेकर हिन्दी भाषा में अपना शोध पत्र भी प्रस्तुत करते हैं।

विज्ञान शिक्षा के प्रति रुचि उत्पन्न करने तथा राजभाषा के माध्यम से विज्ञान के प्रचार प्रसार के उद्देश्य से प्रयोगशाला के निदेशक महोदय विभिन्न विद्यालयों तथा महाविद्यालयों के विद्यार्थियों के लिए विज्ञान संबंधी व्याख्यान हिन्दी में देते हैं।

इसके अलावा प्रयोगशाला की शीर्ष स्तर की प्रबंध परिषद की बैठकों की कार्यसूची द्विभाषी रूप में तैयार की जाती है और इन बैठकों में हिन्दी में भी चर्चा की जाती है। साथ ही प्रशिक्षण कार्यक्रमों में मिला-जुली भाषा का उपयोग किया जाता है।



हिन्दी पखवाड़ा समारोह का आयोजन

भारत सरकार की राजभाषा नीति के संवैधानिक प्रावधान के अधीन सीएसआईआर— राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में प्रतिवर्ष सितम्बर मास में हिन्दी सप्ताह समारोह का आयोजन बड़े उत्साहपूर्वक किया जाता है।

इस वर्ष सीएसआईआर—एनसीएल में 16 से 27 सितम्बर, 2013 की अवधि में हिन्दी पखवाड़ा समारोह का आयोजन किया गया। इस अवधि में प्रयोगशाला स्टाफ तथा विद्यार्थी वर्ग के लिए विभिन्न प्रकार की हिन्दी प्रतियोगिताएँ आयोजित की गईं, जिनमें बड़ी संख्या में वैज्ञानिकों/अधिकारियों/कर्मचारियों/शोधछात्रों ने भाग लिया। दिनांक 16 सितम्बर, 2013 को हिन्दी पखवाड़ा शुभारंभ तथा प्रयोगशाला की वार्षिक राजभाषा पत्रिका एन.सी.एल. आलोक का लोकार्पण समारोह आयोजित किया गया। इस अवसर पर पत्रिका का विमोचन करते हुए मुख्य अतिथि के रूप में समारोह में उपस्थित महाराष्ट्र राष्ट्रभाषा सभा, पुणे के कार्याध्यक्ष तथा सुप्रसिद्ध हिन्दी लेखक श्री सु.मो.शाह ने कहा कि हिन्दी के माध्यम से हम वैज्ञानिक अनुसंधानों को देश की जनता तक सरलता से पहुँचा सकते हैं। उन्होंने सीएसआईआर—एनसीएल जैसी वैज्ञानिक अनुसंधान प्रयोगशाला द्वारा राजभाषा पत्रिका के प्रकाशन पर प्रसन्नता व्यक्त की और कहा कि यह पत्रिका विज्ञान संबंधी जानकारी और राजभाषा संबंधी प्रचार—प्रसार के अपने उद्देश्य में सफल है। इस समारोह में अध्यक्ष के रूप में उपस्थित प्रयोगशाला के वरिष्ठ प्रधान वैज्ञानिक, डॉ. प्रदीपकुमार त्रिपाठी ने अपने सम्बोधन में कहा कि 'एनसीएल आलोक' का प्रकाशन हमारी राजभाषा हिन्दी में काम करने की निष्ठा का प्रतीक है और हमें अधिकाधिक अपना सरकारी कामकाज हिन्दी में करके इस निष्ठा को और अधिक मजबूत बनाना है।

हिन्दी सप्ताह के दौरान दि. 17 सितम्बर को प्रयोगशाला के स्टाफ हेतु हिन्दी शब्दज्ञान प्रतियोगिता, दिनांक 19 सितंबर को सामान्य ज्ञान प्रतियोगिता, दिनांक 20 सितंबर को शुद्धलेखन प्रतियोगिता, दिनांक 24 सितंबर को हिन्दी काव्यपाठ प्रतियोगिता तथा दिनांक 25 सितंबर को चतुर्थ श्रेणी वर्ग के लिए हिन्दी शुद्धलेखन प्रतियोगिता का आयोजन किया गया। इन सभी प्रतियोगिताओं में प्रयोगशाला के कुल 104 स्टाफ सदस्यों तथा शोध छात्रों ने प्रतिभागिता की।

हिन्दी पखवाड़ा का समापन समारोह दि. 27 सितम्बर, 2013 को अपराह्न 3.00 बजे आयोजित किया गया, जिसकी अध्यक्षता प्रयोगशाला के भौतिक रसायन विभाग के प्रमुख एवं प्रशासन के प्रभारी डॉ. अनिल कुमार ने की। इस समापन समारोह में पुणे नगर के प्रख्यात हिन्दी सेवी तथा सुप्रसिद्ध हिन्दी चिंतक एवं लेखक डॉ. केशव फालके मुख्य अतिथि के रूप में उपस्थित थे। डॉ. केशव फालके एवं डॉ. अनिल कुमार ने इस अवसर पर विभिन्न प्रतियोगिताओं के विजेताओं को पुरस्कार प्रदान किए। इसके अलावा हिन्दी में अपना समस्त सरकारी कामकाज हिन्दी में करने वाले कर्मचारियों को भी नकद प्रोत्साहन पुरस्कार प्रदान किए गए। डॉ. फालके ने इस अवसर पर कहा कि आज हिन्दी अपनी राष्ट्रीय सीमाएं लाँघकर अन्तर्राष्ट्रीय स्तर पर जा पहुँची है। इससे हिन्दी के प्रयोग के क्षेत्र की विशालता और व्यापकता सिद्ध होती है। उन्होंने कहा कि हिन्दी हमारे देश की पहचान है तथा विश्व में भारत की पहचान हिन्दी भाषा के द्वारा ही होती है। हिन्दी का एक अति सुदृढ़ सांस्कृतिक एवं सामाजिक आधार है। इस कारण ही इसे भारतीय संविधान में राजभाषा के रूप में प्रतिष्ठित किया गया है और आज हिन्दी विश्व भाषा का खिताब पाने के लिए सबसे बड़ी दावेदार है।

समारोह के अध्यक्ष डॉ. अनिल कुमार ने इस अवसर पर कहा कि हमारी राजभाषा ही हमारे विकास का प्रतीक है। विदेशी भाषा को अपनाकर हम आगे नहीं बढ़ सकते। उन्होंने जानकारी देते हुए कहा कि सीएसआईआर—एनसीएल में प्रशासकीय स्तर पर हिन्दी भाषा में कामकाज किया जाता है और इसका प्रयोग बढ़ाने के विभिन्न उपाय भी किये जाते हैं। उन्होंने उपस्थित स्टाफ सदस्यों का आह्वान किया कि वे राजभाषा के माध्यम से राष्ट्र के उन्नयन में अपना बहुमूल्य योगदान दें।

समारोह के आरंभ में श्री उमेश गुप्ता, वरिष्ठ हिन्दी अधिकारी ने सभी उपस्थित लोगों का स्वागत किया और हिन्दी सप्ताह की प्रासंगिकता की रूपरेखा प्रस्तुत की। समारोह की कार्यवाही का संचालन हिन्दी अधिकारी श्रीमती स्वाति चट्ठा ने किया। श्रीमती प्रेमा बालकृष्णन, प्रशासन अधिकारी ने अन्त में सभी के प्रति धन्यवाद ज्ञापित किया।

विज्ञान संगोष्ठी का आयोजन

सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में भारत सरकार की राजभाषा नीति का कड़ाई से अनुपालन किया जाता है और राजभाषा के सुचारु रूप से कार्यान्वयन हेतु हरसंभव प्रयास किए जाते हैं। इसके अधीन समय-समय पर विभिन्न विषयों पर हिन्दी संगोष्ठियों का भी आयोजन किया जाता है। इसी क्रम में प्रयोगशाला में दिनांक 7 मई, 2013 को “कार्बनिक रूपान्तरण में उत्प्रेरक का प्रयोग” नामक विषय पर एकदिवसीय विज्ञान संगोष्ठी का आयोजन किया गया।

इस संगोष्ठी में मुख्य अतिथि के रूप में वरिष्ठ वैज्ञानिक एवं विज्ञान संचारक, डॉ. डी.डी. ओझा उपस्थित थे। उन्होंने संगोष्ठी में उपस्थित वैज्ञानिकों को सम्बोधित करते हुए कहा कि हिन्दी केवल हमारी राष्ट्रभाषा या राजभाषा ही नहीं है, बल्कि वह अब वैश्विक भाषा बन गई है। इसके स्पष्टीकरण हेतु उन्होंने वर्तमान स्थापित आँकड़ों का विवरण सभी के सामने रखा। उन्होंने आगे कहा कि जब तक हिन्दी में विज्ञान-साहित्य विशाल स्तर पर उपलब्ध नहीं होता तब तक वैज्ञानिक तथा औद्योगिक अनुसंधान का लाभ सबको नहीं मिल सकता। उन्होंने कहा कि विज्ञान-नीति देश के जनमानस तक पहुँचनी चाहिए। विज्ञान सत्य उजागर करता है। इसका लाभ अंधविश्वास निर्मूलन, स्वास्थ्य के प्रति जागरूकता तथा आर्थिक वृद्धि के स्रोत प्राप्त करने के लिए होता है।

अपने मूल अभिभाषण में डॉ. ओझा ने “रसायन विज्ञान : जीवन का आधार” नामक विषय पर अपने विचार विस्तार से प्रकट किए। उन्होंने आगे कहा कि रसायन विज्ञान के अनेक अविष्कार हम हर दिन देखते हैं और आजमाते हैं। अपनी विशिष्ट शैली में डॉ. ओझा ने उपस्थित वैज्ञानिकों एवं शोधछात्रों से कहा कि रसायन विज्ञान का प्रादूर्भाव भारत में वैदिक काल में हुआ था। कणाद, चरक, नागार्जुन आदि के कार्यों के उदाहरण देते हुए उन्होंने भारत के प्राचीन एवं समृद्ध इतिहास को उजागर किया। उनके अनुसार मानव जीवन से सम्बद्ध सभी प्रक्रियाओं में रसायन विज्ञान जुड़ा हुआ है। रसायन विज्ञान को चिकित्सा विज्ञान, कृषि विज्ञान, पदार्थ विज्ञान, जीवविज्ञान आदि में प्रयोग में लाया जाता है। भारत के अलावा अन्य किसी भी देश में अपनी भाषा का दिवस नहीं मनाया जाता है। यह हमारे लिए बहुत ही गंभीर एवं विचारणीय विषय है कि क्यों हम अपनी भाषा को छोड़कर विदेशी भाषा को अपनाने में गौरव का अनुभव करते हैं? डॉ. ओझा ने आगे कहा कि

किसी भी देश की पहचान उसके राष्ट्रध्वज, राजमुद्रा और राजभाषा से होती है। आज हम अपनी राजभाषा को भूलकर अपनी राष्ट्रीयता भी खो रहे हैं। उन्होंने सभी को आह्वान किया कि हमें अपने आत्मसम्मान की रक्षा के लिए अपनी भाषा को ही अपनाना चाहिए।

डॉ. ओझा ने विज्ञान के क्षेत्र में उल्लेखनीय योगदान के लिए इंडियन सोसायटी ऑफ हेल्थ ऐंड एनवायरनमेंट रिसर्च, जोधपुर, राजस्थान की ओर से सीएसआईआर-एनसीएल के निदेशक, डॉ. सौरव पाल को विज्ञान पार्षद (साइन्स कौन्सिलर) पुरस्कार से सम्मानित किया।

संगोष्ठी में अध्यक्ष के रूप में उपस्थित प्रयोगशाला के निदेशक, डॉ. सौरव पाल ने संगोष्ठी के आयोजन पर प्रसन्नता व्यक्त करते हुए सभी प्रतिभागियों का अभिनंदन किया। उन्होंने कहा कि इस प्रकार के आयोजनों से ही हम हिन्दी के माध्यम से अपने शोधकार्यों को जनमानस तक पहुँचा सकते हैं। अपने सम्बोधन में उन्होंने कहा कि देश के विकास में विज्ञान का महत्वपूर्ण योगदान है और वर्तमान युग विज्ञान और प्रौद्योगिकी का युग है। वैज्ञानिकों को अपने मौलिक शोधकार्यों को जनता के सामने लाने के लिए उनकी प्रस्तुती जनभाषा अर्थात् हिन्दी में ही होनी चाहिए। हम अपने विचार अपनी भाषा में बड़ी सहजता और सरलता से व्यक्त कर सकते हैं। डॉ. सौरव पाल ने शोधछात्रों को भविष्य के वैज्ञानिक बताते हुए कहा कि उनके अनुसंधान कार्यों को हिन्दी में प्रस्तुत करने हेतु इस विज्ञान संगोष्ठी का आयोजन किया गया है। उन्होंने कहा कि यह हम सब के लिए बड़े ही हर्ष और गौरव की बात है कि हम अपने वैज्ञानिक अनुसंधान को राजभाषा के माध्यम से समाज के सामने रख रहे हैं। उन्होंने आशा व्यक्त की कि ऐसे आयोजनों से समाज के लोग निश्चित ही लाभान्वित होंगे और इससे देश का विकास होगा। उक्त संगोष्ठी में सभी प्रतिभागी वैज्ञानिक अपने मौलिक अनुसंधान कार्य हिन्दी माध्यम से प्रस्तुत करके राष्ट्रसेवा में अपना योगदान देंगे।

संगोष्ठी के संयोजक एवं प्रयोगशाला के उत्प्रेरण प्रभाग के अध्यक्ष, डॉ. ए.पी. सिंह ने संगोष्ठी की रूपरेखा प्रस्तुत करते हुए विज्ञान की विभिन्न विधाओं में उत्प्रेरण के विभिन्न अनुप्रयोगों पर प्रकाश डाला।

संगोष्ठी का आरम्भ टाटा केमिकल्स के मुख्य वैज्ञानिक, डॉ. राजीव कुमार की प्रस्तुती से हुआ। उन्होंने अपशिष्ट बायोमास से स्वच्छ और वितरित ऊर्जा का सृजन नामक विषय पर अपना शोधपत्र प्रस्तुत

किया। डॉ. राजीव कुमार ने अपने व्याख्यान में जैवभार से ऊर्जा के निर्माण पर मौलिक विचार व्यक्त किए। तत्पश्चात प्रयोगशाला के वरिष्ठ प्रधान वैज्ञानिक, डॉ. प्रदीप कुमार ने “हरित रसायन – चुनौतियाँ एवं अवसर” पर शोधपत्र प्रस्तुत किया। उन्होंने अपने व्याख्यान में हरित रसायन के विभिन्न नियमों एवं कुछ नए प्रयोगों के बारे में जानकारी दी। तदुपरान्त सीएसआईआर-एनसीएल के डॉ. रवि प्रकाश सिंह ने “उत्प्रेरण – अणु परिवर्तन” पर तथा डॉ.ए.जे. वर्मा, अध्यक्ष, बहुलक रसायन एवं अभियांत्रिकी प्रभाग ने “सेलुलोस – जलअपघटन एवं आक्सीकरण के द्वारा उत्पाद” पर शोधपत्र प्रस्तुत किए। इसी प्रकार प्रयोगशाला के वैज्ञानिकों और शोधछात्रों ने इस संगोष्ठी में भाग लेकर अपने-अपने विषयों पर शोधपत्र प्रस्तुत किए। इनमें अनुज कुमार, पी. एल. डेपे, प्रीति शर्मा, संजय सिंह नेगी, काकासाहेब नंदीवाले, अंजनी

दुबे ने बड़ी सहजता और सरलता से हिन्दी में अपने अनुसंधान कार्यों को प्रस्तुत किया। संगोष्ठी के प्रथम सत्र का संचालन डॉ. डी.डी. ओझा ने तथा द्वितीय सत्र का संचालन डॉ. प्रदीप कुमार त्रिपाठी ने बड़ी कुशलता से किया। उन्होंने प्रत्येक प्रस्तुती के बाद उसकी समीक्षा करते हुए उस विषय पर अपने मौलिक विचार भी व्यक्त किए। शोधपत्र के प्रत्येक प्रस्तुतकर्ता को स्मृतिचिह्न देकर सम्मानित किया गया।

संगोष्ठी का संचालन करते हुए प्रयोगशाला के वरिष्ठ हिन्दी अधिकारी, श्री उमेश गुप्ता ने प्रयोगशाला में राजभाषा के उन्नयन एवं विकास हेतु किए जा रहे प्रयासों पर प्रकाश डालते हुए इस संगोष्ठी के आयोजन की भूमिका स्पष्ट की।





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CSIR-National Chemical Laboratory

(Council of Scientific & Industrial Research)

Dr. Homi Bhabha Road, Pune 411 008 (INDIA).

Tel. : +91-20-2590 2600