सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला
CSIR-National Chemical Laboratory

वार्षिक प्रतिवेदन 2012 - 13

Annual Report 2012 - 13

वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद

Published by

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

Printed by

Typographica Press Services, Pune

सीएसआईआर – राष्ट्रीय रासायनिक प्रयोगशाला
CSIR - National Chemical Laboratory

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

वार्षिक प्रतिवेदन
ANNUAL REPORT
2012-13

PERFORMANCE INDICATORS

RESEARCH & DEVELOPMENT REPORTS

RESOURCE CENTERS

S & T SUPPORT SERVICES

ANNEXURES

निदेशक की कलम से...

वर्ष 2012–13 के लिए सीएसआईआर राष्ट्रीय रासायनिक प्रयोगशाला का वार्षिक प्रतिवेदन प्रस्तुत करते हुए मुझे अत्यंत हर्ष हो रहा हैं। वार्षिक प्रतिवेदन अप्रैल 2012 से मार्च 2013 तक की अवधि के हमारे प्रदर्शन को प्रस्तुत करती हैं। प्रतिवेदन में हमारे प्रदर्शन के कई मापदंडों को प्रस्तुत किया जाता है और मैं यह जानकर अत्यंत प्रसन्न हूँ कि पिछले कुछ वर्षों में हमारे प्रदर्शन में निरंतर सुधार आ रहे हैं। विशेष रूप से, हमारे प्रकाशनों के साथ ही एकस्व प्रस्तुत करने में सुधार हुआ है और हमने देश और समाज के लिए प्रौद्योगिकी विकसित करने के लिए बड़े पैमाने पर उद्योगों के साथ हमारे सहयोग को मजबूत किया है, इस बात की भी मुझे बहुत प्रसन्नता है। हमारी बाहरी नकद आय भी पिछले वर्ष की आय के अनुरूप है और मैं इस प्रयोगशाला को गौरवान्वित करने के लिए सभी एनसीएल स्टाफ को बधाई देता हूँ।

वर्ष 2012–13 भी बहुत विशेष वर्ष था, जो 12 वीं पंचवर्षीय योजना की परियोजनाओं का पहला वर्ष था और औपचारिक रूप से 1 अप्रैल 2012 से आरंभ हुआ था। सीएसआईआर–एनसीएल रासायनिक और साथ ही जैविक विज्ञान क्लस्टर दोनों में योजना परियोजनाओं की एक बड़ी संख्या में सम्मिलित है। योजना अवधि के पहले वर्ष में हमने ढांचागत सुविधाओं का निर्माण किया और परियोजनाओं में वर्णित मील के पत्थर को प्रदत्त करने के लिए हम प्रतिबद्ध हैं।

वर्ष 2012–13 में, डॉ. अश्विनी कुमार, तत्कालीन माननीय राज्य मंत्री–योजना, विज्ञान और प्रौद्योगिकी तथा पृथ्वी विज्ञान, भारत सरकार, द्वारा एनसीएल का दौरा किया गया था। उन्होंने हमारे स्टाफ को संबोधित किया और प्रयोगशाला के लिए अपने सहयोग का आश्वासन दिया। इस दौरान सौर ऊर्जा के दोहन के क्षेत्र में हमारी प्रमुख उपलब्धियों में से कुछ का प्रदर्शन उनके सामने किया गया।

वर्ष 2012–13 में, हमने एनसीएल में प्रख्यात वैज्ञानिकों की उपस्थिति में कई कार्यक्रम आयोजित किए । प्रो. इची नेगिशी, नोबेल पुरस्कार विजेता, ने सीएसआईआर – एनसीएल स्थापना दिवस पर "मैजिकल पावर ऑफ ट्रांजिशन मैटल्स – पास्ट, प्रेजेंट एंड फ्यूचर" पर व्याख्यान दिया। इसके अलावा इस वर्ष हमने कई अन्य प्रतिष्ठित व्यक्तियों को आमंत्रित किया। डॉ. प्रकाश आमटे ने प्रो. बी. डी. तिलक स्मृति व्याख्यान, प्रो. एस. चंद्रशेखरन ने प्रो. के. वेंकटरमण स्मृति व्याख्यान प्रस्तुत किया और डॉ. एस. आर. शेटे, कुलपति, गोवा विश्वविद्यालय ने सीएसआईआर स्थापना दिवस पर व्याख्यान दिया। हमारे द्वारा कई संगोष्ठियों और आर. ए. माशेलकर प्रतिभा व्याख्यान का आयोजन भी किया गया।

27–29 दिसम्बर, 2012 के दौरान आईएनएसए वार्षिक साधारण बैठक का आयोजन भी एनसीएल द्वारा किया गया। कई प्रतिष्ठित विदेशी विद्वानों के अलावा, प्रोफेसर माइकल ग्रेटजेल ने भी एनसीएल का दौरा किया जो रंजक संवेदी सौर कोशिकाओं के क्षेत्र में एक प्रख्यात वैज्ञानिक हैं। प्रयोगशाला द्वारा एक दिवसीय संगोष्ठी के रूप में एसीएस का आयोजन भी किया गया, जो अमेरिकन केमिकल सोसायटी और आरएससी इंडिया रोड शो की एक पहल थी। साथ ही प्रो. डी. बालसुब्रमण्यन, प्रो.शैलादित्य सेनगुप्ता और प्रो. प्रदीप देशपांडे द्वारा प्रतिष्ठित सार्वजनिक व्याख्यान का आयोजन भी किया गया।

हमने प्रौद्योगिकी विकास तथा उसे उद्योग जगत को हस्तान्तरित करने के अपने प्रयास जारी रखे हैं। पिछले वर्ष हमने मिनिएचराइज्ड मिक्सरों एवं रिएक्टर उपकरणों, मिल्टेफोसिन हेतु प्रक्रिया, अक्रिस्टलीय बहुलकों का कार्यात्मक ग्रूप एवं खंडीय गति जाँच द्वारा उनके मेकैनिकल गुणधर्मों से सम्बद्ध अध्ययन, प्रकार्यात्मक रूप से समापित ब्लॉक तथा ग्राफ्ट सहबहुलकों से युक्त परफ्लुओरोपोलीइथर्स (पीएफपीई) एवं पीएफपीई की डिज़ाइन एवं संश्लेषण, भूमिगत कोयला गैसीकरण हेतु प्रतिरूपण फ्रेमवर्क, प्राकृतिक गैस हाइड्रेट्स से मिथेन रिकवरी के काइनेटिक्स से सम्बद्ध अध्ययन, ठोस अम्ल उत्प्रेरक के प्रयोग द्वारा ओ– जाइलीन के नाइट्रेशन की प्रक्रिया, निम्न तापमान डिमल्सिफायर्स का विकास, तथा कोकोआ बीन फर्मेन्टेशन एवं ड्राइंग से सम्बन्धित महत्वपूर्ण अध्ययन हेतु हमने प्रक्रिया तथा तकनीक का लाइसेन्स प्रदान किया।

इस प्रतिवेदन में वर्ष 2012–13 के दौरान विभिन्न क्षेत्रों में किए गए अनुसंधान की सूचना प्रस्तुत की गई है तथा मुझे आशा है कि इसमें आपको सीएसआईआर-एनसीएल में हमारे द्वारा किए जा रहे अनुसंधान एवं विकास का परिदृश्य दिखायी देगा।

हमने अपने स्टाफ में नए एवं होनहार मानव संसाधन भी शामिल किए हैं और मैं उम्मीद करता हूँ कि कुछ ही वर्षों में हम अपने स्टाफ की सहायता से अपने अनुसंधान को और सुदृढ़ करते हुए देश की सेवा में बने रहेंगे।

अन्त में मैं प्रयोगशाला के 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। उनके प्रयास, सहयोग, सलाह और विश्वास के कारण ही हमारी अधिकाँश उपलब्धियाँ संभव हुई हैं। मुझे पूरा विश्वास है कि हममें उनका दृढ़ विश्वास भविष्य में हमें नई ऊँचाइयों पर ले जाएगा।

सौरव पाल

(सौरव पाल)

From the Director's Desk ...

I am very happy to present the Annual Report of CSIR-National Chemical Laboratory for the year 2012-13. The Annual Report presents our performances of this period. The report presents several parameters of our performances and I am very happy to note that our performances are continuing to improving in last few years. In particular, our publications as well as filling of patents have improved and I am also happy to note that we have strengthened our association with industry to develop technology for the country and society at large. Our external cash earnings have also matched earnings of the previous year and I congratulate all NCL staff for making this laboratory proud.

The year 2012-13 was also very special, since this was the first year of the 12th five year plan projects which formally started from 1st April 2012. The CSIR-NCL is involved in a large number of plan projects in both chemical as well as biological sciences cluster. We also built infrastructural facilities in the first year of the plan period and committed ourselves to the delivery of the milestones as stated in the projects.

In the year 2012-13, we had a visit by Dr. Ashwani Kumar, the then Hon'ble Minister of State for Planning, Science and Technology and Earth Sciences, Govt. of India. He also addressed our staff and extended his support to the laboratory. We also demonstrated some of our key achievements in the area of solar energy harnessing.

In the year 2012-13, we had many events and talks by eminent scientists at CSIR-NCL. Prof. Ei-ichi Negishi, Nobel Laureate, delivered CSIR-NCL Foundation Day lecture on "Magical Power of Transition Metals: Past, Present and Future". In addition, we had several other invitees. Renowned social worker Dr. Prakash Amte delivered Prof. B. D. Tilak Memorial Lecture, Prof. S. Chandrasekaran delivered Prof. K. Venkataraman Memorial Lecture and Dr. S. R. Shetye, Vice Chancellor, Goa University delivered CSIR Foundation Day Lecture. We also hosted several symposia and R. A. Mashelkar Endowment Lectures. We also organized INSA Annual General Meeting during 27-29 December 2012. Among the distinguished foreign visitors, we had Prof. Michael Graetzel who is an eminent scientist in the area of dye sensitized solar cells. We have also organized ACS on campus event which was an initiative from the American Chemical Society and a RSC India Road Show in the form of one day symposium. Distinguished public lectures by Prof. D. Balasubramanian, Prof. Shiladitya Sengupta and Prof. Pradeep Deshpande were organized.

We have continued our efforts on the development of technology and its delivery to the industry. In the last year, we have licensed the processes and know-how for miniaturized mixers and reactors devices, process for Miltefosine, studies related to the mechanical properties of amorphous polymers by probing their functional group and segmental motions, design and synthesis of functionally terminated Perfluoropolyethers (PFPEs) and PFPE containing block and graft copolymers, modeling framework for underground coal gasification, studies related to kinetics of methane recovery from natural gas hydrates, nitration process of *o*-xylene using solid acid catalyst, process for continuous flow nitration of acetophenone, low temperature demulsifiers development, and significant studies related to cocoa bean fermentation and drying.

This report presents before you research that took place in 2012-13 in different areas and I hope this provides you an overview of research and development that we are carrying out at CSIR-NCL. We have also added new bright human resources and I am hopeful that in few years, with the help of all our staff, we will continue to strengthen our research and serve the nation.

Finally, I wish to acknowledge the support and cooperation 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

(Sourav Pal)

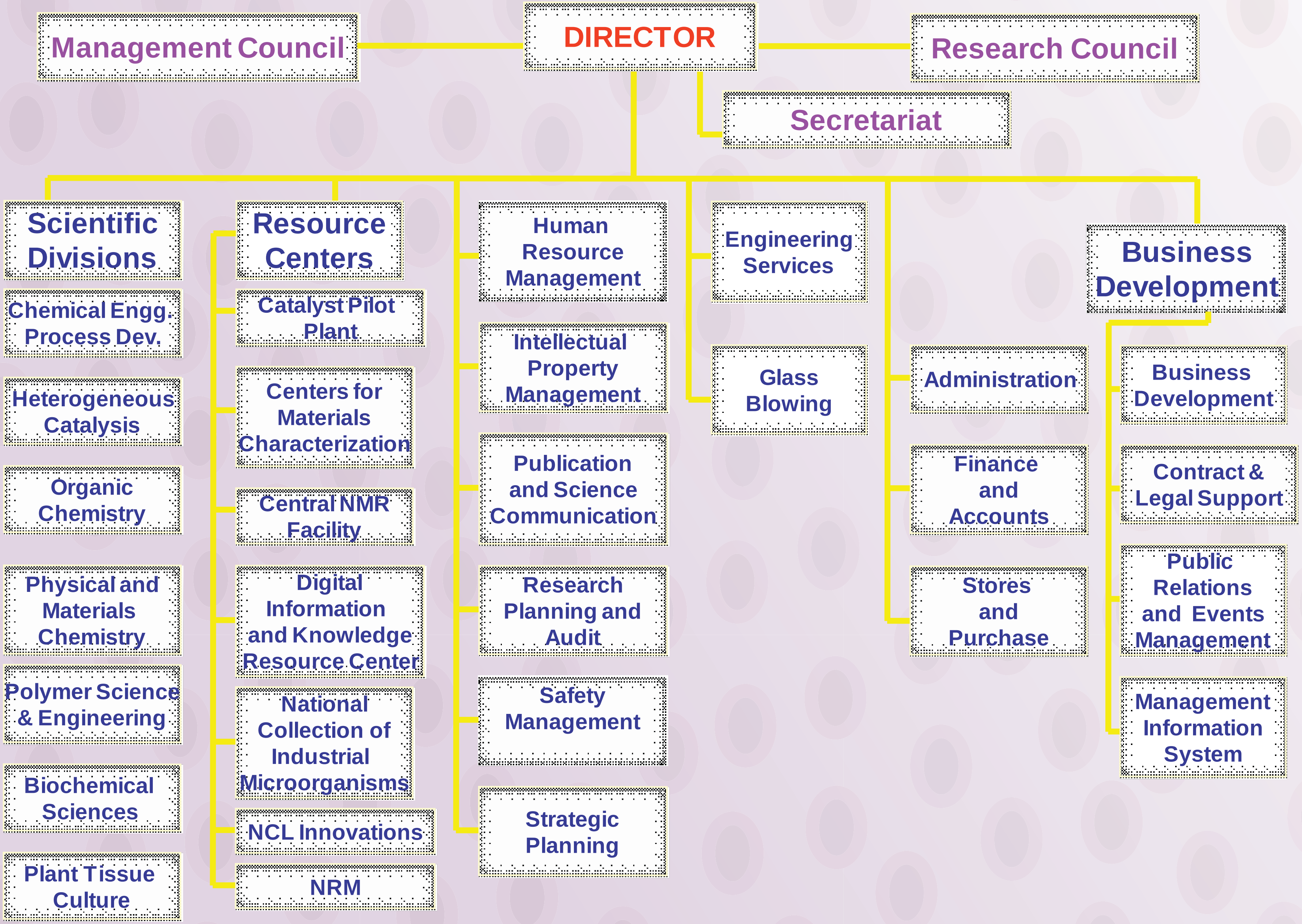
Vision, Mission & Guiding Principles & Values

- 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 themselves 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

- 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

- 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

Organisation Chart



- **DIRECTOR**
  - Management Council
  - Research Council
  - Secretariat
  - Scientific Divisions
    - Chemical Engg. Process Dev.
    - Heterogeneous Catalysis
    - Organic Chemistry
    - Physical and Materials Chemistry
    - Polymer Science & Engineering
    - Biochemical Sciences
    - Plant Tissue Culture
  - Resource Centers
    - Catalyst Pilot Plant
    - Centers for Materials Characterization
    - Central NMR Facility
    - Digital Information and Knowledge Resource Center
    - National Collection of Industrial Microorganisms
    - NCL Innovations
    - NRM
  - Human Resource Management
  - Intellectual Property Management
  - Publication and Science Communication
  - Research Planning and Audit
  - Safety Management
  - Strategic Planning
  - Engineering Services
  - Glass Blowing
  - Administration
  - Finance and Accounts
  - Stores and Purchase
  - Business Development
    - Business Development
    - Contract & Legal Support
    - Public Relations and Events Management
    - Management Information System

RESEARCH AREAS

Catalysis

- Heterogeneous catalysis
- Organometallic chemistry
- Surface science

Biochemical Sciences

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

Organic Chemistry

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

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

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

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

CSIR-NCL serves to various sectors such as

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

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

RESEARCH COUNCIL

Chairperson

Prof. D. D. Sarma
Solid State & Structural Chemistry Unit
Indian Institute of Science
Bengaluru- 560 012

Members

Prof. S. Ramakrishnan
Department of Inorganic and Physical Chemistry
Indian Institute of Science
Bengaluru – 560 012

Prof.(Ms.) Charusita Chakravarty
Department of Chemistry
Indian Institute of Technology
New Delhi – 110 016

Prof. (Ms.) Saswati Lahiri
Indian Association for the Cultivation of Science
Jadavpur
Kolkata – 700 032

Dr. Balu Sarma
President & Chief Technology Officer
Praj Matrix – The Innovation Center
Mulshi
Pune – 411 042

Dr. R. Brakaspathy (Agency Representative)
Advisor
Department of Science and Technology
New Mehrauli Road
New Delhi – 110 016

Dr. Ayyappanpillai Ajayaghosh
(DG's Nominee)
Head
Chemical Sciences and Technology Division
National Institute for Interdisciplinary Science
and Technology
Thiruvanathapuram – 695 019

Dr. Rajesh S. Gokhale (Sister lab.)
Director
Institute of Genomics and Integrative Biology
Mall Road
Delhi – 110 007

Dr. M. O. Garg (Cluster Director)
Director
Indian Institute of Petroleum
Dehradun – 248 005

Dr. Sourav Pal
Director
CSIR-NCL

Head
Planning & Performance Division or
his nominee (Permanent Invitee)
CSIR
Anusandhan Bhavan
New Delhi – 110 001

Member Secretary

Dr. G. S. Grover
Head, Research Planning and Audit Unit
CSIR-NCL

MANAGEMENT COUNCIL

Chairperson

Dr. Sourav Pal
Director, CSIR-NCL

Members

Mr. G. Prabhakaran
Scientist (CSIR-NCL)

Dr. S. Ravindranathan
Scientist (CSIR-NCL)

Dr. Ashish Lele
Scientist (CSIR-NCL)

Dr. N. P. Argade
Scientist (CSIR-NCL)

Dr. Rahul Banerjee
Scientist (CSIR-NCL)

Ms. M. P. Chirmule
Technical Officer (CSIR-NCL)

Dr. B. D. Kulkarni
Distinguished Scientist (CSIR-NCL)

Dr. Ganesh Pandey
Scientist (CSIR-NCL)

Dr. V. V. Ranade
Scientist (CSIR-NCL)

Mr. R. P. Purandare
Head, ESU (CSIR-NCL)

External Members

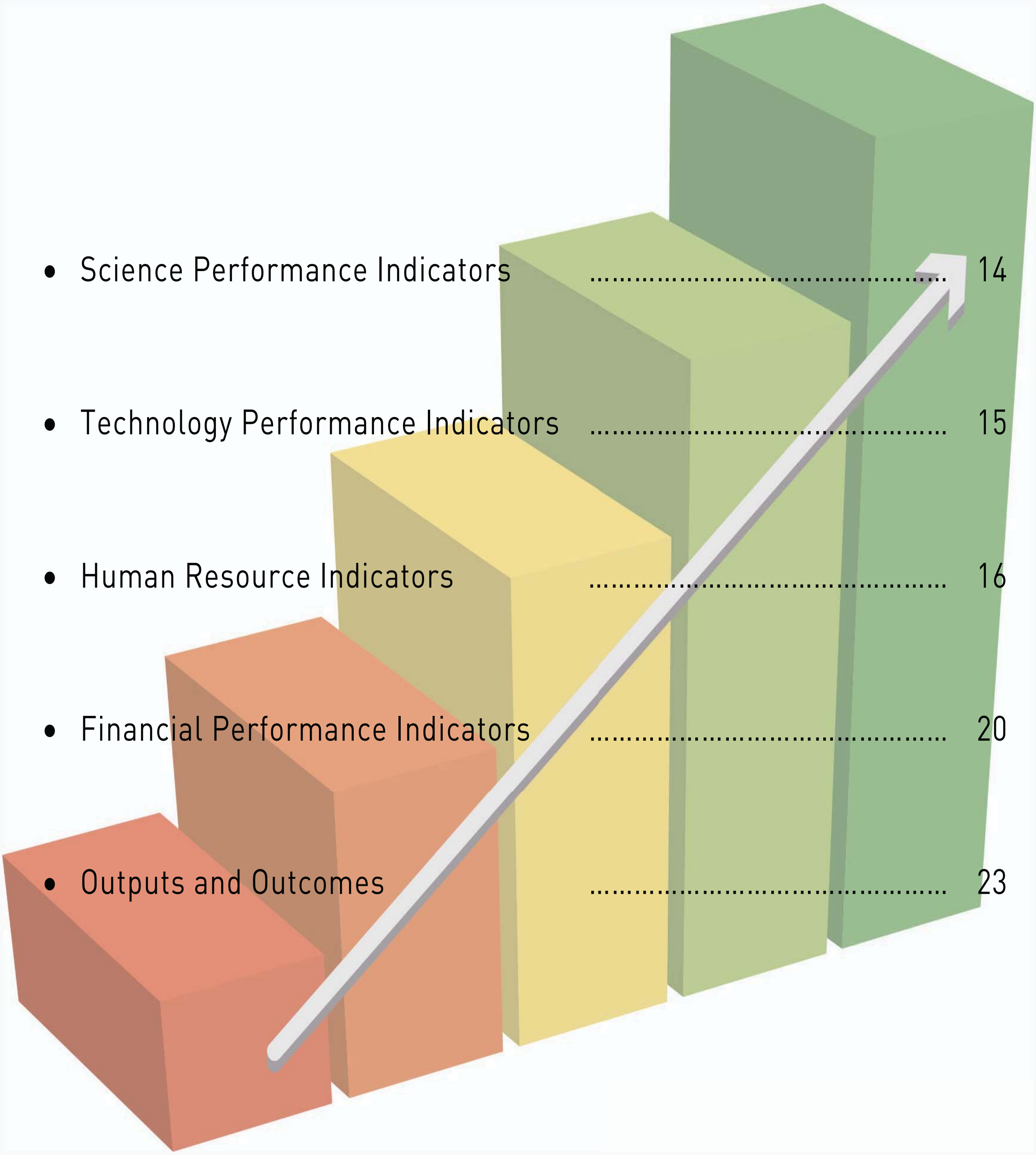
Dr. R. R. Hirwani
Head, URDIP

Dr. Satish Shetye
Director,
CSIR-NIO, Goa

Member Secretary

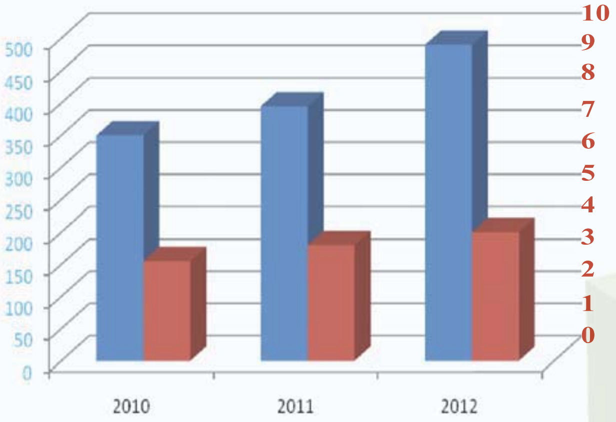
Mr. S. K. Gupta
Controller of Administration, CSIR-NCL

PERFORMANCE INDICATORS



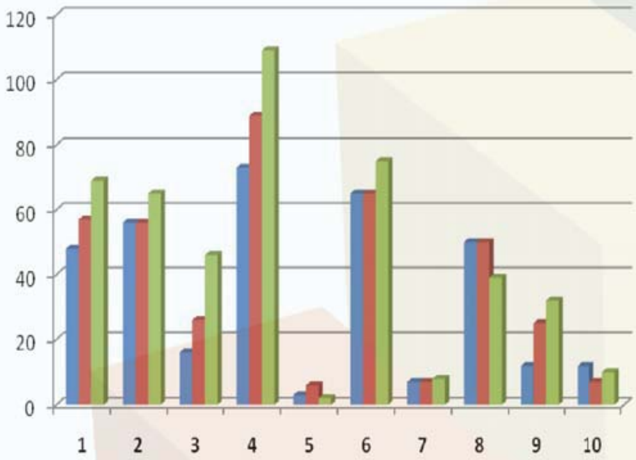
Science Performance Indicators

Research Output: Publications



Year	2010	2011	2012
Total Papers	344	389	460
Avarage Impact Factor	2.83	3.29	3.69

Area-wise Publications



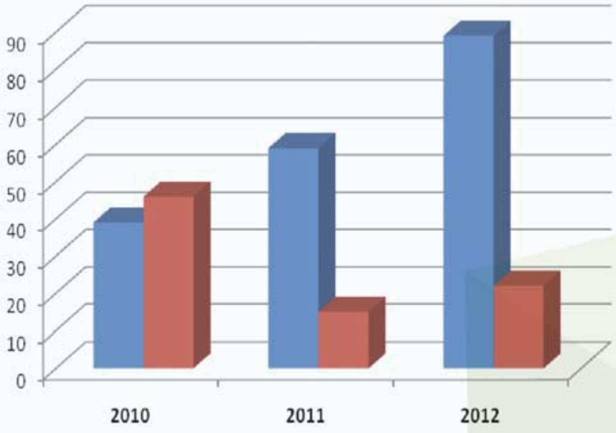
Year	2010	2011	2012
Biological Sciences and Engineering	48	57	69
Catalysis and Surface Science	56	56	65
Chemical Engineering Sciences	16	26	46
Materials Chemistry	73	89	109
NMR	3	6	2
Organic Chemistry	65	65	75
Physical Chemistry	7	7	8
Polymer Science and Engineering	50	50	39
Structural Chemistry	12	25	32
Theory and Computational Science	12	07	10

Ph.D. Theses

Year	2010	2011	2012
No. of Theses	53	58	52

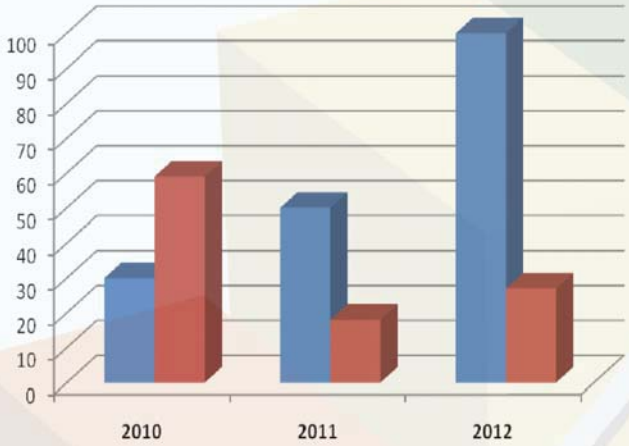
Technology Performance Indicators

Indian Patents : Filed and Granted



Year	🟦 Filed	🟫 Granted
2010	36	42
2011	56	12
2012	86	19

Foreign Patents: Filed and Granted



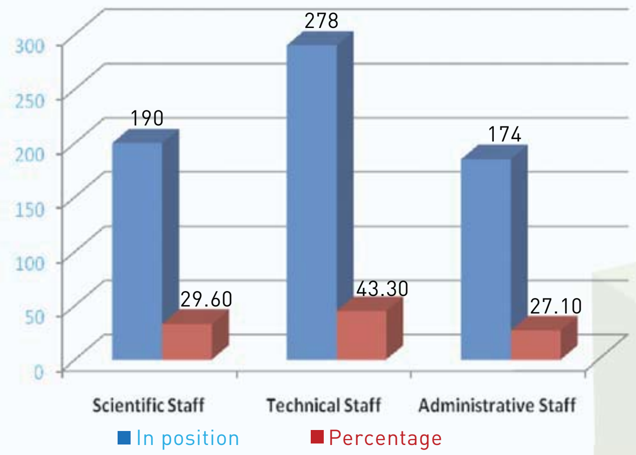
Year	🟦 Filed	🟫 Granted
2010	27	55
2011	46	13
2012	96	22

Premia/ Royalty Earnings

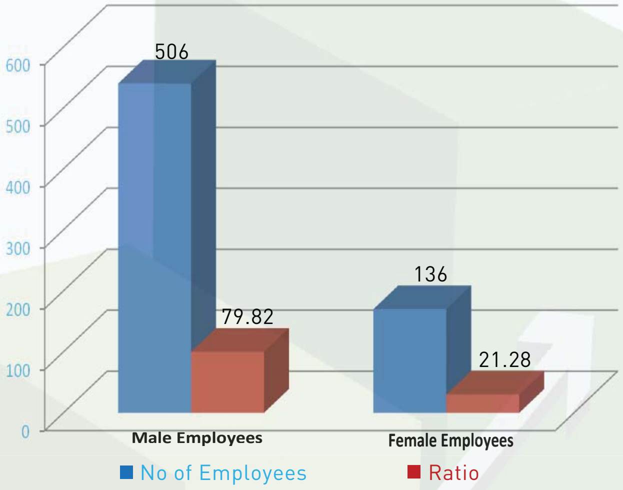
Year	🟦 ₹ in lakhs
2010-11	64.73
2011-12	369.71
2012-13	480.96

Human Resource Indicators

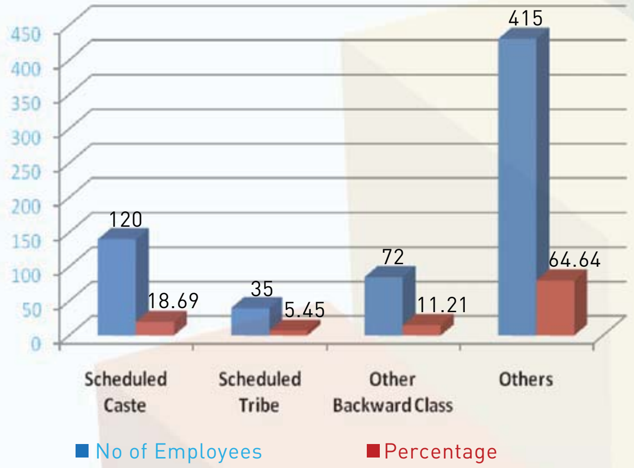
Total Staff: 642



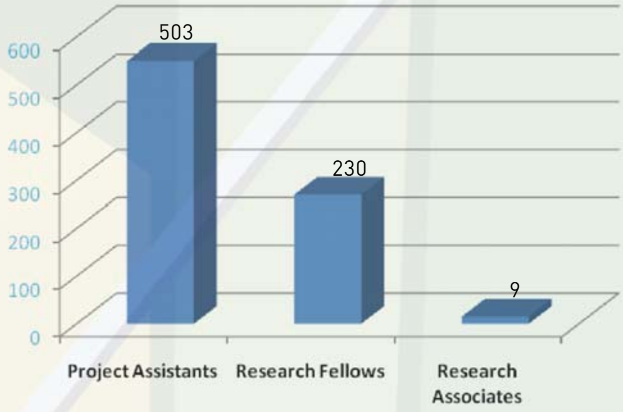
Male and Female Employees



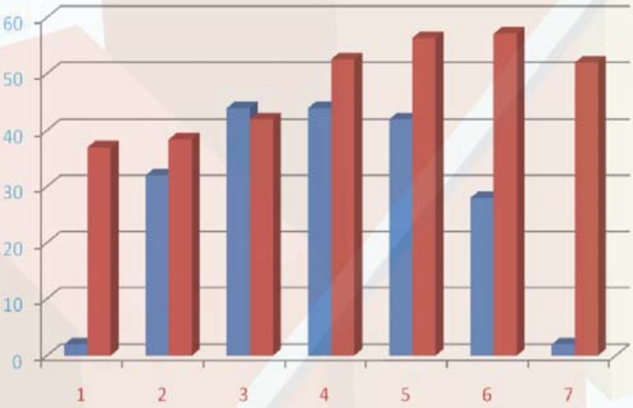
SC, ST, OBC and Others



Students and Project Staff



Scientific Staff: Age wise distribution



Grade	Nos	Average Age
Sci. B/ Trainee Scientists	1	37
Sci. C/ Scientists	32	38.41
Sci. E- I / Sr. Scientists	44	41.87
Sci. E- II / Principal Scientists	44	52.58
Sci. F/ Sr. Principal Scientists	40	56.36
Sci. G/ Chief Scientists	28	57.15
Sci. H/ Outstanding Scientists	1	50
Total	190	

We Welcome

Dr. Meitram Niraj Luwang
(12.06.2012)

Materials Science, Luminescent nanomaterials and its applications

- ☐ Ph. D. Manipur University (2012)

Dr. Mahesh S. Dharne
(22.6.2012)

Microbiology and Biotechnology

- ☐ Research Scientist (ICMR-NIV), Pune (2011-2012)
- ☐ Post-doctoral Fellow, University of Maryland, Baltimore, United States (2010- 2011)
- ☐ Visiting scientist- US Department of Agriculture, Beltsville, Maryland, United States (2007-2010)
- ☐ Ph. D. Biotechnology, University of Pune (DBT-National Centre For Cell Science) (2003-2008)

Mr. Yogesh Suryawanshi
(13.07.2012)

Process, Product Development, Automation, Pilot Plant Design & Building

- ☐ Director- Tridiagonal Process Engineering Pvt. Ltd. (April 2009 - June 2012)
- ☐ Head- Reactor and Pilot Plant Division – Chemito Technologies Pvt. Ltd. (August 2007 - February 2009)
- ☐ M.Tech – Chemical Engineering , Dr. B. A. T. U., Lonere (July 2005 - August 2007)

We Welcome

Dr. Debashree Ghosh
(31. 07. 2012)

Theoretical and Computational Chemistry

☐ Postdoctoral research associate, University of Southern California, Los Angeles, USA (September 2009 - June 2012)

☐ Ph.D., Chemistry and Chemical Biology, Cornell University, Ithaca, NY, USA (August 2005 - September 2009)

☐ M.S., Chemical Sciences, Indian Institute of Science, Bangalore

Dr Syed G. Dastager
(01. 08. 2012)

Microbial Systematic and Plant-Microbe Interaction

☐ Scientist, CSIR-National Institute of Oceanography, Regional Center, Mumbai (May 2011 - July 2012)

☐ Scientist (Ad-hoc), CSIR-National Institute of Oceanography, Goa (July 2010 – April 2011)

☐ Fellow Scientist (QHS), CSIR-National Institute for Interdisciplinary Science and Technology, Trivandrum (May 2008 - July 2010)

☐ Post-Doc Research Associate, Korea Research Institute of Bioscience and Biotechnology, South Korea (December 2006 - December 2007)

☐ Ph. D. Gulbarga University (August 2002 - December 2006)

Dr. Sachin B. Agawane
(20.08.2012)

Biochemical Sciences

☐ Scientist, CSIR-Indian Institute of Chemical Technology, Hyderabad (August 2005 – August 2012)

☐ Assistant Manager, Venkateswara Hatcheries, Hyderabad (January 2004 – August 2005)

☐ Veterinarian, Raj Biotech, Wing (December 1999 - May 2000)

☐ M.V.Sc. Pathology from Bombay Veterinary College, Mumbai

We Welcome

Dr. Shashank G. Gaikwad
(27. 08. 2012)

Extraction and Process Development

- ☐ Research Professional, GE Bangalore (March 2008 - August 2012)
- ☐ Ph. D. (Tech.), Institute of Chemical Technology, Mumbai (July 2003 - December 2007)

Dr. Sayan Bagchi
(30.11.2012)

Ultrafast Spectroscopy and Dynamics

- ☐ Post-Doctoral Research Scholar, Stanford University, USA (2008- 2012)
- ☐ Ph. D. University of Pennsylvania, Philadelphia, USA (2002 - 2008)

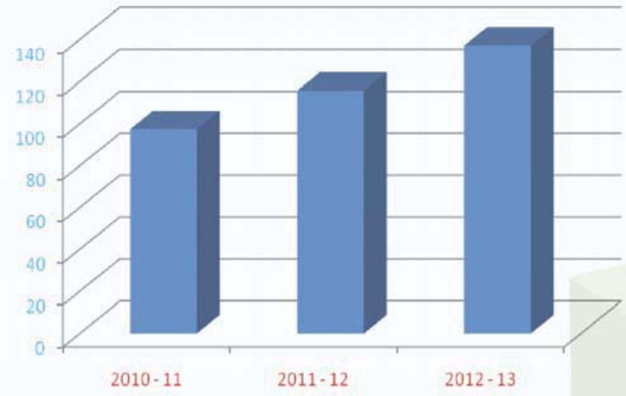
Dr. Kiran Kulkarni
(18.03.2013)

Structural Biology, Cellular Signalling Networks

- ☐ Post-Doctoral Fellow, Institute of Cancer Research, London, UK (2009- 2013)
- ☐ Application Scientist, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru (2007-2009)
- ☐ Ph. D. Indian Institute of Science (2007)

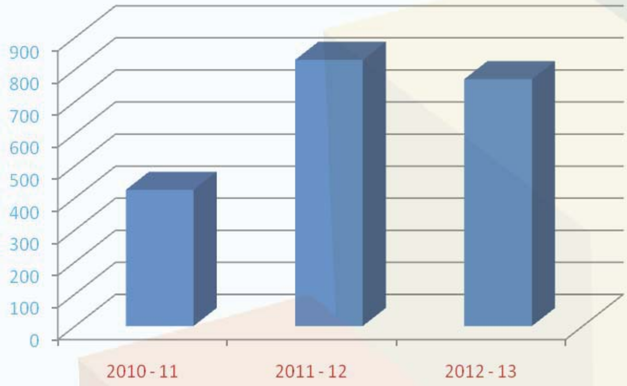
Financial Performance Indicators

CSIR Budget



Year	₹ in Crores
2010-11	95.31 (CSIR Budget : 76.88 + Network Project : 17.42 + NMITLI Projects : 01.01)
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)

Laboratory reserve: Receipts



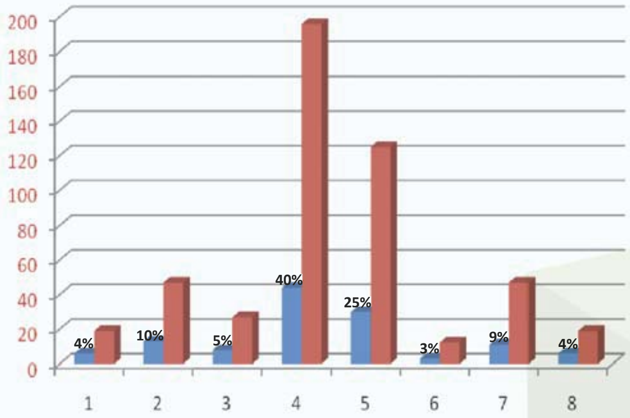
Year	₹ in Lakhs
2010-11	390
2011-12	795
2012-13	719

Laboratory reserve: Expenditure

Year	₹ in Lakhs
2010-11	260
2011-12	433
2012-13	483

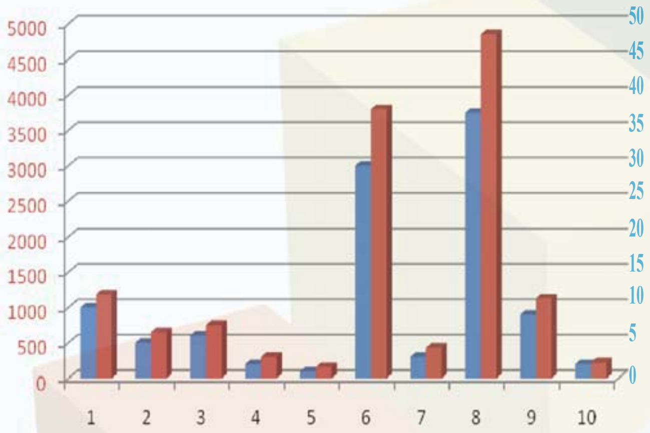
Financial Performance Indicators

Expenditure: Laboratory reserve 2012-13 (₹ in Lakhs)



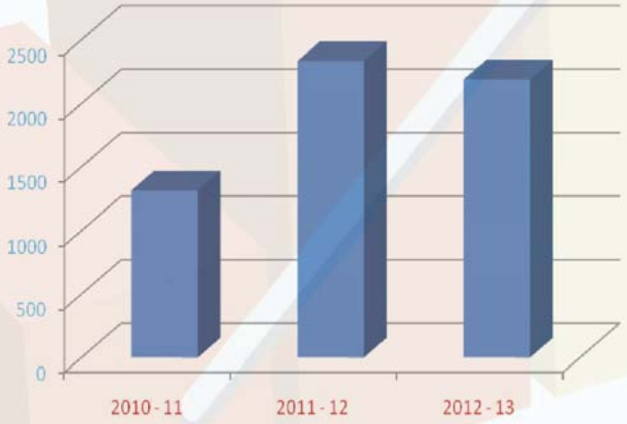
1. Salary linked allowances	4%	19.002
2. Library	10%	46.98
3. Appliances and equipment + Comp. equip.	5%	24.187
4. Contingencies	40%	195.783
5. Maintenance (Lab. + Staff quarter)	25%	121.519
6. Chemicals & Consumables	3%	12.244
7. Work and services	9%	44.368
8. Furniture	4%	18.915

Expenditure: CSIR and Network Projects 2012-13 (₹ in Lakhs)



1. Appliances and equipment + Comp. equip.	9%	1185.002
2. Chemicals	4%	555.744
3. Contingency	5%	600.775
4. Library (Books, Journals and Electronic Journals)	2%	300
5. Maintenance (Lab. + Staff quarter)	1%	160
6. Network projects	29%	3765.999
7. NMITLI projects	3%	422.042
8. Salaries (Pay & Allow.)	37%	4852.714
9. Staff quarter: construction	8%	1040
10. Work and services	2%	198.5

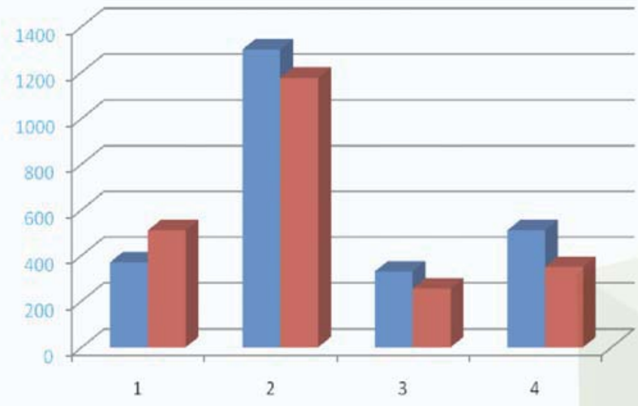
External Income



Year	₹ in Lakhs
2010-11	1315
2011-12	2335
2012-13	2191

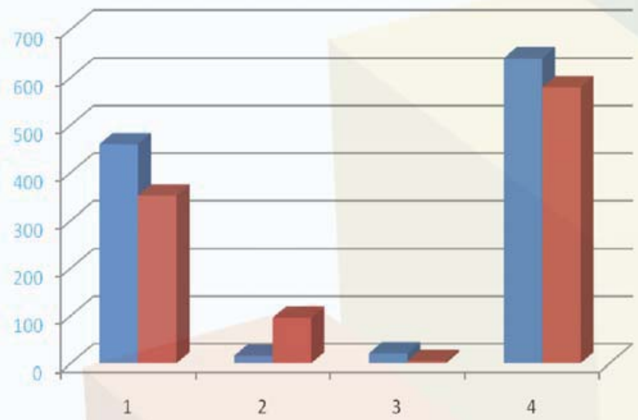
Financial Performance Indicators

ECF by Source



	2011-12 ₹ in Lakhs	2012-13 ₹ in Lakhs
Knowhow & Royalty/IP	370	481
Grant-in-aid-projects	1231	1176
Consultancy / technical services	283	204
Sponsored / collaborative projects	451	330
Total	2335	2191

ECF from Industry



	2011-12 ₹ in Lakhs	2012-13 ₹ in Lakhs
Indian Industry (Private)	449	352
Indian Industry (Public)	16	96
Government Sector	21	05
Foreign Sector	617	565
Total	1103	1018

Outputs and Outcomes

Category of benefits	Benefit	Indicators	2010-11	2011-12	2012-13
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)	5.59	11.03	10.18
	Continuing education	Total earnings from continuing education/ training programs (₹ in Crore)	NA	NA	NA
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (₹ in Crore)	0.65	3.70	4.81
Strategic goods and options	Other tactical and strategic developments	Total earnings from patent related transaction (₹ in crore)	1.50	3.44	-
		No of patents in new Licensing /assignment/ option arrangements	3	7	-
		No of unique Licensing /assignment/ option cases	1	1	-
		No of Indian patents granted (Calendar year)	42	12	19
		No of foreign patents granted** (Calendar year)	55	13	22
	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (₹ in Crore)	1.80	8.95	4.74
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (₹ in Crore)	7.56	12.31	11.73
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	No of Indian patents granted (Calendar year)	42	12	19
		No of foreign patents granted** (Calendar year)	55	13	22
		Number of papers in foreign peer-reviewed journals	318	370	431
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	22	NA	NA

* - 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

Outputs and Outcomes

Category of benefits	Benefit	Indicators	2010-11	2011-12	2012-13
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in foreign journals / publications (Calendar year)	318	370	431
		Number of papers published in Indian journals(Calendar year)	24	19	26
		Average Impact Factor	2.83	3.29	3.69
		Number of invention disclosure (Calendar year)	54	85	116
		Number of patents filed in India (Calendar year)	36	56	86
		No of foreign patents filed ** (Calendar year)	27	46	96
		Number of PCT applications filed (Calendar year)	16	28	36
		No of US applications filed	6	14	26
	Highly trained man-power	Number of PhDs produced (Calendar year)	53	59	52
		Number of NET/GATE qualified students joined (including DBT JRF)	124	140	90
	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	4	6	9
	Pride and standing among nations; National image	Number of international awards won	-	-	-
		Memberships of major international academies and learned societies	9	12	12
		Memberships of editorial boards of international peer-reviewed journals (Cumulative membership years)	54	NA	NA
		Number of papers in foreign journals	318	370	431
		Number of IF research papers	323	355	434

1 Crore = 10 Million

RESEARCH & DEVELOPMENT REPORTS

Magnetostrictive smart materials

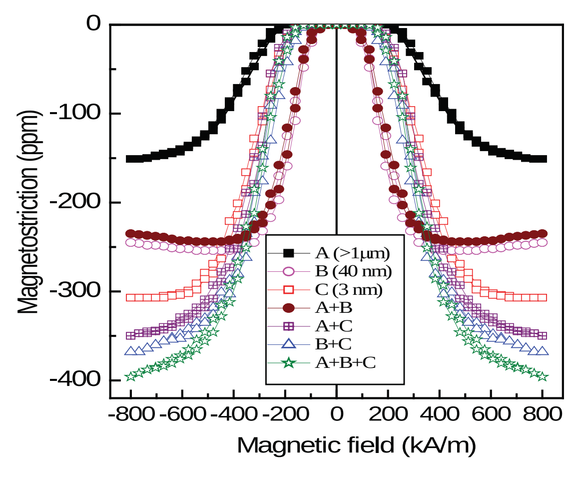
P. A. Joy
pa.joy@ncl.res.in

Publications: ACS Appl. Mater. Inter., 2012, 4, 6421; Appl. Phys. Lett., 2012, 101, 72405; Curr. Appl. Phys., 2013, 13, 1697

The use of sintered polycrystalline cobalt ferrite as amagnetostrictive material for various applications is limited by the low value of magnetostriction coefficient (λ) and strain derivative ($d\lambda / dH$) of the material obtained under usual processing conditions. Research was aimed to enhance the magnetostrictive performance parameters of sintered cobalt ferrite by simple and novel processing techniques.

Sintered self-composites of cobalt ferrite

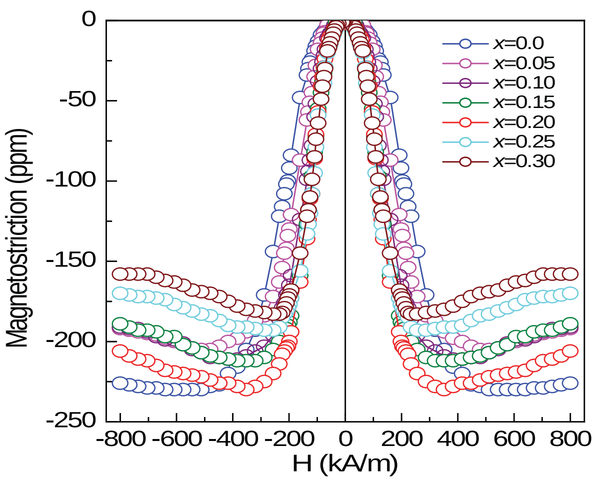
Much higher values of the magnetostriction coefficient were obtained for sintered polycrystalline cobalt ferrite by a novel concept and simple process of making self-composites obtained by sintering compacts made from a physical mixture of nanosized and micron sized particles of cobalt ferrite with different sizes. The self-composites were made from nanosized particles and micron sized particles as starting materials. It was compacted under very low hydrostatic pressures which showed enhanced magnetostriction. Maximum magnetostriction up to 400 ppm and maximum value of strain derivative of 2.0×10^{-9} $A^{-1}m$ was achieved for a self-composite made from powder particles of three different sizes in the nano and micron levels, whereas the individual components gave values up to 310 ppm.



Comparison of the magnetostriction coefficient of sintered cobalt ferrite compacts

Manganese substituted cobalt ferrite

The relatively low value of the slope of the magnetostriction or the strain derivative ($d\lambda / dH$) at low magnetic fields is a major concern for various applications for the sintered cobalt ferrite. The strain derivative of sintered polycrystalline cobalt ferrite was increased by the substitution of Mn for Fe in $CoFe_2O_4$, but at the cost of the value of magnetostriction coefficient which was considerably reduced after substitution. The higher strain derivative was achieved without affecting the magnetostriction coefficient by suitable substitution for Mn in cobalt ferrite and when the sintered compacts were made from nanocrystalline powders.



Magnetostriction coefficient of different compositions in $CoFe_{2-x}Mn_xO_4$

Synthesis assemblies and applications of functional nanoparticles

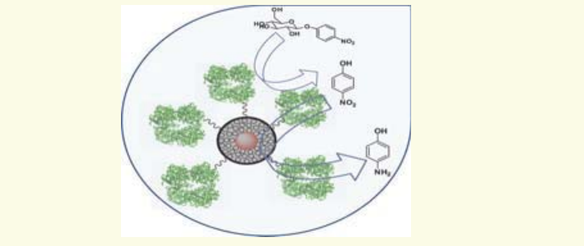
B. L. V. Prasad
pl.bhagavatula@ncl.res.in

Publications: Colloid. Surface. A, 2012, 414, 296; 2013, 422, 181; RSC Adv., 2013, 3, 2186; Chem-Asian J., 2013, 8, 369; Nanoscale, 2013, 5, 1768

The aim was to develope new methods for material synthesis, bio-nanoparticle conjugates and their applications, surface modification of nanoparticles and their assemblies and molecular assemblies etc.

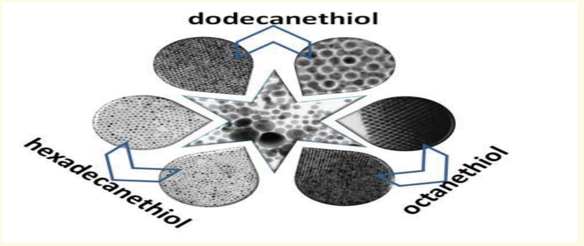
Development of a multifunctional catalyst for a "relay" reaction

A multifunctional catalyst that can carry out a "relay" reaction was developed with the amalgamation of the nanoparticles and enzymes. The catalyst consisted a surface bound enzyme on a metalcore-silicashell nanoparticle architecture. The enzyme catalyzed the first reaction and the metal nanoparticles acted as a catalyst for the second reaction on the product released from the first reaction. The catalytic activity of glucosidase grafted Au@mSiO$_2$ on 4-nitrophenyl-β-glucopyranoside was studied; where glucosidase will catalyse the first step to generate 4-nitrophenol, which acted as a substrate for the next reduction step which is catalysed by Au nanoparticles present inside the mesoporous silica shell.



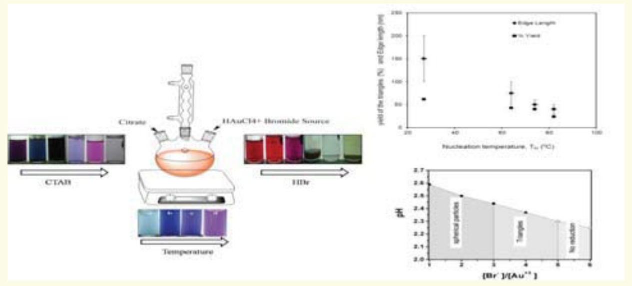
Fine control on nanoparticle sizes and size distributions

A fine control over the size and size distribution of nanoparticles was achieved using digestive ripening at different temperatures using different ligands. Such variations in size and size distributions hugely influenced the self-assembled processes in nanoparticles and resulted in superlattice structures that were controlled by subtle interplay between ligand orientational entropy, their interdigitation and the Van der Waal attraction between the metal cores.



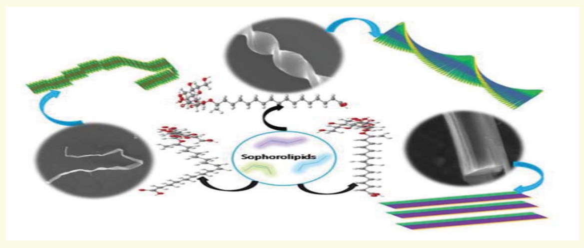
Investigations on the role of bromide ion and temperature during the synthesis of triangular gold nanoplates

Through a conventional batch mode process the effect of temperature on nucleation and growth of gold triangular nanoplates was studied and obtained some insight of the temperature on the final yield and edge length of triangles. The results showed that, while CTAB controls the edge length and yield of triangles, its use is not mandatory to attain plate like morphology. It was showed that, while the initial temperature of the reaction mixture governs the nucleation rate and the rate of temperature rise governs the growth rate of particles. The concentration of Br$^-$ ions controlled the edge length and yield.



Remarkable influence of a small change in the molecular structure on the self-assembled structures of sophorolipids

The fascinating self-assembled structures of three sophorolipids were differentiated by very small molecular level change. The elaidic acid sophorolipids form the most interesting twisted ribbon structures due to favourable π overlap that leads to a squeeze in the middle of the molecule leading a higher steric repulsions of the sophorose moieties ensuing a twist and leading to the helicity. All the sophorolipids can be obtained in large quantities, so self-assembled structures can be formed in large scale. This posseses great application potential as possible scaffolds in tissue engineering or for condensing inorganic oxides such as silica.



Advanced materials for electrochemical powersources

Sreekumar Kurungot
k.sreekumar@ncl.res.in

Publications: J. Mater. Chem., 2012, 22, 44, 22506, 23668, 23799; Nanoscale, 2012, 4, 890; Inorg. Chem., 2012, 51, 9766

Objective was to design and develope non platinum and low platinum electro catalysts for polymer electrolyte membrane fuel cell (PEMFCs) and development of high energy storage electrodes for supercapacitors using novel hybrid materials.

Non platinum electrocatalysts for PEMFCs

The work on highly dense N- and FeN_x doped nano porous graphene (FeNGr) showed 40 mV higher positive onset potential shift compared to N-Gr. A well structured nanoporous graphene and green luminescent graphene quantum dot (GQDs) was simultaneously generated by a chemically assisted oxidative treatment of graphene by H_2O_2. The nitrogen doping on porous Gr (NpGr) showed an onset potential of +0.02 V, which is 50 and 90 mV positive compared to NGr and pGr, respectively. Three dimensional arrangement of nitrogen doped graphene with carbon nitride back-bone (CNG) opens a new strategy to activate reaction centers of nitrogen doped graphene to perform as a non metal electrocatalyst in acidic condition for ORR.

The prepared catalyst was highly active towards ORR through a four electron pathway with less than 3% peroxide formation in the entire potential range in 0.1 M $HClO_4$. Similarly, CNG showed extraordinary electrochemical stability and fuel selectivity. In parallel, the synthesized N-doped porous carbon derived from MOF-5 was used as a basic scaffold for the *in-situ* C_3N_4 formation and the potential of composite was tested as an ORR catalyst. The MOFCN900 showed higher performance towards oxygen reduction reaction in terms of higher onset potential (0.035 V vs Hg/HgO) and enhanced current density of (4.6 mA/cm^2).

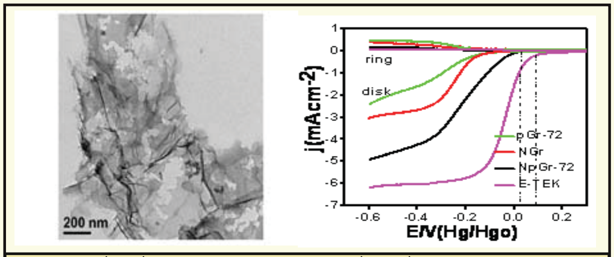


Fig. 1: (Left) HRTEM image of FeNGr, (Right) RRDE test of pGr-72, NGr, NpGr-72 and E-TEK

Electrode materials for supercapacitor applications

Highly conducting porous 1-dimensionally *(1-D)* confined nanohybrid of polyethylene-dioxythiophene (PEDOT) were synthesised using a cup-stacked hollow carbon nanofiber (CNF) as a solid template for supercapacitor charge storage and dye-sensitized solar cell (DSSC) counter electrode. This made the material a potential candidate for super capacitor application and promising material to replace Pt counter electrode in DSSC's.

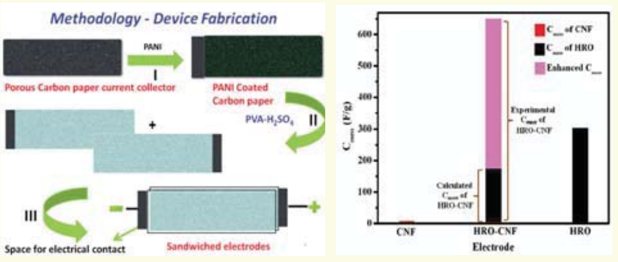


Fig. 2: (Left) Methodology of fabrication of supercapacitors using (PVA+H_2SO_4), (Right) Mass specific capacitance values of electrode

Multifunctional materials for electrochemical applications

A high aspect ratio material was derived by confining acid doped polybenzimidazole along the inner and outer walls of a carbon nanofiber matrix which showed enhanced capacitance values. Porous carbons were obtained on direct carbonization of non-porous Zn-based MOFs. The linear relations between Zn/C ratio of the MOF vs. surface area of the resulting carbon, microporosity vs. H2 uptake, surface area vs. specific capacitance of the end carbons were studied and the inter-dependence of the capacitive behavior on the surface area was analyzed using BET adsorption adsorption isotherms and elctrochemical studies. Maximal surface area of 1378 m^2/g was obtained from C-MOF-2 along with a specific capacitance of 170 F/g at 1 A/g. Tuning of functionality of a Pt-RuO_2-CNF ternary system from charge storage to oxygen reduction behavior by means of oxidative functionalization of the CNF surface is an interesting development.

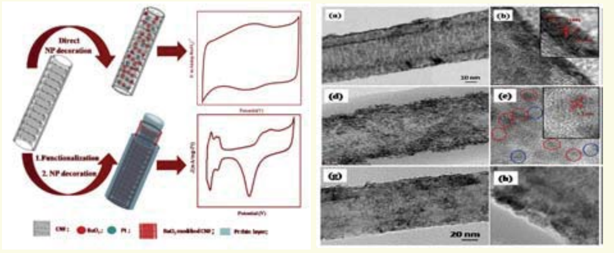


Fig. 3: (Left) The switchover from charge storage to oxygen reduction activity; (Right) TEM images showing the exposed Pt thin layer and underlying RuO_2 bed

Materials for hydrogen storage and carbon capture

Rahul Banerjee
r.banerjee@ncl.res.in

Publications: J. Am. Chem. Soc., 2011, 133, 17950; 2012, 134, 19524; 2013, 135, 5328; Chem. Commun., 2013, 49, 6197

The aim of this work was to design porous Covalent Organic Framework materials (COFs) with hydrogen binding energies intermediate between physisorption and chemisorption. Such materials need to reach a binding energy for hydrogen in the range of 15 – 25 kJ/mol averaged over all sorption sites. Group was also engaged in design and synthesis of COFs for proton conduction for fuel cell applications.

Syntheses of significant COFs

The synthesis of two new COFs by a combination of reversible and irreversible organic reaction was reported. These COFs were stable and remained crystalline in acid (9N HCl), base (9N NaOH) and water. These COFs were synthesized by a reaction between 1, 3, 5-Triformyl phloroglucinol (Tp) and Paraphenylenediamine (Pa-1) or 2, 5-dimethylparaphenylene-diamine (Pa-2). The total reaction was divided in two steps. Reversible Schiff base reaction led to the formation of crystalline framework in the first step, followed by irreversible enol to keto tautomerisation in the second step (Fig. 1) which enhanced the chemical stability. The irreversible nature of the tautomerism did not affect the crystallinity of the COF since the transformation involved only shifting of bonds keeping atomic positions almost same in both the cases. These COFs showed exceptional resistance towards boiling water, acid and base treatment. Both COFs retained their crystallinity and gas adsorption property at these above mentioned conditions.

Mechanochemistry was efficiently employed to carry out various organic and inorganic transformations, nanostructures formation and metal-organic framework construction. It has thus become a good alternative to classical solution based synthesis. Modified mechanochemical synthesis was employed for the rapid synthesis of MOFs by using liquid assisted grinding (LAG) to enhance the topological selectivity and was employed to construct *0D* porous organic cages. In general, harsh experimental conditions such as, reaction in a sealed pyrex tube, inert atmosphere, suitable solvents, longer time for crystallization etc. is required during COF synthesis to form well ordered crystalline frameworks.

The synthesis of two highly stable COFs was also reported by using modified Schiff base reactions, where the proton tautomerism brought exceptional stability (water, acid and base) into the framework. This outstanding chemical stability of these COFs led the group to attempt for alternative simple, solvent free, rapid and scalable room temperature construction of covalent organic frameworks through mechanochemistry.

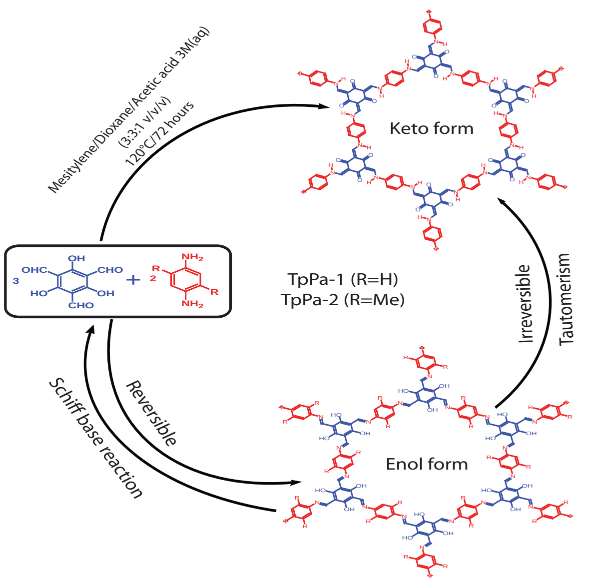


Fig. 1: Schematic representation of synthesis of TpPa-1 and TpPa-2

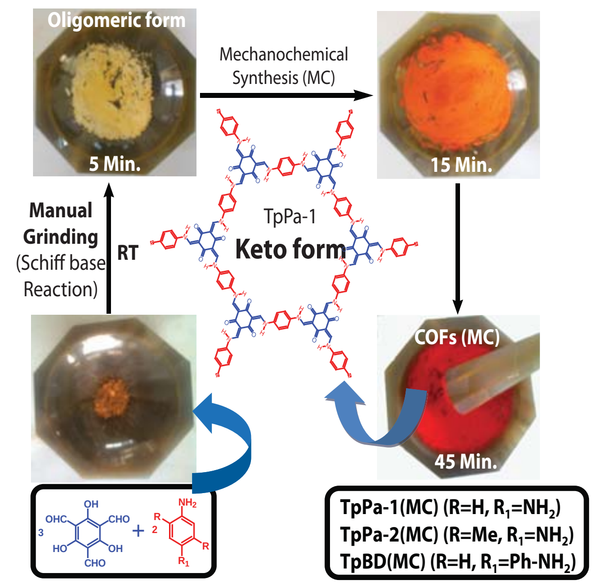


Fig. 2: Schematic representation of the synthesis of TpPa-1 (MC), TpPa-2 (MC) and TpBD (MC)

Synthesis and applications of multifunctional nanomaterials

Manjusha V. Shelke
mv.shelke@ncl.res.in

Publications: J. Mater. Chem., 2012, 22, 22922; J. Mater. Chem. C, 2013, DOI:10.1039/C3TC30904E; Appl. Catal. B-Environ., 2013, 130, 270; Colloid. Surface. B, 2013, 105, 128

The objective behind the work was to explore the full potential of nanostructured materials. For this, the materials were fabricated rationally following designed patterns with a high degree of control over the size, location, packing manner, dimensionality, uniformity and shape.

Nanostructured arrays for high efficiency electron field emission

Nanoscale heterostructures are important building blocks for functional devices to achieve multifunctionality. A complementary secondary particle was added to existing nanostructure which derived nanomaterials with a desired combination of physicochemical attributes. Silicon nanowires (SiNWs) were particularly important in this context of integration and connection of various functional nanostructures with SiNWs. These SiNWs were used as a fundamental component of novel miniature devices. Efficient field emitters based on SiNWs/nanoZnO and SiNWs/Graphene Oxide (GO) nanosheets were developed successfully. These nanostructured arrays displayed excellent field emission current densities at low electric field.

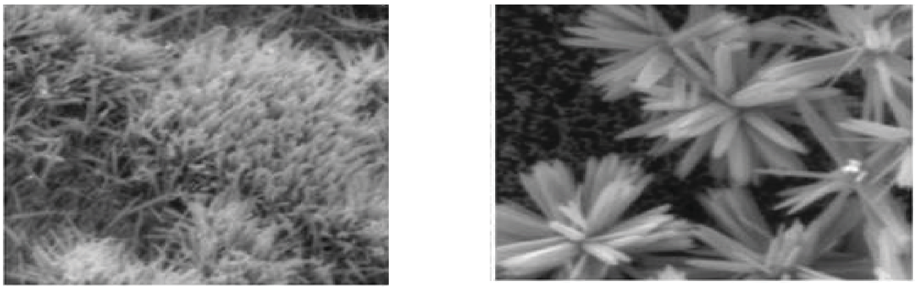


Fig. 1: SEM images and Field emission performance of SiNWs/nanoZnO arrays

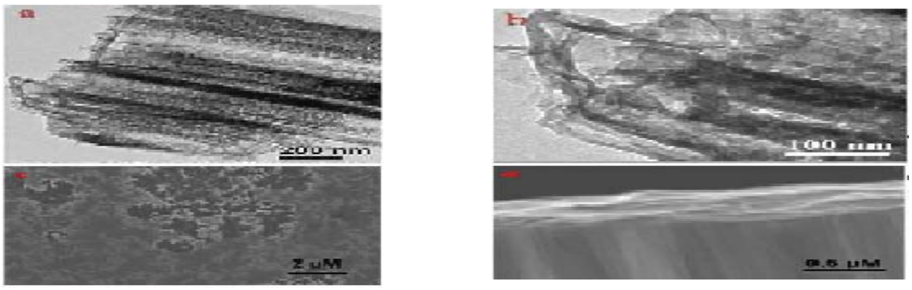


Fig. 2: TEM/SEM images and Field emission current stability of SiNWs/GO nanosheets

New electrode materials for charge storage

The focus of the work was on classical supports like nanostructure carbon forms (e.g. CNT, Graphene, CNF). Despite of high theoretical specific capacitance; low cost of Fe_3O_4 and the relatively low gravimetric capacitance is the major obstacle for broad use of Fe_3O_4 as electrode material in Supercapacitor. Highly stable and porous SWCNH supported the design of new electrode; it has boosted the applications of this functional materials. The synthesis of new SWCNH-Fe_3O_4 nanocomposite for supercapacitor was reported and the electrochemical performance was also examined.

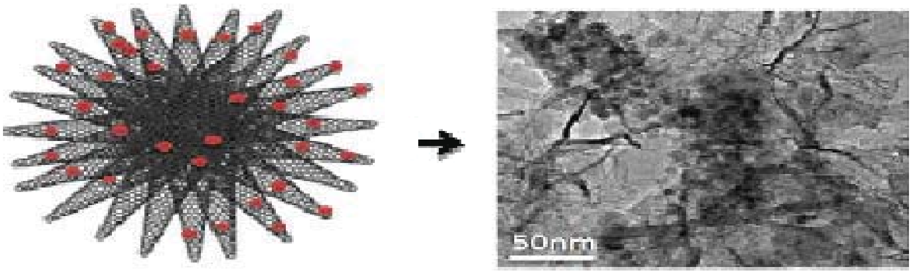


Fig. 3: Single walled carbon nanohorns-Fe_3O_4 nanocomposite supercapacitor electrode

Long-length, highly graphitized SWNTs

S.P.Gokhale
sp.gokhale@ncl.res.in

Long-length, highly graphitized SWNTs

Carbon nanotubes (CNTs) were modified with a suitable post-synthesis functionalization or during the synthesis itself by controlling the process conditions depending on the requirement of a particular application. Selective growth of single-walled CNTs (SWNTs) was achieved during nucleation by changing the catalyst composition or structure and controlling the kinetic parameters. The highly graphitized SWNTs were synthesized by employing improved nitrogen-pretreated Fe-Mo/MgO catalyst nanoparticles in a thermal CVD and studied the effects of nitrogen pretreatment of the catalyst on the structure and properties of SWNTs. Simple nitrogen pretreatment was demonstrated to enhance the catalytic activity, which in turn promoted the CNT growth mechanism to form long length, isolated and highly graphitized SWNTs. It also improved the thermal properties of SWNTs.

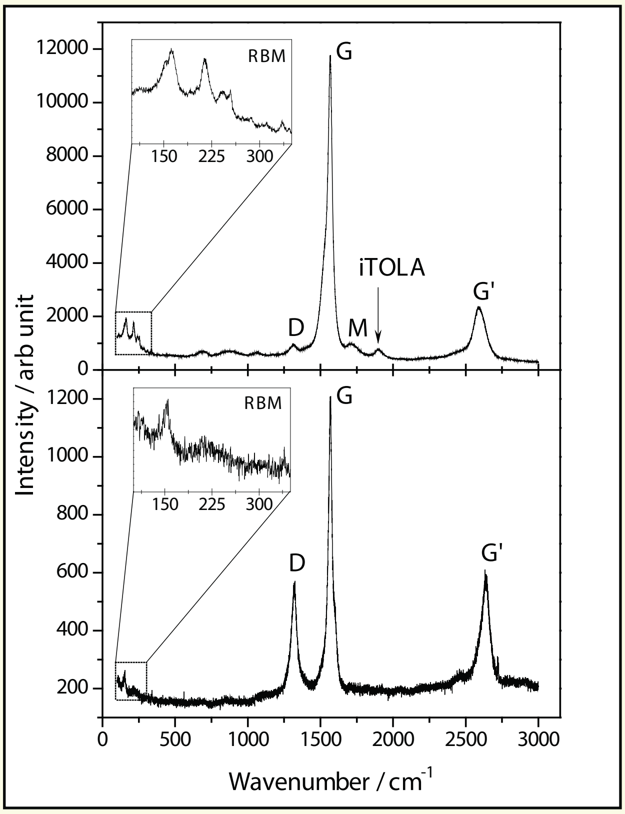


Photo-responsive materialsfor dye sensitized solar cells and organic solar cells

J. Nithyanandhan
j.nithyanandhan@ncl.res.in

The objective of this work was to design and synthesize photoactive molecules for photovoltaic devices. Research activities were focused on modulation of the photo-physical properties of dyes by encapsulation towards increasing the photovoltaic efficiencies. It also aimed to design and synthesize the organic dyes for panchromatic light absorption. Focus was also on photo chemical reactions for processing the semiconducting materials.

Modulating the photo-physical properties of dyes towards increasing the photovoltaic efficiencies

Conversion of light energy to electrical energy in dye sensitized solar cells (DSSCs) comprised of 4 steps; light absorption to promote an electron from HOMO to LUMO of the dye; charge injection from LUMO of the dye to conduction band of the TiO_2, dye regeneration with the aid of electrolyte/hole transport material and charge collection at metal counter electrode. Dye aggregation and charge recombination processes reduced the efficiency of a DSSC. Both molecular and supramolecular approaches were utilized to isolate the dyes from the bulk in order to avoid the molecular aggregation on TiO_2 surface and to avoid the charge recombination by tailoring hydrophobic functionalities that prevent the diffusion of electrolyte near to TiO_2 surface.

Photo chemical reactions for processing the semiconducting materials

Processing semiconducting materials is a key issue to achieve high efficient devices. Solution based processing is an attractive method over high vacuum based thermal evaporation methods as it provides control on morphology of the active layer. Most of the organic semiconducting materials are not soluble in common organic solvents. A series of soluble precursors that provide insoluble and highly conjugated materials upon photolysis was designed to overcome such problem. The soluble precursors were solution processed to obtain the film upon exposure to light and intra-molecular cyclisation nature; the photoreaction affords the conjugated product.

Multi-functional nanohybrid materials for clean energy and health

Kaliaperumal Selvaraj
k.selvaraj@ncl.res.in

Publication: Biol. Trace Elem. Res., 2013, DOI10.1007/s12011-014-9891-0

2-D Carbon-Inorganic oxide based multifunctional nanohybrid materials

Morphology controlled high surface area inorganic components, remarkable nanohybrid materials with tunable semi-conductance have been created in the lab. A spectrum of characterization reveals their high potential for applications where challenging electrical isolations at nanoscopic domains are demanded such as super/ultra-capacitors. This interesting case of invention of a novel near-ambient way of making 3D graphene material has led to filing a patent recently. This simple and fast method to make 3D graphene has potentiality for its large scale production which is still considered to be a difficult task. An activated self-assembly mechanism (supported through DFT based first principle calculations) observed to make this possible. By this way, it allows to fine tune its electrical conductivity up to about 4 - 5 orders of magnitude. The fabrication through stacking the highly conducting GO and poorly conducting inorganic layer alternatively in nanometric dimensions increases its potential to be used as super/ultra-capacitors. A confinement experiment of magnetic nanoparticles showed a further larger scope for material confinement and isolation at nanoscale. In addition, a great deal of mechanistic understanding has been achieved through a concerted approach using molecular spectroscopies and density functional theory based quantum chemical calculations on the direct dimensional conversions of layered carbon materials.

Graphene – inorganic nanohybrid materials for bio-imaging applications

Inorganic ordered mesoporous materials with large surface area and pore volumes in combination with carbon layers of graphene and its oxides have been synthesized that showed interesting characteristics to hold drugs and high contrast agents for bio-imaging. Mesoporous silicates such as MCM-41 of controlled particle sizes (~ 100nm) have been hybridized with 1 to 3 layered isolated graphene oxide sheets. The nano-hybrid material developed showed relatively higher drug/dye loading efficiencies of up to 1.6 and 1.31 wt. % for the dyes used in imaging techniques such as Indocyanine green (ICG) and Rhodamine B (RhB). They showed a quantum yield of about 0.04 to 0.08.

A systematic spectroscopic studies suggest that chemical modifications for improving with designed functionalities help in achieving this. Similar material synthesized to entrap magnetic nanoparticles of iron oxide (Fe_3O_4) showed excellent model drug loading efficiencies. This interesting case of invention has been further studied to know the interfaces between the different components involved. In collaboration, small metal nanoparticles having potential in similar applications were synthesized through biological means and were investigated for their stability and toxicities.

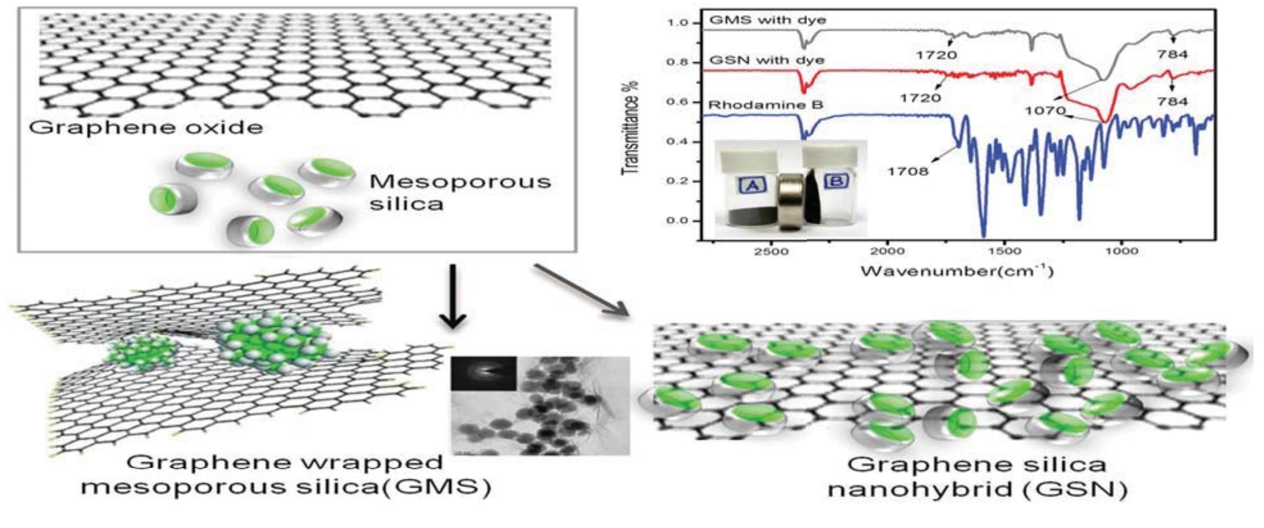


Illustration of the nanohybrid system using mesoporous silica and graphene oxide and confinement of magnetic nanoparticles (TEM image: inorganic nanoparticle wrapped by graphene oxide sheets, Right Image: Materials without (A) and with (B) magnetic nanoparticles)

Biodegradable polymers and functionalization of cellulose

A. J. Varma
aj.varma@ncl.res.in

Publications: Adv. Mater. Phys. Chem., 2013, 3, 112;
Trends Carbohyd. Res., 2013, 5, 7

Polymers from renewable resources

Sugar was used to functionalize hydrocarbon polymers so as to build properties like biodegradability and biocompatibility.

Oxidized cellulose shows ever increasing applications in anti-microbial medical products and many hi-tech electronic applications including hybrid materials. Investigations were done for fundamental and application aspects of various oxidation products of cellulose. These products were prepared using a variety of oxidation systems, structural analysis of the functional groups on the oxidized cellulose, and their stabilities, solubilities, biodegradability and anti-microbial properties.

Biodegradable polymers

Commodity elastomers like SBS have become an integral part of society. However, these synthetic polymers resist microbial degradation when discarded in landfills. One possible method of introducing biodegradability into non-biodegradable hydrocarbon polymers some functional groups along the SBS polymer chain has to introduce. It was previously demonstrated that functionalization of maleated polystyrenes with minute quantities of sugars lead to a significant increase in the extent of their biodegradation. This work was further demonstrated that functionalization of a commodity elastomer like SBS with sugars is possible by employing click chemistry technique. Preliminary studies showed such polymers biodegrade to a significant extent.

It was observed that incorporation of minute quantities of sugar (0.09 - 0.37 wt %) pendants on SBS copolymer main chain renders it biodegradable. ~4-14 fold weight loss for bacterial pseudomonas sp. and ~7-36 fold weight loss for fungal cultures (Aspergillus niger) were observed as ratio of percent weight loss to percent sugar content of SBS. These results were corroborated by SEM studies, where biodegraded samples showed distinct cavities, whereas un-degraded samples showed smooth surfaces.

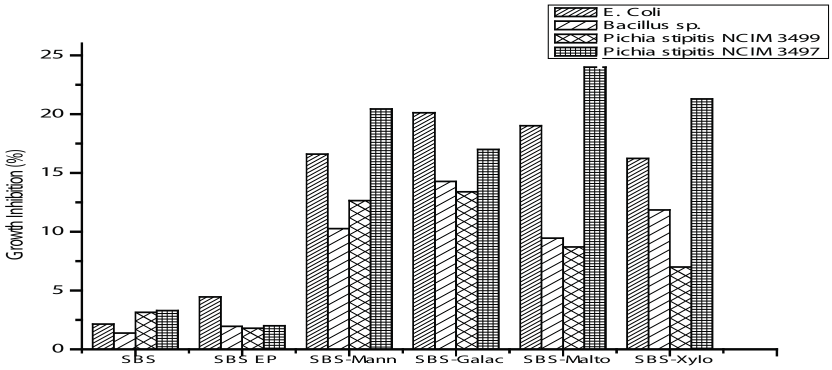


Fig. 1: Growth inhibition after 24h with carbohydrate functionalized SBS having cationic nitrogen pendants against *E. coli, Bacillus sp., Pichia stipitis* NCIM 3499 and *Pichia stipitis* NCIM 3497.

Conjugated polymers for sensors and photovoltaic applications

Asha S. K.
sk.asha@ncl.res.in

Publications: Adv. Funct. Mater 2013, 23, 2033; J. Polym. Sci. A Pol. Chem., 2012, 51, 509; J. Mater. Chem. 2012, 22, 15235; Macromolecules 2013, 46, 2159

Conjugated polymers provide a good platform for a wide variety of applications such as light emitting diodes, polymer solar cells, field effect transistors and sensors.

Self-assembly in tailor-made polyfluorenes: Synergistic effect of porous spherical morphology and FRET for visual sensing of bilirubin

A conjugated polymer based sensor for sensing bilirubin was reported. The work described the selective and sensitive detection of Bilirubin using conjugated polymer based on Polyfluorene. Abnormal level of bilirubin in body fluids is potentially toxic. By taking advantage of overlapping photophysical properties of bilirubin and polyfluorenes; a model Polyfluorene sensor to detect unconjugated bilirubin via FRET process was developed for the first time. Efficient energy transfer between polyflourene and bilirubin enabled naked eye detection of bilirubin using hand-held UV lamp.

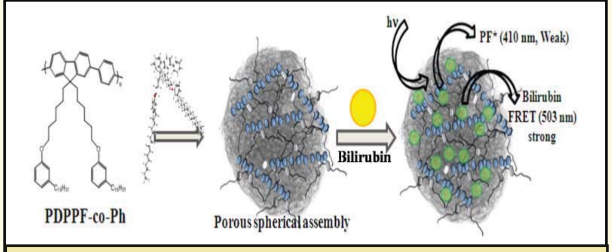


Fig. 1: Schematic representation of the mechanism of FRET induced bilirubin sensing using Polyfluorene

Nanostructured crystalline comb polymer of perylenebisimide by directed self-assembly: Poly(4-vinylpyridine)- pentadecylphenol perylenebisimide

Non-covalent interaction like hydrogen bonding was used to obtain well defined nanostructured polymeric supramolecular assemblies between poly (4-vinylpyridine) (P4VP) and perylene-bisimide (PBI). Thin film morphology of the 1:1 complex (P4VP(PDP-UPBI)) was analyzed by using transmission electron microscopy (TEM) which showed uniform lamellar structures in the domain range of 5 – 10 nm. A clear trend of improved electrical parameters was observed for the complex compared to pristine PBI from space charge limited current (SCLC) measurements.

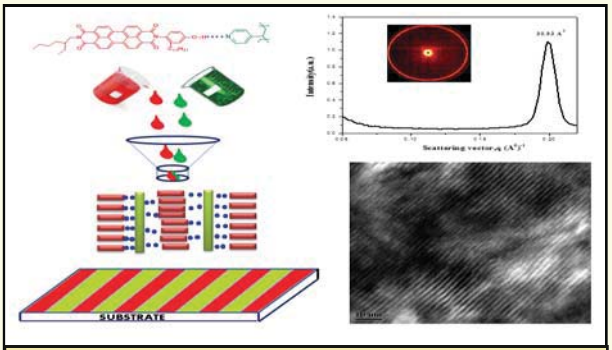


Fig. 2: 1:1 Supramolecular complex formation of an unsymmetrical perylenebisimide (PDP-UPBI) with poly (4-vinylpyridine) (P4VP) resulting in the formation of uniform lamellar structures in the domain range of 5 – 10 nm

A facile one-pot reactive solution blending approach for main chain donor-acceptor polymeric materials

A high temperature solution blending process was used to incorporate donor-acceptor semiconducting materials based on oligo(p-phenylene vinylene) (OPV) and Perylenebisimide (PBI) into the backbone of an engineering thermoplastic polyester [Poly(1,4-cyclohexylenedimethylene-1,4-cyclohexanedi-carboxylate)] (PCCD). Transesterification was achieved in presence of minimum amount of a high boiling solvent like ortho-adichlorobenzene (ODCB) at high temperature (150- 185°C) in presence of a transesterification catalyst. The advantages of solution blending over melt condensation are its ease of synthesis, high incorporation (> 30 mole % of PBI) of the desired chromophore while still retaining high molecular weight and solubility in common organic solvents.

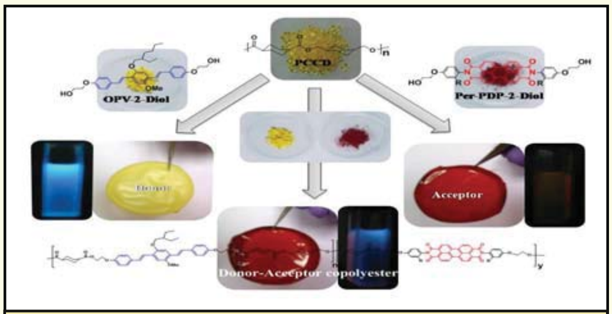


Fig 3: Structure of the high temperature solution blended donor (OPV) / acceptor (PBI) polymer incorporated into the engineering thermoplastic polyester PCCD

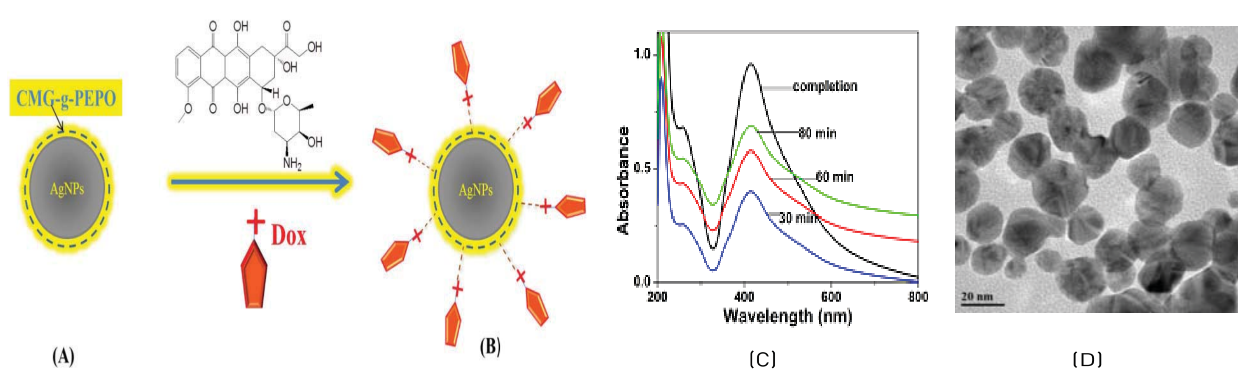
Synthesis of Ag-nanoparticles using thermo-associating polymer

M. V. Badiger
mv.badiger@ncl.res.in

Development of new associating polymers from renewable resources and their applications

The purpose was to find alternative, eco- friendly chemicals for the synthesis of nanoparticles. The synthesis and characterization of silver nanoparticles (Ag-NPs) using thermo-associating polymer namely, Carboxymethylguargum-g-Poly (ethylene oxide-co-propylene oxide) [CMG-g-PEPO] as reducing agent as well as capping agent was done. The advantage with CMG-g-PEPO was that, it played a dual role of capping as well as reducing agent during the synthesis of Ag-NPs.

Further, the polymer layer on the nanoparticles was made hydrophilic or hydrophobic with a small change in the temperature which helped in the controlled drug delivery. The conformation of formation of Ag-NPs was performed using UV/Vis spectroscopy. The optical and morphological properties of the Ag-NPs were studied using XRD, XPS, TEM and Raman spectroscopy. Use of these nanoparticles in controlled drug delivery of Doxorubicin hydrochloride (DOX), a well-known anticancer drug was demonstrated.



(C)

(D)

Fig. 1: (A) End-capped Ag-NP; (B) Ag-NP with DOX; (C) UV-Vis spectra of Ag-NP; (D) TEM image of Ag-NPs

Transition metal catalyzed reaction enhanced by supramolecular ligands and polymerization

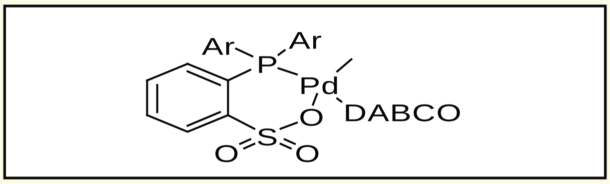
Samir H. Chikkali
s.chikkali@ncl.res.in

Publication: ChemCatChem., 2013, 5, 2785

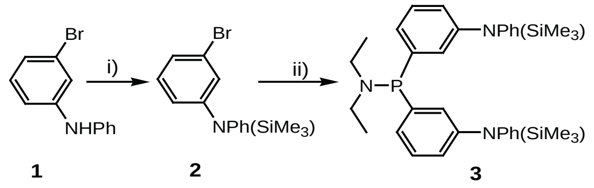
This work was aimed to design catalysts with inbuilt hydrogen bonding motif and test these catalysts in various catalytic transformations. The purpose was to address the limitations of the existing catalytic systems by employing hydrogen bonding motifs and thereby facilitate the transformation to achieve the desired targets.

Insertion (co)polymerization of functional olefins

A phosphinesulfonate-Pd complex with DABCO as a labile donor was developed. It incorporated various functional olefins. It is possible that DABCO can be replaced by olefin and the (functional) olefin insertion (co)polymerization will be facilitated.



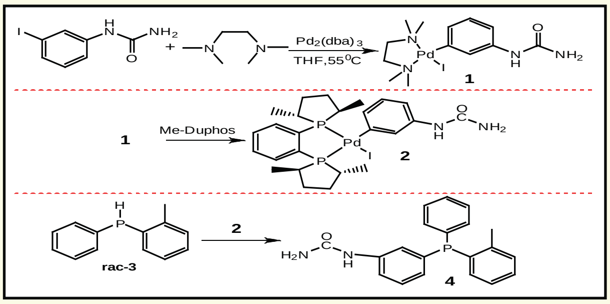
Highly desirable synthesis of a phosphine-sulfonate ligand bearing a hydrogen bonding motif was aimed. The synthesis of aminophosphine intermediate 3 was done to implement a special strategy. The intermediate was utilized to prepare the desired hydrogen bonding phosphine-sulfonate ligand.



Scheme 1: Synthesis of hydrogen bonding ligands

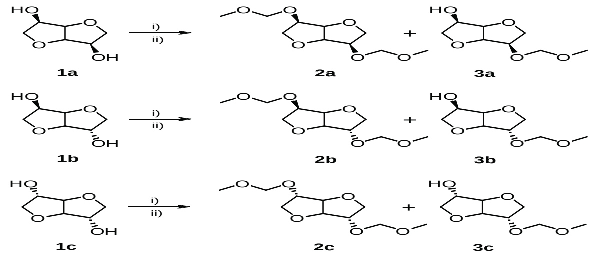
Synthesis of *p*-stereogenic supramolecular ligands

Although *P*-chiral phosphines were the first chiral ligands applied in homogeneous catalysis, it was supplanted by phosphines having the chirality on the backbone and the development of *P*-chiral phosphines was incredibly slow. This was due to the difficulty of synthesis of *P*-chiral compounds which were traditionally generated with stoichiometric amount of chiral auxiliary or through resolution techniques. One objective was to circumvent the stoichiometric process and develop catalytic protocol. Thus a catalytic synthesis of *P*-stereogenic supramolecular phosphine 4 was established in a catalytic protocol.

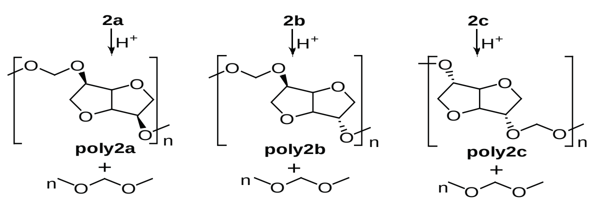


Renewable and sustainable polymers

The synthesis of isohexide-based diacetal monomers, leading to fully biobased polycondensate was established. The polymerization was catalyzed by *para*-toluenesulfonic acid and was performed at 70-100°C under 0.1 mbar vacuum. The molecular structure of the novel polyacetals was unambiguously established using various spectroscopic and analytical tools. In a typical *2D* NMR experiment [HSQC (^{1}H-^{13}C-)], all protons with matching multiplicities from a polymer repeat unit were correlated with the corresponding carbon signals at anticipated chemicals shift values. Furthermore, end-group analysis by ^{1}H NMR revealed a molecular weight in the range of Mn = 2800 (isomannide-polyacetal) to 42000 (isosorbide-polyacetal). The NMR molecular weights were corroborated by Gel Permission Chromatographic (GPC) analysis in DMF at room temperature. The significantly high molecular weight of polymers at rather low polymerization temperature and short reaction time indicated the enhanced reactivity of the monomers 2a-c compared to the parent isohexides 1a-c.



i) 3 eq.NaH, RT, 24h; ii) 3 eq.CH_3OCH_2Cl, RT, 24h.



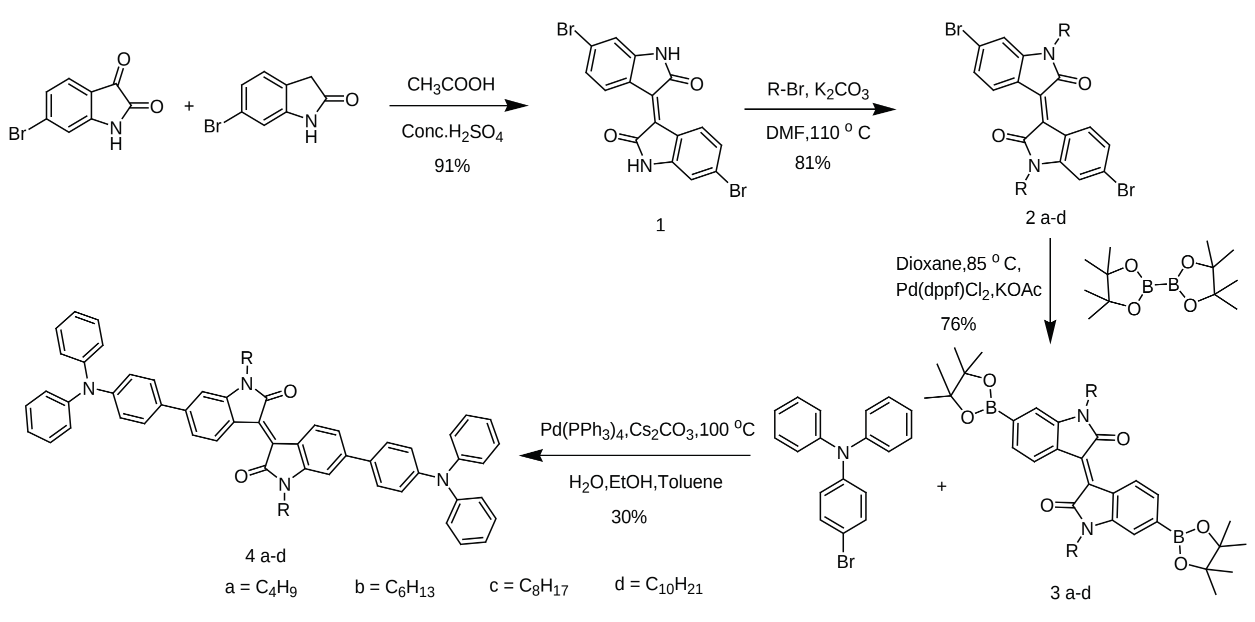
Small molecules based efficient organic field effect transistors

K. Krishnamoorthy
k.krishnamoorthy@ncl.res.in

Small molecules can be synthesized with precise molecular weight and high purity unlike its polymeric analogs. However, it does not show high efficiency in electronic devices while processing from solution. The research group imparted the advantages of polymers into a small molecule and fabricated a field effect transistor with high efficiency.

Small molecules and oligomers can be synthesized with very high purity and precise molecular weights, but they often don't form uniform thin films while processing from solution. Decreased intermolecular contact between the small molecules is another disadvantage. To increase the intermolecular contact in small molecules, group has chosen *i*-indigo, as one of the conjugated molecular unit. These *i*-indigo molecules also facilitate intermolecular contacts due to quadrupole interactions. The electron poor *i*-indigo was connected with electron rich triphenylamine to synthesize a donor-acceptor-donor type small molecule. The propeller shaped triphenylamine helped to increase the solubility of the small molecule as well as isotropic charge transport. Four D-A-D small molecules were synthesized with varying alkyl chain length (butyl, hexyl, octyl and decyl). The intermolecular spacing increased as a function of increase in alkyl chain length.

However, overall the intermolecular spacing between the molecules was found to be low compared to similar molecules and doesn't vary as a function of thermal annealing. This implies that the intermolecular contacts between the small molecules are enhanced and it doesn't vary as function of thermal annealing. Organic field effect transistors (OFET) were fabricated using a small molecule exhibited a hole carrier mobility (μ) of 0.3 cm^2/Vs before thermal annealing. A marginal increase in μ was observed upon thermal annealing at 150°C, which was attributed to changes in thin film morphology. The morphology of the thin films plays an important role in charge transport in addition to the intermolecular spacing that can be modulated with judicious choice of the conjugated molecular unit.



Scheme 1. Synthesis of D-A-D small molecules

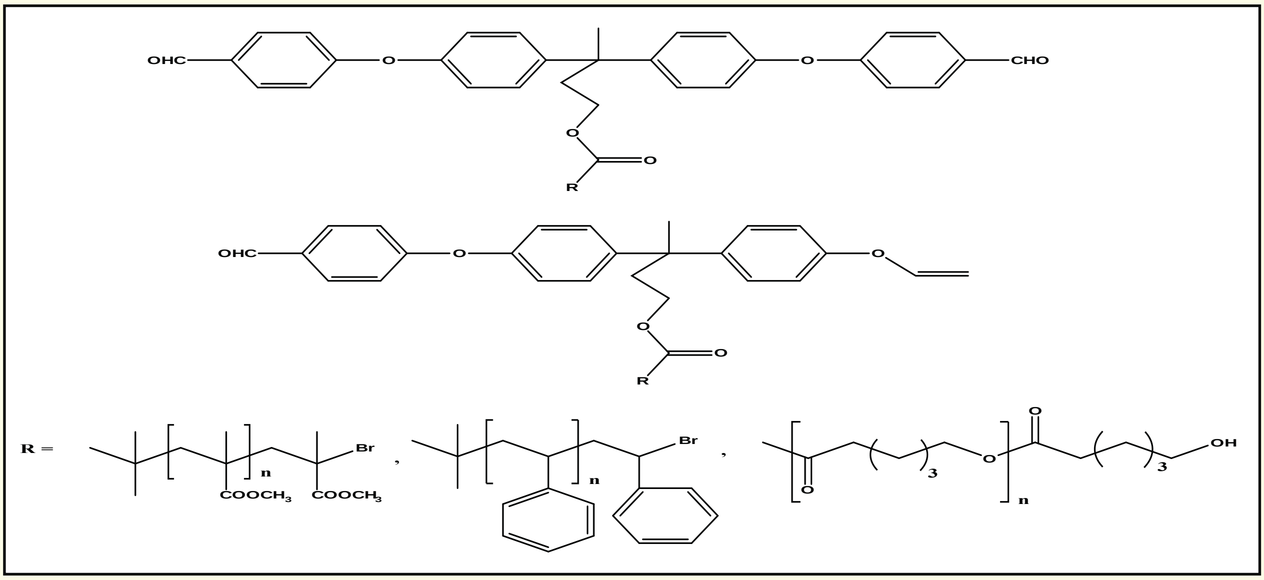
Design of macromolecular architectures by controlled polymerization methods

Prakash Wadgaonkar
pp.wadgaonkar@ncl.res.in

Publications: React. Funct. Polym., 2012, 72, 713; J. Polym. Sci. Pol. Chem., 2013, 51, 2091

Research was aimed to design and synthesize well-defined functionally-terminated polymers by employing controlled polymerization methods such as Atom Transfer Radical Polymerization (ATRP), Ring Opening Polymerization (ROP), etc. These polymers are useful as building blocks for the construction of complex polymer architectures.

α,α’-homodifunctional and α,α’-heterodifunctional polymers possessing active functional groups were synthesized based on monomers such as methyl methacrylate, styrene and ε-caprolactone using appropriately substituted functional group containing ATRP and ROP initiators as depicted below. Functional group containing ATRP and ROP initiators were in turn synthesized starting from levulinic acid which was a platform chemical obtained from biomass and were demonstrated to be useful initiators for controlled polymerization of the intended monomers. α,α’-homodifunctional and α,α’-heterodifunctional polymers represent a valuable precursor for the synthesis of block shaped and Y-shaped Miktoarm star copolymers.



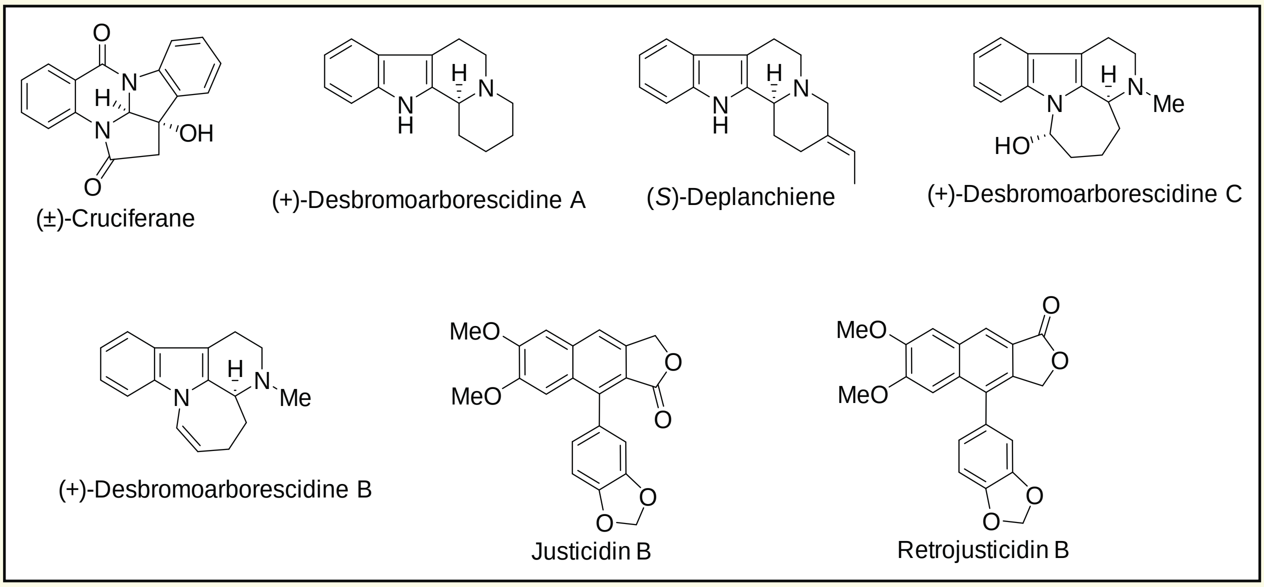
Total synthesis of recently isolated bioactive natural products

N. P. Argade
np.argade@ncl.res.in

Publications: Org. Lett., 2013, 15, 14, 4006; J. Org. Chem., 2013, 78, 6802

Total synthesis of bioactive natural products occupies a keystone position in organic chemistry. The real challenge was to design these molecules with highly efficient practical routes. Total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors was done by employing variety of new synthetic strategies.

The list of natural products synthesized included cruciferane, desbromoarborescidines A–C, deplancheine, justicidin B and retrojusticidin B. The remarkable selective aryne insertion reactions, stereoselective reductive intramolecular cyclization, exchange of nitrogen regioselectivity in intramolecular cyclization and the palladium-promoted [2+2+2] cocyclization were the involved key steps.



(±)-Cruciferane

(+)-Desbromoarborescidine A

(*S*)-Deplanchiene

(+)-Desbromoarborescidine C

(+)-Desbromoarborescidine B

Justicidin B

Retrojusticidin B

C–C Bond formations using aryne chemistry and NHC organocatalysis

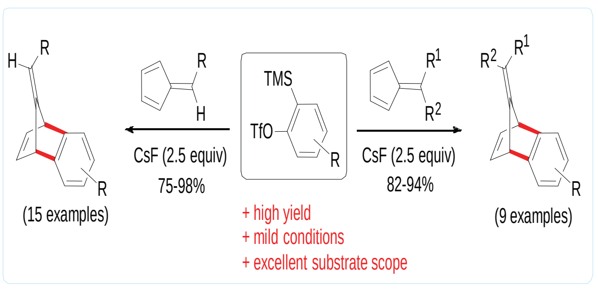
A. T. Biju
at.biju@ncl.res.in

Publications: Org. Lett. 2012, 14, 2830, 6238, 2013, 14, 1756; Adv. Synth. Catal., 2013, 355, 1089; Green Chem., 2013, 15, 1608

The transition-metal-free carbon-carbon bond-forming reactions using arynes resulted in the one-pot construction of molecular complexity, which were applied to the synthesis of various heterocyclic scaffolds and 1,2-disubstituted arenes. The application of arynes in transition-metal-free multicomponent coupling reactions, pericyclic reactions and insertion reactions were examined. The group has been working on NHC-organocatalyzed umpolung (reversal of normal mode of reactivity) of aldehydes, which can lead to the formation of nucleophilic acyl anion intermediates, homoenolate intermediates and enolate intermediates depending on the reaction conditions. It resulted in the construction of various carbocycles and heterocycles via unique carbon-carbon and carbon-heteroatom bond-forming reactions.

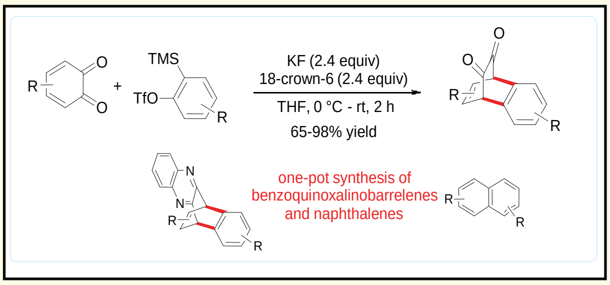
Diels-Alder reaction of pentafulvenes with arynes

A high-yielding, versatile and practical Diels-Alder reaction of pentafulvenes with arynes under mild reaction conditions was developed. The aryne generated by the fluoride induced 1,2-elimination of 2-(trimethylsilyl)aryl triflates undergoes efficient cycloaddition with 6-substituted and 6,6-disubstituted pentafulvenes leading to the formation of benzonorbornadiene derivatives. Broad substrate scope, high yields, and mild reaction conditions are the noteworthy features of the present reaction. The benzonorbornadienes have potential applications in organic chemistry. Ring opening metathesis polymerization (ROMP) by using Mo carbene initiators afforded highly stereoregular polymers. Also, the addition of benzonorbornadienes to 4-phenyl-4H-1,2,4-triazole-3,5-dione (PTAD) resulted in a convenient entry to polycyclic azoalkanes, which were valuable target molecules.



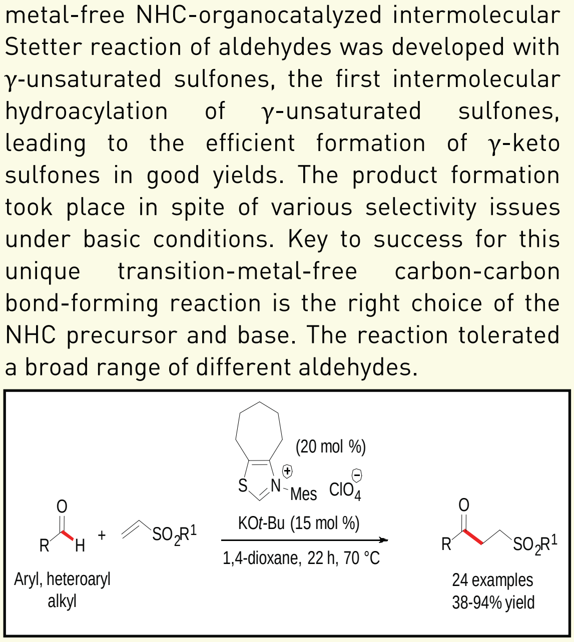
Diels-Alder reaction of 1,2-benzoquinones with arynes

A new protocol for the efficient Diels-Alder reaction of 1,2-benzoquinones with arynes was reported. The aryne generated by the fluoride induced 1,2-elimination of 2-(trimethylsilyl)aryl triflates undergone a facile Diels-Alder reaction with 1,2-benzoquinones affording the dioxobenzobicyclooctadienes in good to excellent yields. In addition, this methodology was applied to the one-pot synthesis of benzoquinoxalinobarrelene and naphthalene derivatives. The dioxobenzobicyclooctadiene derivatives are potentially amenable to a number of synthetic transformations including various photochemical reactions of the bicyclo [2.2.2] octadiene moiety as well as the reaction of 1,2-diketo group.



Synthesis of γ-Keto sulfones by NHC-catalyzed intermolecular stetter reaction

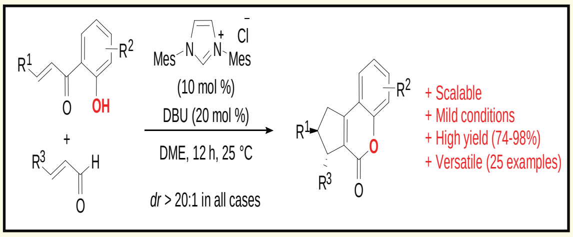
In the area of NHC-organocatalysis, a transition-metal-free NHC-organocatalyzed intermolecular Stetter reaction of aldehydes was developed with γ-unsaturated sulfones, the first intermolecular hydroacylation of γ-unsaturated sulfones, leading to the efficient formation of γ-keto sulfones in good yields. The product formation took place in spite of various selectivity issues under basic conditions. Key to success for this unique transition-metal-free carbon-carbon bond-forming reaction is the right choice of the NHC precursor and base. The reaction tolerated a broad range of different aldehydes.



C–C Bond formations using aryne chemistry and NHC organocatalysis

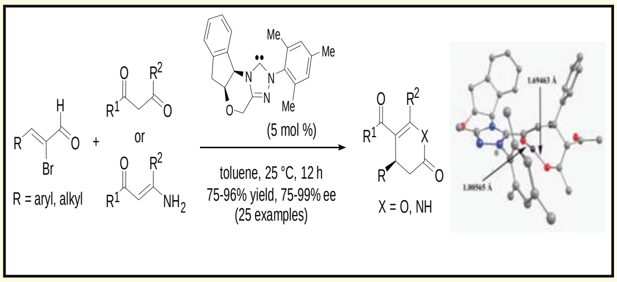
NHC-catalyzed reaction of enals with hydroxy chalcones: Diastereoselective synthesis of functionalized coumarins

The N-Heterocyclic carbene-catalyzed annulation of enals with 2′-hydroxy chalcones was uncovered which afford cyclopentane-fused coumarin derivatives with excellent level of diastereocontrol. The reaction tolerated a broad range of functional groups and proceeded under mild conditions; 25 examples were given and a preliminary mechanistic investigation was done. Notably, functionalized coumarin derivatives are important synthetic targets due to their biological properties and some of them are endowed with important fluorescent properties.



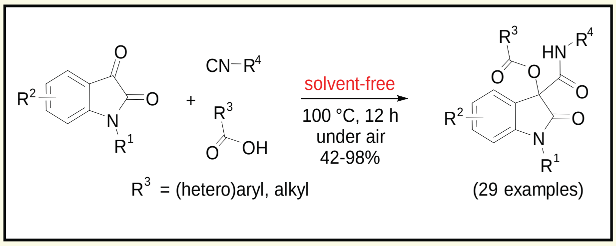
Enantioselective NHC-catalyzed annulations of 2-bromoenals with 1,3-dicarbonyl compounds and enamines via chiral α,β-unsaturated acylazoliums

The NHC-catalyzed generation of chiral α, β-unsaturated acyl azoliums from 2-bromoenals followed by its interception with 1,3-dicarbonyl compounds or enamines, the formal [3+3] annulation reaction was exposed. The reaction resulted in the enantioselective synthesis of synthetically and medicinally important dihydropyranones and dihydropyridinones and tolerated a wide range of functional groups. It was noteworthy that the reaction took place under mild reaction conditions utilizing relatively low catalyst loadings. In addition, based on DFT calculations, a mechanistic scenario involving the attack of nucleophile from below the plane of the α, β-unsaturated acyl azoliums, and the mode of enantioinduction was realized.



Engaging isatins in solvent-free, sterically congested passerini reaction

A facile, atom-economic and environmentally-benign protocol was developed for the synthesis of biologically important 3-acyloxy 3-carbamoyl indol-2-ones in high yields by employing isatins as carbonyl compound surrogates in Passerini reaction carried out under solvent-free conditions. In addition, electron-deficient phenols can also be used as the acid component in this reaction. Notably, oxindoles having a quaternary benzylic centre represent a common structural motif in many natural products and biologically active compounds.



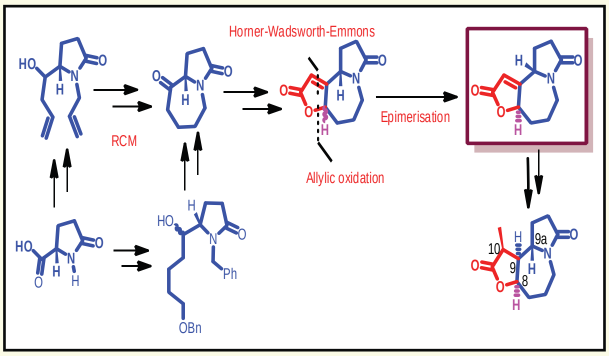
Methodologies, asymmetric synthesis and organometallics

S. P. Chavan
sp.chavan@ncl.res.in

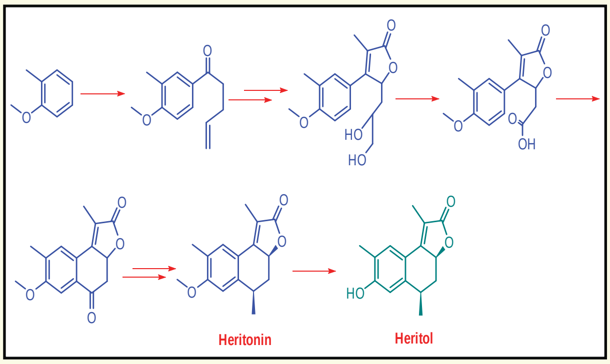
Publications: Tetrahedron Lett., 2012, 53, 2647, 4683, 2013, 54, 1528, 2137; Tetrahedron, 2012, 68, 8509; Tetrahedron-Asymmetr., 2012, 23, 1410, 1496; Eu. J. Org. Chem., 2012, 6841

Synthesis of natural products and biologically active compounds

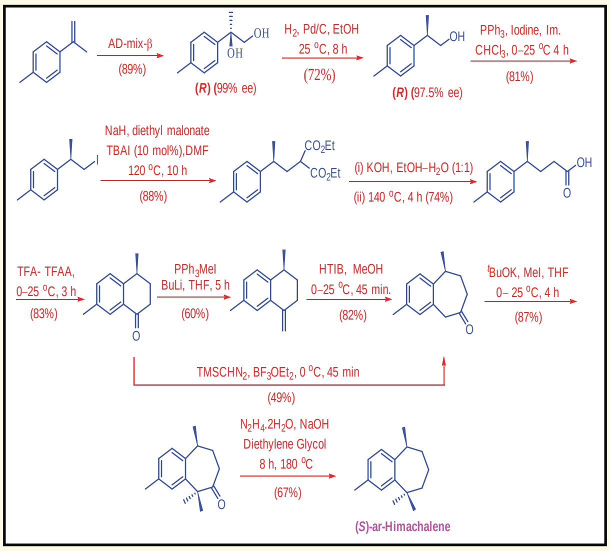
Synthesis of stemoamide: (–)-Stemoamide, one of the stemona alkaloids was isolated by Xu and coworkers in 1992 from *Stemona tuberosa* Lour and related stemona species. The research group accomplished the formal total synthesis of (–)-stemoamide by taking advantage of Ring closing Metathesis (RCM) and allylic oxidation in eleven steps in 15% overall yield. The alternate route to seven membered ring construction was developed using Grignard reaction and base induced cyclisation to furnish butenolide in fourteen steps in 11% overall yield.



Diastereoselective synthesis of (±) heritonin and (±) heritol: Miles and co-workers have isolated cadinane sesquiterpene lactones Heritol and Heritonin from the sap of the mangrove plant *Heritiera littoralis* of Philippines and other tropical countries. These plants possess ichthyotoxicity in ppm quantities to *Tilapia nilotica* fingerlings and are used by native fishermen to kill fish. The highly distereoselective total synthesis of racemic heritonin and heritol was achieved from cheap and commercially available starting materials in eight and nine purification operation in 43% and 33% overall yield, respectively which was highest overall yield reported so far.

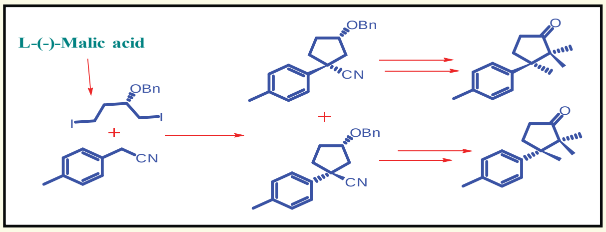


Enantioselective synthesis of pheromonal component *ar*-Himachalene: Himachalene is a structurally and biologically important class of the naturally occurring sesq-uiterpene hydrocarbons containing the synthetically challenging benzoannulene ring system. The essential oil and different constituents of *C. deodara* account for the insecticidal and larvicidal action therefore it can be used in pest management. The research group accomplished the enantioselective synthesis of both isomers of ar-himachalene. The synthetic sequence involved a sharpless asymmetric dihydroxylation reaction, hydrogenolysis, and the use of TMSCHN2 or a hypervalent iodine reagent for the ring expansion. This protocol could be of general interest and also useful for the synthesis of several complex bioactive natural and unnatural products.

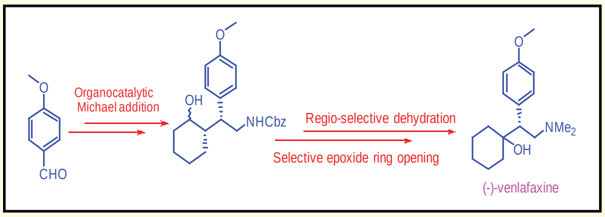


Synthesis of (+) cuparenone and (-) cuparenone: α-Cuparenone is a bicyclic sesquiterpene which exhibits itself in two isomeric forms. This sesquiterpene is a synthetic challenge to organic chemists due to presence of two contiguous quaternary centers, one of which is stereogenic in cyclopentane ring. The synthesis of both the enantiomers of α-αuparenone was achieved in ten steps involving one diastereomeric separation, starting from L- Malic acid and 4-methyl benzyl cyanide, led to (*S*)-(+)-cuparenone and (*R*)-(-)-cuparenone in ≥99 % and 15 % overall yield.

Methodologies, asymmetric synthesis and organometallics

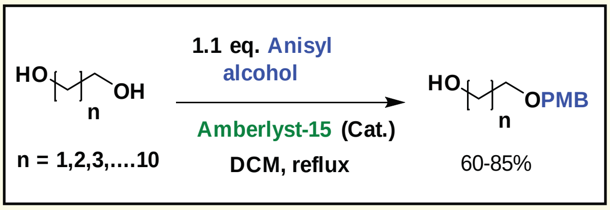


Asymmetric synthesis of antidepressant venlafaxine: Venlafaxine, a new generation antidepressant drug is being used for the treatment of major depressive disorder (MDD), generalized anxiety disorder and comorbid indications in certain anxiety disorders for depression. Research group accomplished asymmetric total synthesis of (–)-venlafaxine from commercially available, cheap starting material by using an environmentally friendly proline-based catalyst. By using different enantiomers of proline-based catalyst both the enantiomers of venlafaxine in a very concise manner can be accessed.

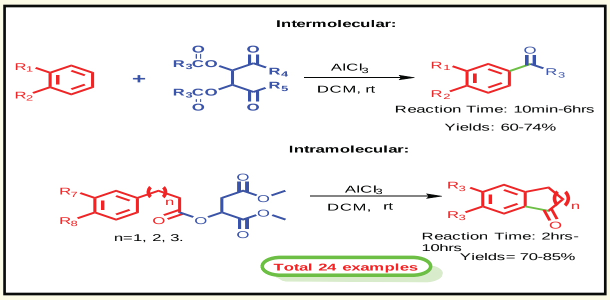


Development of synthetic methodologies

A mild, convenient and practical methodology for PMB protection of alcohols: 4-Metho-xybenzyl (PMB) protection of alcohols is an important step in the synthetic sequence. Conventional methods for the PMB protection of alcohols require the use of strong bases like NaH, *n*-BuLi *etc* and the use of unstable *p*-methoxy benzyl bromide/chloride as the reactant. A methodology was devised which utilized a commercially available Ambertlyst-15 resin as a heterogenous catalyst and anisyl alcohol as the reactant. The use of heterogenous catalyst offers advantages over conventional reagents in terms of selectivity, ease of operation and reusability of the resin and simple work-up after the reaction is over. This methodology allows selective mono PMB protection of diols and di-PMB protection of diols as per requirement.



Unprecedented, mild, efficient and simple Friedel-Crafts acylation reaction using esters: Esters normally do not undergo Fridel-Craft's acylation reactions. An important synthetic methodology was developed for the inter- and intra-molecular Friedel-Crafts acylation reaction of wide variety of activated esters with different aromatic compounds and mechanistic aspects were studied carefully by both theoretically and experimentally.



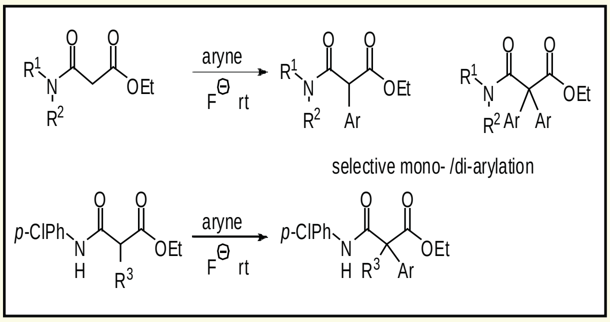
Development of synthetic methods and total synthesis of natural products

Santosh B. Mhaske
sb.mhaske@ncl.res.in

Publications: *Org. Lett.*, 2012, 14, 3994, 5804; 2013, 15, 2218; *Synth. Commun.*, 2013, 43, 1

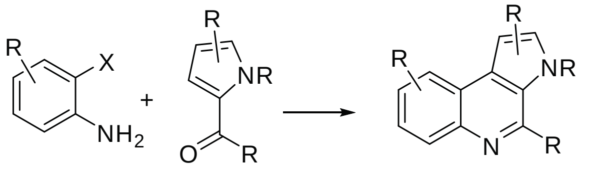
A facile, fluoride-induced transition-metal-free chemoselective α-arylation of β-dicarbonyl compounds (malonamide esters) at room temperature using aryne intermediates was demonstrated. Selective mono- or diarylation and generation of a quaternary benzylic stereocenter were also achieved. The methodology is useful for the synthesis of a library of CNS depressant barbiturate drugs like Phenobarbital.

Facile C-arylation using arynes

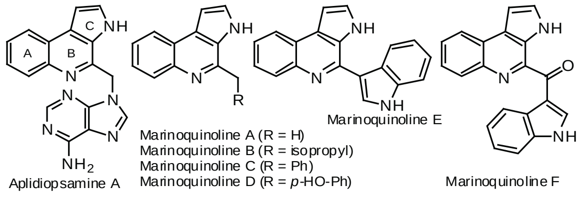


C-H activation: Direct access to pyrroloquinolines

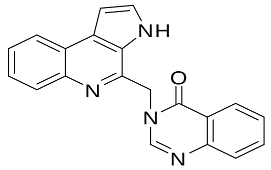
A method for palladium-catalyzed cyclization of imines was developed to construct the extremely rare 3*H*-pyrrolo[2,3-*c*]quinoline ring system for diversity oriented first total synthesis of antimalarial marine natural product Aplidiopsamine A, Marinoquinoline A and potential natural product hybrid NCLite-M1.



Two natural products, 8 entries, one new chemical entity



PDE4 inhibitors for CNS disorders

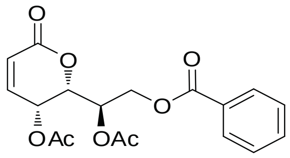


NCLite-M1

CNS / Malaria
NCE of pharmaceutical interest

Protecting group-free total synthesis of celistenolide

A short, efficient and expedient protecting group-free diastereoselective total synthesis of (±)-Cleistenolide was achieved in five steps with 60% overall yield. Achmatowicz reaction, chemoselective oxidation of secondary alcohol and diastereoselective 1,3-*anti* reduction of β-hydroxy ketone are the key features of this linear total synthesis. The synthetic strategy demonstrated herein has a potential to explore it for an asymmetric total synthesis of (–)-Cleistenolide and related bioactive natural products.



(-)-Cleistenolide

Anti-Tuberculotic

Asymmetric synthesis of biologically important compounds

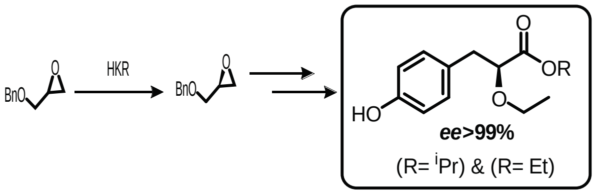
M. Muthukrishnan
m.muthukrishnan@ncl.res.in

Publications: Bioorg. Med. Chem. Lett., 2013, 23, 1416; Tetrahedron Asymmetr., 2011, 22, 1353, 2012, 23, 1512; Tetrahedron Lett., 2011, 52, 2387

Hydrolytic kinetic resolution (HKR) method is one such elegant strategy, which utilizes chiral (salen) Co complex catalysts for the preparation of terminal epoxides and vicinal diols in high enantiopurity. Easy access of terminal epoxides, high levels of selectivity, low loading and easy availability of the catalyst made this method well amenable for the preparation of plethora of biologically important compounds. The group has utilized the elegant HKR strategy for the preparation of many pharmaceutically important compounds.

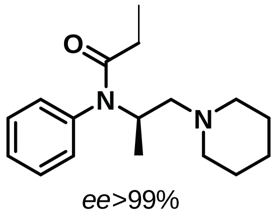
Asymmetric synthesis of ethyl-(*S*)-2-ethoxy-3-(4-hydroxyphenyl) propanoate (EEHP), a key intermediate of PPAR agonists

Ethyl-(*S*)-2-ethoxy-3-(4-hydroxyphenyl) propanoate (EEHP), is an important pharmaceutical intermediate, present in many PPAR (Peroxime proliferator-activated receptors) agonists. PPAR plays a significant role in regulating lipid and carbohydrate metabolism and their agonists have shown therapeutic application for the treatment of diabetes and dyslipidemia. In addition EEHP derivatives found application in photosensitive materials, sweetening agents, treatment of certain eating disorders, etc. Development of a practical and highly enantioselective synthetic route to EEHP was done by employing HKR strategy as a key step and a source of Chirality.

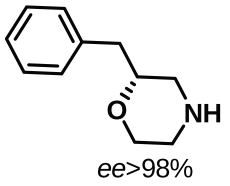


Asymmetric synthesis of EEHP employing HKR strategy

Similarly, group has utilized the HKR strategy for the synthesis of some other chiral drugs as following.



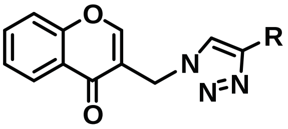
(R)-Phenampromide
(Opioid analgesic)



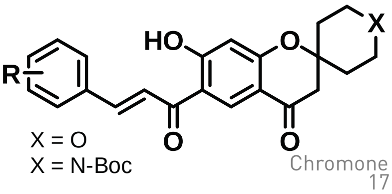
(R)-2-Benzylmorpholine
(appetite suppressant agent)

Development of novel chromone based derivatives as potent antitubercular agents

Chromone is recognized as a privileged structural motif, observed in plethora of natural products and in various therapeutic agents. Although many of the naturally occurring chromones exhibit interesting anti-TB properties, but no systematic investigations were carried out to explore its anti-TB potential. As part of research program, focus was on design and synthesis of structurally new class of compounds based upon privileged chromone scaffold and studying their anti-TB properties.



Chromone triazole conjugates
20 examples
MIC-1.56-25µg/mL(H37Rv)



Chromone chalcone conjugates
17 examples
MIC-3.25-25µg/mL(H37Rv)

Methodologies, asymmetric total synthesis of biologically active compounds

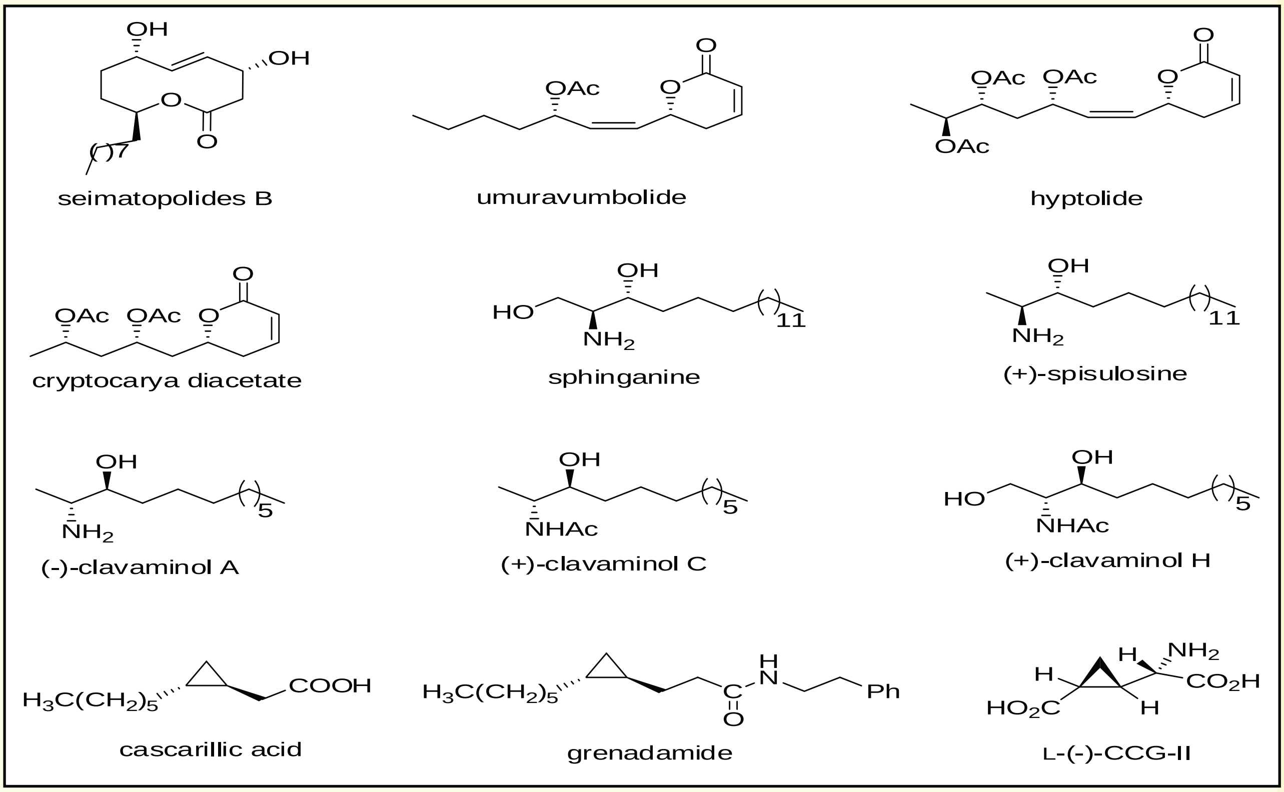
Pradeep Kumar
pk.tripathi@ncl.res.in

Publications : RSC Adv., 2012, 2, 11231; 2013, 3, 15442; Eur. J. Org. Chem., 2013, 4586; Adv. Synth. Catal., 2013, 355, 1719; Accounts Chem. Res., 2013, 46, 289

Research was focused on asymmetric synthesis of naturally occurring lactones and amino alcohols. New methodologies for the preparation of *syn/anti*-1,5-diols and *syn/syn*-1,3,5-triols were developed which serve as useful building blocks for enantioselective synthesis of biologically active natural products.

Research was done on the enantio- and diastereocontrolled conversion of chiral epoxides to trans-cyclopropane carboxylates and applied the methodology to the successful synthesis of cascarillic acid, grenadamide and L-(-)-CCG-II. The total asymmetric synthesis of a wide variety of biologically useful compounds was achieved by employing the Jacobsen hydrolytic kinetic resolution, organocatalysis, indium mediated allylation of α-hydrazino aldehyde as the source of chirality and silicon-tethered ring closing metathesis, cross-metathesis as the key steps. The target molecules including seimatopolide B, aculeatins F, solenopsin, umuravumbolide, hyptolide, cryptocarya diacetate, clavaminols, sphinganine and (+)-spisulosine. Seimatopolide B were synthesized by generating the stereogenic centers by means of Jacobsen`s HKR. In the case of umuravumbolide and hyptolide, the stereogenic centers were generated via proline-catalyzed α-aminoxylation of aldehydes and Brown's asymmetric allylation method and the olefins were constructed by exploiting temporary silicon-tethered ring-closing metathesis (TST-RCM) and Ando's protocol.

A desymmetrization approach was used for the synthesis of enantiopure *syn/anti*-1,5-diols via hydrolytic kinetic resolution (HKR) of functionalized meso bis-epoxides which was further elaborated to the synthesis of *syn/syn*-1,3,5-triols and subsequently applied to the formal synthesis of cryptocarya diacetate. A conceptually different approach was employed for the synthesis of 1,2-amino alcohols such as clavaminol A–H, sphinganine and (+)-spisulosine by proline catalyzed α-amination of aldehyde and one-pot indium mediated allylation of the crude α-hydrazino aldehydes. A DFT based quantum chemical calculations were performed to obtain a quantitative explanation of the stereoselectivity of the reaction. Some of the molecules accomplished in the total synthesis using above reactions were following.



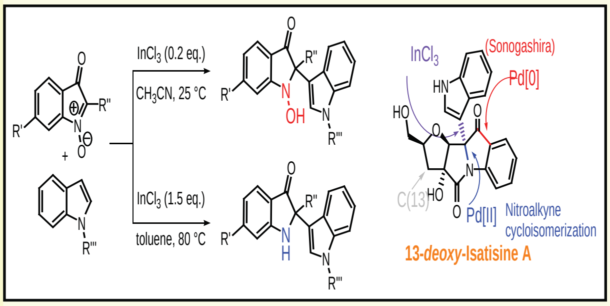
Total synthesis and metal catalysis

C. V. Ramana
vr.chepuri@ncl.res.in

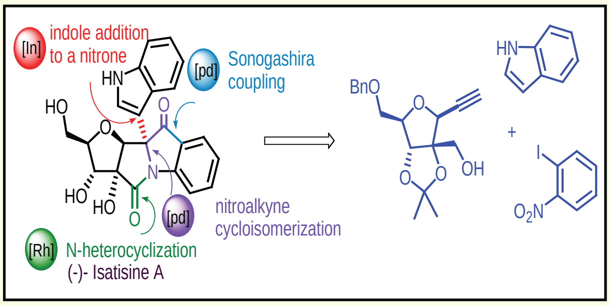
Publications: Chem. Eur. J., 2012, 18, 9601, 13288; J. Org. Chem., 2012, 77, 1566, 2169, 10509; Tetrahedron Lett., 2012, 53, 6347

Total synthesis is focused on creativity in development of new methodologies, modular strategies and providing effective platforms for the synthesis of natural products like small molecule libraries. The use of metal complexes as catalysts addressing the construction of the polycyclic frame works present in the bioactive small molecules in another active area.

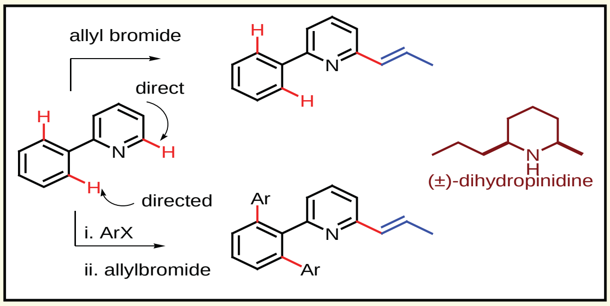
A strategy directed towards the total synthesis of isatisine A was executed. The research group has developed the selective methods for the addition of indoles to isatogens leading to either 2,2-disubstituted-N-hydroxy-indolin-3-one or 2,2-disubstituted-indolin-3-one compounds. The present methods provide the first example of the addition of indoles to the isatogen nucleus. The earlier methodology for the isatogen synthesis, taken together with the current methods has helped to synthesize the 13-deoxy-isatisine A in ten steps from an easily available sugar building block. The strategy that have developed is unique in its own and features several late-stage metal-mediated transformations (coupling, cyclization and additions, the later two being developed in this context) addressing the key carbon–carbon and carbon–hetero atom bond formations, thereby making it highly modular.



The recent total synthesis of isatisine A is a classic example wherein the compatibility of four [metal]-catalyzed / mediated transformations have been executed in a sequence by the group. This is a rare feat in total synthesis. Amongst them were the unprecedented nitroalkyne / nitroalkynol cycloisomerizations, were designed based purely on the mechanistic hypothesis. Also, the application of a [Rh]-catalyzed oxidative γ-aminoalcohol cyclization leading to the γ-lactam in the synthesis of a complex natural product was established for the first time. This paper was appeared as a "Featured article in the Journal of Organic Chemistry.



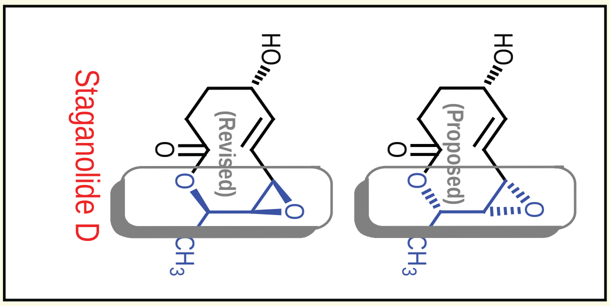
Dealing with the development of complementary C – H activations, research group has revealed the direct C – H activation of pyridine ring which was unprecedented. As an off-shoot to this exercise, the (±)–dihydropinidine was synthesized in two steps, both being catalyzed by the complexes of ruthenium and platinum in sequence. A one-pot directed and direct C–H activation comprising a total three C-H activations in one-pot were explored successfully.



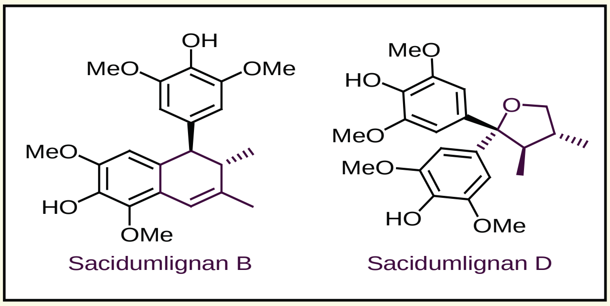
A simple protocol was developed for the stereospecific synthesis of C-arabinofuranosides featuring a furan ring transposition as the key reaction. The stereochemistry present at the C(5) of the starting hexofuranose was translated to the anomeric configuration of the resulting C-glycosides. The carba-disaccharide analogue of motif C (of cell wall AG complex of M.Tb) was also synthesized by applying a double furan ring transposition, where a C(2)-symmetric bis-hexofuranoside was explicitly converted to the corresponding disaccharide. This double furan ring transposition reported herein is the first of its kind.

Total synthesis and metal catalysis

Staganolide D, a target was selected for the (first) total synthesis in order to demonstrate the proposal on how the stereochemistry of the allylic substituents can influence the outcome of a ring closing metathesis (RCM) reaction. The group showed that the proposed structure was not the right one, despite the fact that an earlier total synthesis confirmed its proposed structure. It proved that the group that isolated staganolide D overlooked its existence as equilibrating conformational isomers.



The first total synthesis of naturally occurring sacidumlignans B and D was completed and their relative or absolute configurations were established. The synthesis of sacidumlignan A from an intermediate was executed which was used in the synthesis of sacidumlignan B. For the total synthesis of the sacidumlignan B, a dehydrative cyclization of a γ-arylaldehyde leading to the aryldihydronaphthalene units were used–which was the first of its kind. The adopted strategy employed a single advanced intermediate for all the targets executed. A diastereoselective γ-methylation of a lactone was used as the key step for the control of the chiral centers of the central lignan core.



Total synthesis of biologically active compounds and medicinal chemistry

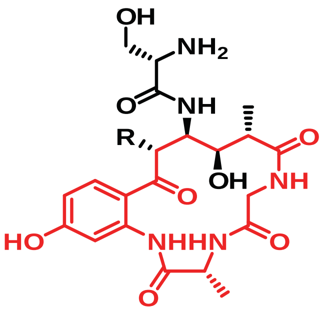
D. Srinivasa Reddy
ds.reddy@ncl.res.in

Publications: Chem. Commun., 2013, 49, 3242; Org. Lett., 2012, 14, 6222; Tetrahedron Lett., 2012, 53, 6343; WO 2013054275 A1, 2013054366 A1

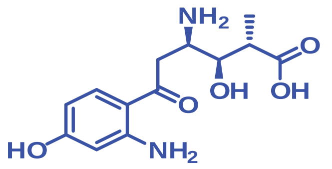
The research was focused mainly on total synthesis of biologically active compounds such as anti-inflammatory, anti-bacterial and anti-cancer agents. Significant progress on "Silicon-switch approach" was made in the medicinal chemistry front.

Synthesis of anti-inflammatory cyclic peptides solomonamides A and B

Two cyclic peptides solomonamide A and solomonamide B with unprecedented chemotype were recently isolated from the marine sponge *Theonella swinhoei* from Italy. Solomonamide A showed significant reduction (~ 60%) of inflammation in the carrageenan induced paw edema model properties at a very low concentration of 100g/kg. Because of potent *in vivo* biological activity, novel chemotype, and scarcity of the material, it is significant to access these important classes of molecules by means of total synthesis and their analog in sufficient quantities for further biological evaluation. The synthesis was accomplished of macrocyclic core and key fragment AHMOA in the program. The feasibility of key reactions was tested and established a synthetically viable route. The total synthesis, synthesis of analogues, and its biological evaluation are currently ongoing.



R = OH Solomonamide A
R = H Solomonamide B

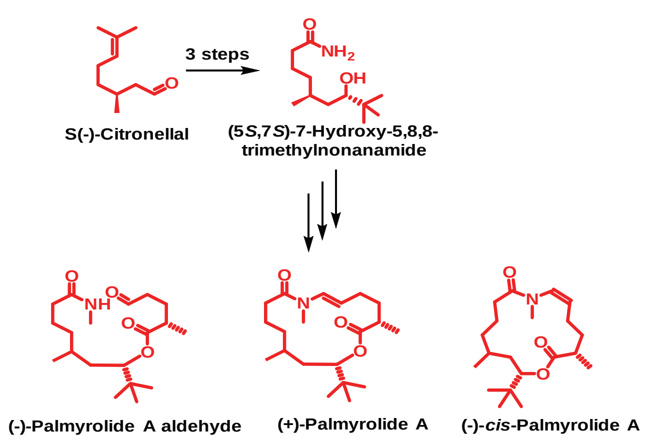


4-amino-6-(2'-amino-4'-hydroxyphenyl)-3-hydroxy-2-methyl-6-oxohexanoic acid (AHMOA)

Highlights:
- macrocyclic core synthesis
- key fragment AHMOA synthesis

Synthesis of palmyrolide A and its cis-Isomer, potential voltage-gated sodium channel blocker

Palmyrolide A, a neuroactive macrolide was isolated from the marine organism by Gerwick and co workers in 2010. Based on findings from initial *in vitro* biological screening, palmyrolide A and their analogues qualify for further biological evaluation as they may function as voltage-gated sodium channel (VGSC) blockers. The interesting biological profile along with its two rare structural units as the tertiary butyl group adjacent to lactone moiety and *trans-N*-methyl-enamide motif, make this compound as an attractive target for synthetic chemists. The total synthesis of (-)-palmyrolide A aldehyde and (+)-palmyrolide A and (-)-*cis*-palmyrolide A was accomplished using chiral pool approach, Zhu's oxidative homologation of an aldehyde to primary amide, access to (–)-*cis*-palmyrolide A, and the protecting group-free total synthesis. Calculations with DFT (with the help of Dr. Vanka Kumar) have provided insight into the *trans-cis* conversion process and corroborated experimental findings.

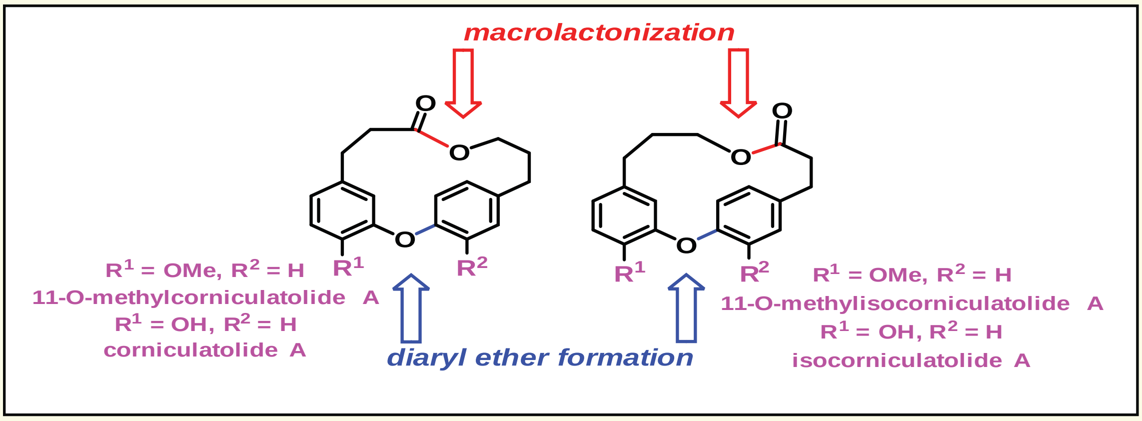


S(-)-Citronellal
(5*S*,7*S*)-7-Hydroxy-5,8,8-trimethylnonanamide
(-)-Palmyrolide A aldehyde
(+)-Palmyrolide A
(-)-*cis*-Palmyrolide A

Total synthesis of biologically active compounds and medicinal chemistry

Synthesis of isomeric corniculatolides

Synthesis of three natural macrolides 11-*O*-methylcorniculatolide A, 11-*O*-methylisocorniculatolide and isocorniculatolide A were reported using simple, straight forward and high-yielding route. The present synthesis confirms the assigned molecular structures and provided an access to sufficient quantities of natural products for the biological evaluation. In addition, it has determined the anti-TB potential of the three natural compounds using Alamar-blue assay (H_37R_v) and found no significant inhibitory activity at 100g/ml. Excellent yield, short sequence, and useful SAR information are the highlights of this work.



Medicinal chemistry: Silicon-switch approach

Significant progress on "Silicon-switch approach" was made in the medicinal chemistry front. The strategic replacement of carbon with silicon within marketed drugs or pre-validated drug scaffolds provided an exciting approach to search for new chemical entities (NCEs) in drug discovery. This approach can be cost-effective and of minimum risk because the corresponding carbon analogues (starting points) are known drugs or drug-like compounds with proved pharmacology/toxicity profiles. Another highlight of this approach is in the anti-infective area, where research group could possibly address the problem of drug resistance through introduction of silicon-based drugs.

Asymmetric synthesis of bioactive molecules and synthetic methodologies

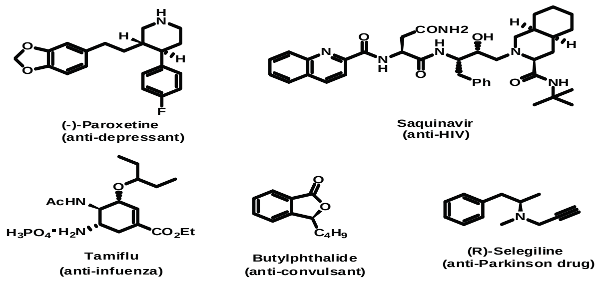
A. Sudalai
a.sudalai@ncl.res.in

Publications: Org. Biomol. Chem., 2012, 10, 3655, 3988; 2013, 11, 1280, 3608; Tetrahedron Asymmetr., 2012, 23, 240, 898, 1534; Tetrahedron Lett., 2012, 53, 148, 3213, 4195; 2013, 54, 2679; RSC Adv. 2013, 3,1695

The research included development of new synthetic methodologies using organocatalysis and transition metal catalysis, newer synthetic methods for C-C and C-N bond formations and their application in multi-step asymmetric synthesis of pharmaceuticals, large number of bioactive natural products from readily available non-chiral sources and metal-free processes for key organic transformations.

Asymmetric synthesis of pharmaceuticals and bioactive molecules

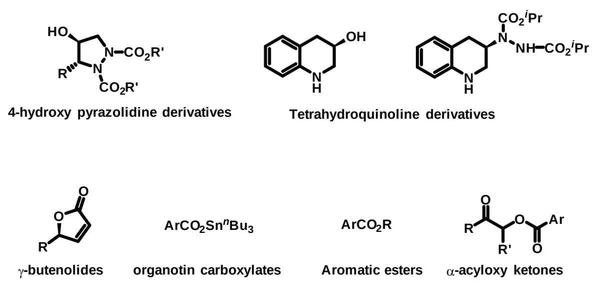
New methods for synthesis of optically active drugs were developed. Drugs such as Tamiflu (anti-influenza), Amprenavir and Saquinavir (anti-HIV), Paroxetine (anti-depressant), (*R*)-Selegiline (anti-Parkinson), Benzphetamine (anerotic drug), Butylphthalide (anti-convulsant drug) and a large number of bioactive natural products such as Stagonolid C (phytotoxic nonenolide), (-) Aspinolide A, Ro 67-8867 (NMDA receptor antagonist), (+)-Elanolide (attractant pheromone), (+)-Deoxoprosophylline (glycosidase inhibitory), Demethyl pestaphthalide, first synthesis of Matteucen C (relieving ostalgia), (–)-Sumanirole (anti-Parkinson), (*S*)-903 (inotropic agent).



Compounds synthesized

Synthetic methodologies involving organocatalysis

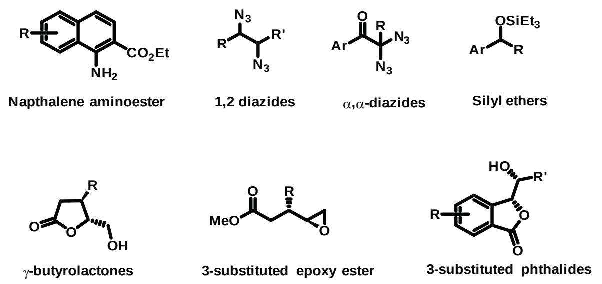
It involved asymmetric synthesis of biologically active molecules using organocatalysts, novel synthetic methods were developed using proline as catalyst for the synthesis of bioactive 4-hydroxy pyrazolidine derivatives through α-amination/Corey-Chaykovsky reaction of aldehydes, γ-butenolides *via* α-aminoxylation and *cis* wittig olefination of aldehydes, tetrahydroquinoline derivatives by α-aminoxylation or amination/ reductive cyclization method. N-heterocyclic carbenes (organocatalyst) were used for oxidative stannylation and esterification of aromatic aldehydes and for regioselective oxo-acyloxylation of alkenes to give α,α acyloxyketones and esters under aerobic condition.



Key organic frameworks synthesized under transition metal catalysis

Synthetic methodologies involving transition metal catalysis

A simple methodology was developed that affords substituted naphthalene amino esters, important building blocks for the synthesis of pharmaceuticals and polycyclic aromatic electronic materials *via* CuCN-promoted cyclization in high yields. Also, it was reported that Pd salts were highly effective catalysts in the presence of triethylsilane as hydride source for selective hydrosilylation of aryl ketones and aldehydes. A flexible, novel single-step method that employs Co-catalyzed HKR to produce substituted γ-butyrolactones and epoxy esters in high optical purities was developed. Additionally, demonstration of a highly practical, novel CN-assisted oxidative cyclization method was done for the synthesis of a wide variety of 3-substituted phthalides. A simple procedure with NaIO$_4$–NaN$_3$ as a new combination for the 1,2-diazidation of alkenes and α,α-diazidation of aryl ketones, that provides direct and efficient entry to vicinal 1,2-diazidoalkanes and geminal 1,1-diazidoarylketones was reported.

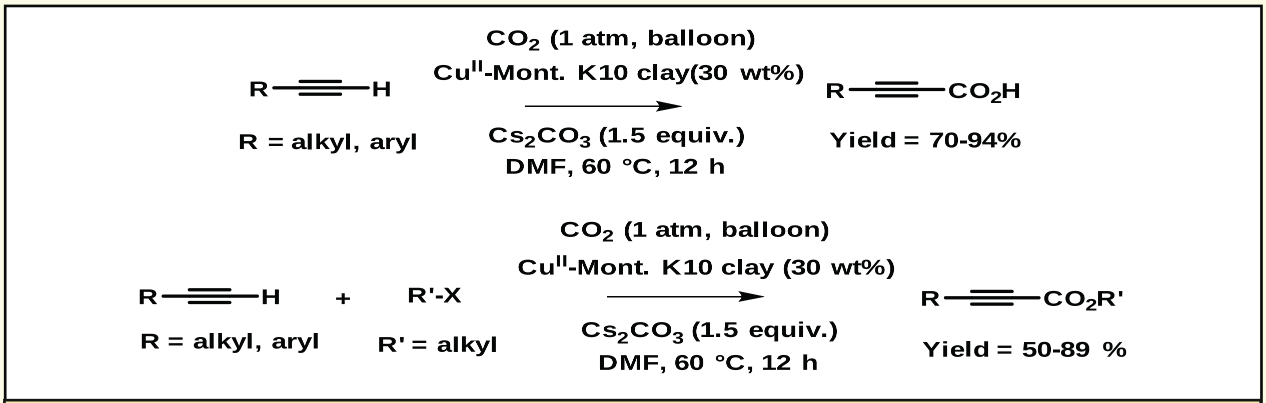


Key organic compounds synthesized using organocatalysis

Asymmetric synthesis of bioactive molecules and synthetic methodologies

Carboxylation of terminal alkynes with carbon dioxide under heterogeneous catalysis

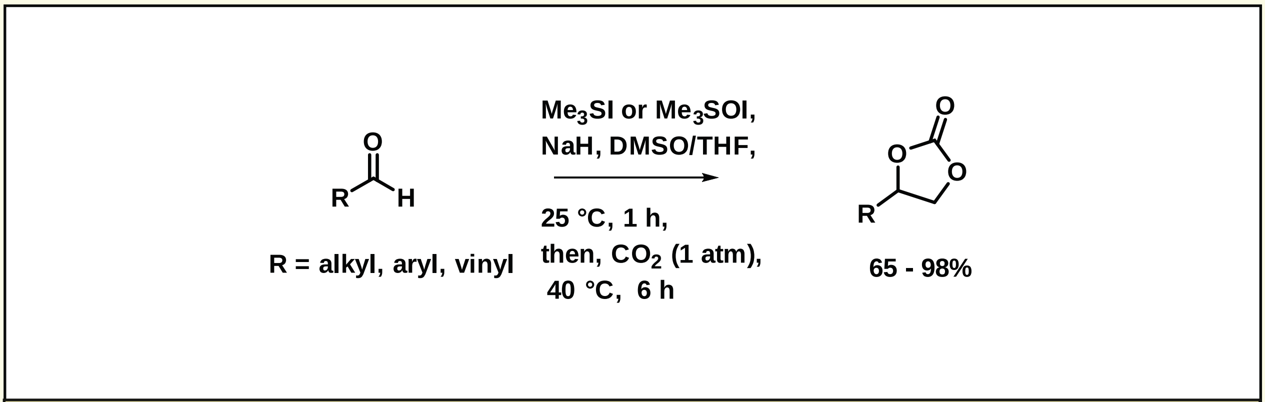
A new protocol for direct carboxylation of terminal alkynes was developed using reusable Cu^{II}-Mont. K10 clay as heterogeneous catalyst and CO_2 as the C1 carbon feedstock (Scheme 1). And also coupling of terminal alkynes with CO_2 (1 atm) in the presence of alkyl halides was achieved under the same reaction conditions, thereby providing access to a variety of functionalized alkyl-2-alkylnoates in high yields.



Scheme 1: Direct carboxylation of terminal alkynes with carbon dioxide

Metal-free one-pot synthesis of cyclic carbonates from aldehydes

An elegant one-pot synthetic method was developed for the preparation of cyclic carbonates in high yields involving reaction of aldehyde with sulphur ylides, followed by CO_2 insertion (Scheme 2). The salient features of the methodology are as follows: (1) inexpensive starting materials, (2) metal-free synthesis, (3) no costly reagents or complex co-catalyst needed, (4) water soluble NaI (by-product) acts as promoter, (5) utilization of CO_2 (1 atm) under ambient reaction conditions at 40°C, and (6) functional group tolerance, and high yields of cyclic carbonates.



Scheme 2: Synthesis of cyclic carbonates from aldehydes and CO_2

Open source drug discovery and outreach programs

The objective of OSDD was to develop an open platform for researchers across the globe to contribute to the cause of fighting against neglected diseases. TB is a disease which is a major threat for the developing and the tropical countries and has been a neglected target in the majority of the Pharmaceutical Industries. The first disease target taken up by OSDD was Tuberculosis (TB). Apart from the lack of any new drugs (for almost the last 40 years), the recent emergence of MDR TB has posed even more challenges. It was aimed to develope new drug candidates for certain diseases like TB in the OSDD platform.

Efforts were made to contribute for the synthesis of small molecules for screening, and for the in-silico modeling for further modulation of the identified hits. Along with this, it has developed a platform for the science students to contribute to the cause of OSDD from their under-graduate phase onwards by participating in the outreach program for synthesis of small molecules.

A diverse array of small molecules comprising of natural products, their analogues, novel heterocyclic scaffolds, derivatives of steroids and carbohydrate analogues were synthesized across the 12 groups (470 compounds) and were screened against the growth of *M. Smegmatis.* The initial screening led to the identification of a good number of initial hits which was sent for further screening against H_37R_v.

OSDD outreach program

It was aimed to attract the young talent to participate in the open source drug discovery program. As part of this training program, the selected students were exposed to the advancements in the scientific research and were informed how to carry out the modern synthetic reactions that they study in their courses to get encouraged to pursue their career in research.

The first batch of the OSDD Outreach Program started from the May 1, 2012. Twelve students who were pursuing B.Sc/M.Sc integrated participated in this program. These students were trained in the selected research groups of CSIR-NCL to carry out the synthesis of small-molecule libraries using simple and easy-to-do reactions in 2-3 steps. Each student or a group of students made a few compounds and learned how to carry out the purification of the compounds by chromatography and also take the NMR, mass spectra, etc. and characterize them. These compounds were screened for anti-tuberculosis activity at CSIR-IICT. A certificate of appreciation was issued to each student.

Having successfully conducted the first Outreach Program over a period of two months, the next program was planned for a period of four–six months for students of M. Sc or M. Pharm during December 2012 to April, 2013. Four students were participated during this session.

Encapsulated microorganisms for environmental protection

R. V. Gadre
rv.gadre@ncl.res.in

Application of a variety of insecticides has become an integral part of agriculture. These insecticides find their way into food, soil and water adversely affecting the food chain, potability of water, productivity of the soil and finally human and environmental health. The current research project involved the isolation, collection, screening and evaluation of several microorganisms that are useful for degradation of phenol as a model compound and monocrotophos as a major target insecticide.

Soil samples were inoculated in mineral medium for enrichment of microbial cultures able to degrade phenol and monocrotophos. Isolates were obtained on nutrient agar to which monocrotophos was added or in mineral medium with phenol as sole source of carbon. The cultures were then grown in deep-well blocks, test tubes and flasks and the degradation of phenol at different concentrations was evaluated. Analysis of the residual phenol and monocrotophos was performed using HPLC and in terms of organic load by Rapid COD method of Merck. Cultures obtained from NCIM were also screened for the purpose.

Pseudomonas putida NCIM 2152, *Pseudomonas putida* 2176 and *Pseudomonas resionovorans* NCIM 2599 degraded up to 600 mg/l phenol in synthetic medium in less than 24 h.
Several isolates obtained from soil samples were evaluated for monocrotophos degradation showed that monocrotophos could not serve as sole source of carbon in the medium for growth. When supported with additional nutrients, 12 isolates showed substantial monocrotophos degradation. The cultures were identified to species level using Biolog phenotypic microarray system for bacterial identification. *Providencia stuartii, Achromobacter insolitus, Gemella sanguinis, Micrococcus lylae D, Pseudomonas aeruginosa, Stenotrophomonas maltophilia, Brevundimonas diminuta, Serratia liquefaciens/grimesii* and *Ochrobacter tritici* degradred the monocrotophos to 50-74% in 18 days when used at 200 mg/l concentration.

Novel glycation inhibitors

Mahesh J. Kulkarni
mj.kulkarni@ncl.res.in

Publication: Sci. Rep., 2013, 15, 2941

Glycation is a series of reaction between reducing sugars and amino groups of proteins leading to formation of advanced glycation end products (AGEs). AGEs interact with receptor for AGEs (RAGE) to cause oxidative stress and activate pro-inflammatory pathways. AGEs were implicated in development of diabetic complication, neurodegenerative disease, cancer and aging. The work was aimed to study various aspects of glycation including AGE-RAGE signalling, screening inhibitors of glycation, and glycation regulation of protein function.

Hydralazine mediated transglycation in diabetes

A mass spectrometry based transglycation assay was developed; this led the formation of hydralazine. Hydralazine mediated transglycation was demonstrated in streptozotocin (STZ) induced diabetic mice who were evidenced by decreased HbA1c, plasma protein glycation and formation of hydralazine glucose conjugates in urine.

The mechanism by which transglycation was undergone by hydralazine is depicted in Fig 1. The reaction between glucose and protein which led formation of Schiff's base and Amadori product is reversible in nature. Hydralazine interfered at the level of Schiff's base or Amadori product formation which removed the protein bound glucose by virtue of its nucleophillic nature. A similar mechanism was proposed in case of glutathione mediated transglycation. Furthermore, hydralazine down regulated the expression of Receptor for Advanced Glycation End products (RAGE), NADPH oxidase (NO_X), and super oxide dismutase (SOD). This search will provide a new dimension for developing intervention strategies for the treatment of glycation associated diseases such as diabetes complications, atherosclerosis, and aging.

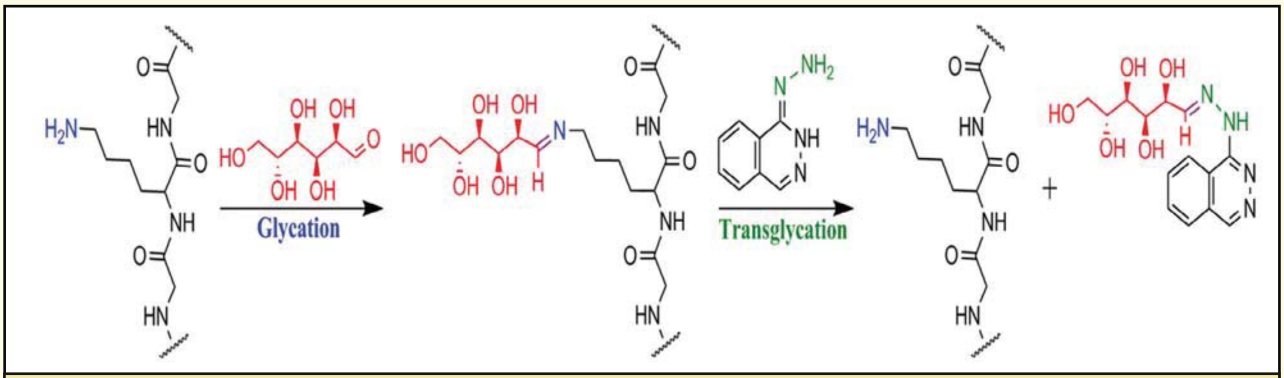


Fig. 1: Mechanism of hydralazine mediated transglycation

Cell culture bioprocessing

Mugdha Gadgil
mc.gadgil@ncl.res.in

Publications: Biotechnol. Progr., 2012, 28, 1605; Comput. Biol. Med., 2012, 42, 1141; RNA Biol., 2012, 9, 891

A hydrogel based system was developed for *in situ* pH maintenance without pH measurement. It was demonstrated to maintain pH between 6.8 to 7.2 for a suspension CHO cell line in CD CHO medium and between 7.3 to 7.5 for adherent A549 cells in DMEM:F12 containing 10% FBS. This system for pH maintenance in shake flasks can allow better mimic bioreactor based fed batch operation for initial screening during cell line and process development for recombinant protein production in mammalian cells.

A meta-analysis of publicly available data on gene expression changes in A549 cells upon treatment with anti-cancer drugs was carried out to identify common changes in cells at a transcriptional level upon treatment with anti-cancer drugs. Simulated datasets and permutation analysis were used to guide choice of ratio cutoff. Out of the genes identified, FDXR was the only gene differentially expressed in six of seven drug treatments.

Development of novel synthetic peptide structures

G. J. Sanjayan
gj.sanjayan@ncl.res.in

Publications: J. Am. Chem. Soc., 2013, 135, 11477;
Chem. Commun., 2012, 48, 8922, 9747, 11205; 2013, 49, 2222

Secondary structure mimics found to have extensive application in biomedical science. Efforts were made to mimic the secondary structural features of proteins such as reverse turns, helices and sheets. Research was aimed to develop novel scaffolds. Development of diverse mimetics / molecular architectures was done successfully.

Design and development of complex synthetic zipper peptides

Exclusive design of complex synthetic architectures using non-covalent interactions was a challenge, owing to the poor understanding of interplay of such interactions. A robust new class of synthetic zipper structures was developed by using a collection of non-covalent forces. Extensive structural studies unequivocally confirmed their zipper-like architecture – both in the solution and solid-state.

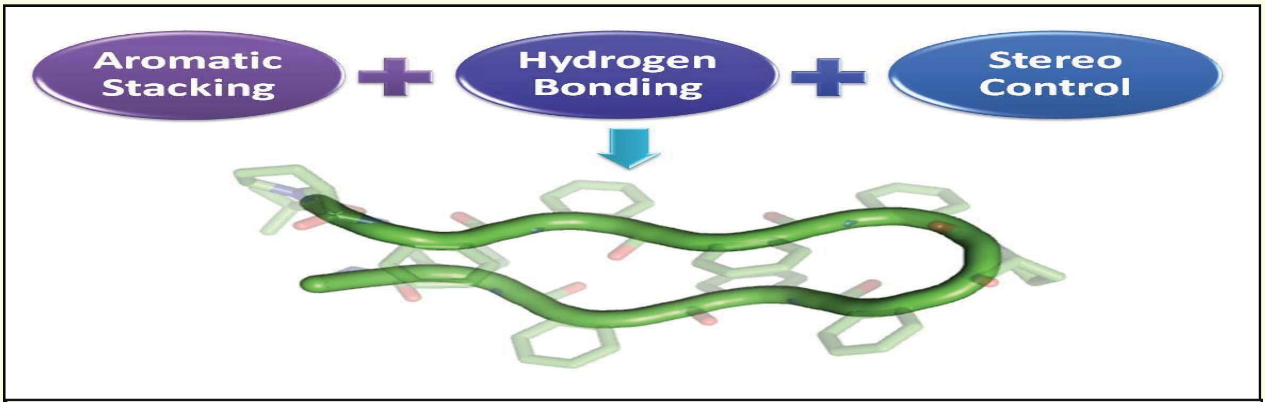


Fig.1: Engineering synthetic peptide zippers using non-covalent interactions

Dynamic transition upon protein-RNA complex formation

Sapna Ravindranathan
sapna.ravindranathan@ncl.res.in

The interaction of the N-terminal RNA recognition motif domain (RRM1) of the Polypyrimidine Tract Binding (PTB) protein was examined with a stem-loop RNA that contains a UCUUU penta-loop present in the Internal Ribosomal Entry Site (IRES) of Foot-and-Mouth disease virus (FMDV), Encyphalomyocrditis virus (EMCV) and Theiler's Murine Encephalomyelitis virus (TMEV). PTB has 531 amino acids and is comprised of four RNA recognition motifs. In EMCV IRES, the pyrimidine tracts occurred as hairpin loops or bulges. A stem loop structure with a UCUUU penta-loop is also common to FMDV and TMEV and is essential for IRES activity.

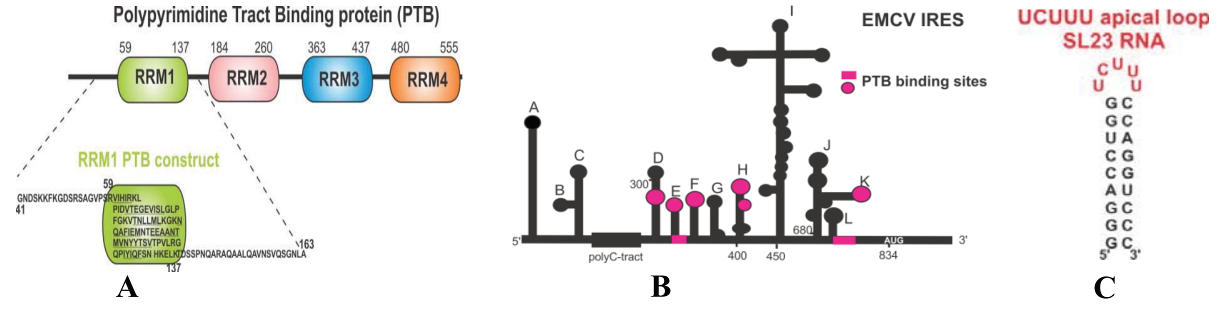


Fig.1: A) Schematic of full length PTB with RRM domains, B) Schematic of EMCV IRES, C) Stem-loop RNA construct

Previous structure determinations of PTB-RRM1 bound to the single stranded RNA CUCUCU showed that recognition was achieved through canonical RRM-RNA interactions via the β-sheet surface of RRM1 and the loops connecting the β strands. However when PTB-RRM1 binds to stem-loop RNA, the C-terminal tail of RRM1 which included part of the extensive linker connecting RRM1 to RRM2 in PTB formed an additional α -helix which docks to β - 2 strand (Fig. 2). Also the binding affinity was much higher for the stem loop RNA than the single strand RNA. Newly formed α - helix made no contacts to RNA. This raised the question of how the C-terminal part of RRM1 was able to sense the binding of a structured RNA to the β - sheet. It was also found that the C-terminal helix was crucial for PTB function in promoting IRES mediated translation.

The structural reorganizations occurred in PTB-RRM1 as a result of stem-loop RNA binding; it implies that significant dynamics changes must also occur as a result of this interaction. This prompted the detailed dynamics investigations in this system. Dynamics characteristics underlying the conformational changes resulted from RNA binding were examined. These measurements revealed that a dynamic network connected the C-terminal tail with the adjacent β -sheet and remote structural elements which were involved in binding the stem-loop RNA (Fig. 3).

This network which coupled binding of RRM1 to a stem-loop RNA with the formation of an additional secondary structure element showed how PTB can adapt to recognize an ordered RNA target in the context of IRES mediated translation.

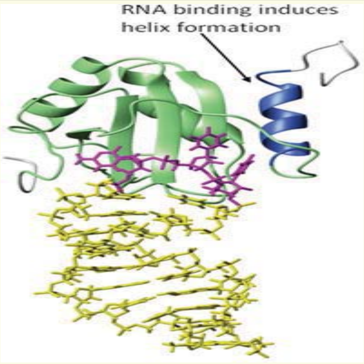


Fig. 2: Structure of PTB-RRM1 stem-loop RNA complex

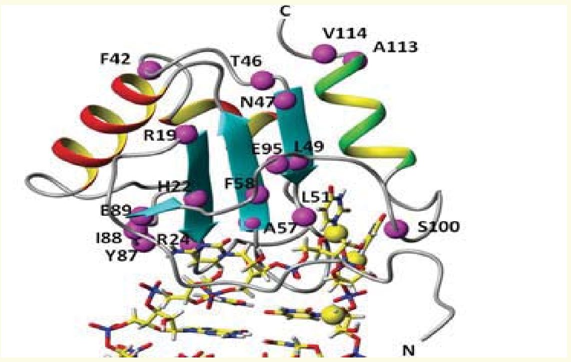


Fig.3: Network of residues showing milli-second time scale dynamics events

Chemoreception in insects

A. Sen
a.sen@ncl.res.in

Publications: J. Insect Sci., 2013, 13, 52; J. Vector Borne Dis., 2013, 49, 1-3;
J. Pest Sci., DOI-10.1007/s10340-013-0502-1

Research efforts were focused on olfaction and gustation in insect-plant interactions with emphasis on identification of semiochemicals that evoke insect behavior(s) for use in agriculture and vector control. Discrimination of nutrients and potentially toxic compounds were achieved with the help of gustatory sensilla present on the mouthparts of the larvae. Besides, plant feeding by insects resulted in triggering biochemical pathways that released a blend of volatiles different from undamaged plants.

In addition, there is a diurnal difference in the release of volatiles by plants which has significance in egg laying patterns by the adult female. The research group has been studying these aspects in various tritrophic interactions involving a) *Helicoverpa armigera* –Pigeonpea - *Chelonus blackburni*, *H.armigera*- Chickpea - *Chelonus blackburni*; b) *Persea bombycina/Litsea polyantha-Antheraea assama-Exorista sorbillans* and c) *Terminalia arjuna/T.tomentosa-Antheraea mylitta - Exorista sorbillans* using behavioral and electrophysiological analysis.

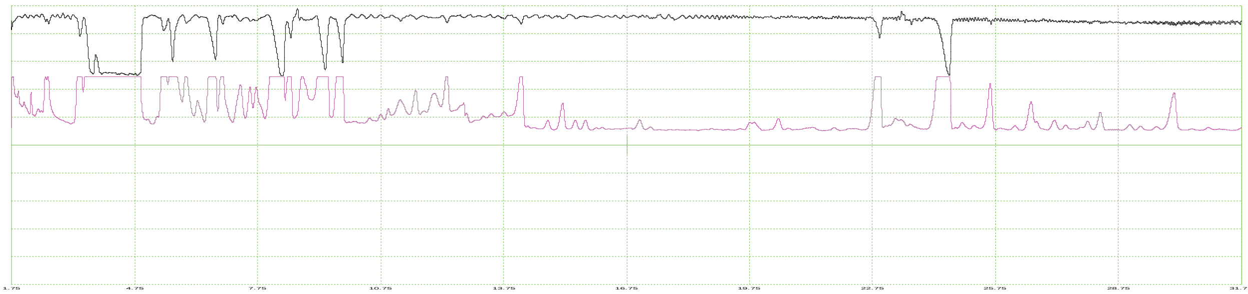


Fig. 1: GC-EAD recording of female Uzi fly, *Exorista sorbillans*to volatiles collected from muga silkworm *(Antheraea assamensis)* damaged leaves of Som *(Machilus bombycina)*

Gustation in Antheraea species

Electrophysiological characterisation of the medial and lateral sensilla styloconica as well as the epipharyngeal sensilla in *A. assama* and *A. mylitta* reveal that they are sensitive to a wide group of chemical compounds including sugars and sugar alcohols, salts, deterrents and plant saps. Thus, feeding behavior of *A. assama* and *A. mylitta* allows for the acceptance of different plants that is determined by the relative activity levels in the four chemosensory neurons in each of the sensilla styloconica present on the galea and the three neurons in the epipharynx.

Volatiles from human sweat mediating host selection in *Anopheles stephensi*

Human skin emanations attract mosquitoes. Group is studying components in human sweat (from forehead, feet, forearm and armpits) and how they influence behavior in adult mosquitoes, particularly the malaria vector, *Anopheles stephensi.* Electrophysiological and behavioral studies indicate that adult females of *A. stephensi* have a broad spectrum of olfactory receptor neurons on the antennae to detect various olfactory signals from human sweat comprising primarily of carboxylic acids, aldehydes, alcohols and ketones.

Interaction of peptides with bio-membranes to produce membrane curvature

Durba Sengupta
d.sengupta@ncl.res.in

Publication: J. Phys. Chem. B, 2012, 116, 14556

Biological functions at the membrane interface including membrane fission are difficult to probe by current experimental methods and require complementary computational approaches. Coarse-grain simulations were used to understand the composition-dependent interaction of caveolin-1 with cholesterol rich and cholesterol depleted lipid membranes.

Caveolin-1: A membrane curvature generating peptide

Caveolin-1 (cav-1) is the most common member of the caveolin family and plays multiple roles in cellular signaling, lipid exchange, endocytosis and intracellular delivery of bacterial toxins. 1–3 interactions of cav-1 with cholesterol-rich membranes resulted in changes in membrane morphology. Molecular dynamics simulations were carried out using the coarse-grain MARTINI force-field to analyze association of cav-1 with cholesterol-rich and cholesterol-depleted bilayers. Focus was on the intramembrane and caveolin scaffolding domains to extract out the functionally relevant differences in binding and topology between cholesterol-rich and cholesterol-depleted bilayers. The structural properties of cav-1 as well as the binding modes in the presence and absence of cholesterol were compared. The results highlight the molecular details of cav-1–membrane interactions and provide an understanding of the effects of the peptide tuning the morphology of cholesterol-rich membranes.

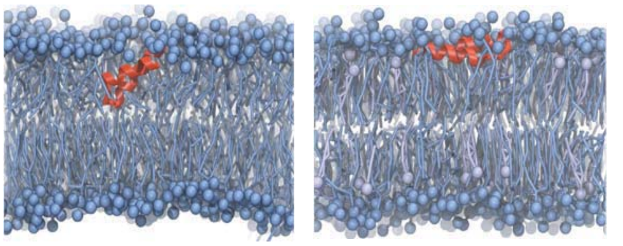


Fig.1: Snapshot of cav-1 peptides bound to DPPC (top) and DPPC-cholesterol (bottom) bilayers. The peptide is represented in red, the DPPC molecules in blue, and the cholesterol molecules in violet

Cholesterol modulates the depth of insertion of caveolin-1

Coarse-grain molecular dynamics simulations were performed and observed that caveolin-1 peptides were bound at the membrane–water interface and penetrate to different depths in the five bilayer systems simulated. The depths of insertion reached equilibrium values at a nanosecond time scale and were surprisingly stable even at a microsecond time scale. Fig. 1 shows the depth of insertion of the peptide for the two representative systems DPPC and DPPC–cholesterol mixed bilayers. A comparison of the values of the depth of binding reveals that the peptide inserts the most in pure DPPC bilayers and the least in DPPC–cholesterol mixed bilayers. Insertion in POPC and DOPC as well as POPC–cholesterol mixed bilayers was similar and was in between that of DPPC and DPPC–cholesterol bilayers. Interestingly, the insertion of the peptide (both COM and maximum insertion) was greater in pure DPPC bilayers compared to DPPC–cholesterol but was marginally less in POPC compared to POPC–cholesterol bilayers.

Biocatalysis and biosynthesis

Thulasiram H. V.
hv.thulasiram@ncl.res.in

Publications: Analyst, 2012, 137, 4564; Curr. Mol. Med., 2012, 12, 952; J. Biol. Chem. 2012, 287, 24844; Bioresource Technol. 2012, 115, 70

The research was focused on isoprenoid biosynthetic pathway, biocatalysis and metabolomics.

Expedient preparative isolation of basic limonoids from Neem fruits

Basic limonoids, characterized by 4,4,8-trimethyl-17-furanylsteroid skeleton possess a vast array of pharmacological activities. But due to the complexity in the natural extract, the isolation of these limonoids especially in the gram-scale was unattained. Again, rapid identification in the crude phytochemical extract is also desirable for high-throughput screening. An automated medium pressure liquid chromatography (MPLC) based scaling-up process was developed for the preparative isolation of three major limonoids (Azadirone, epoxyazadiradione and azadiradione) from Neem (*Azadirachta indica*) fruit-coats. They were individually quantified using HPLC in different developing stages of fruit-coats. A LC-ESI-MS/MS based rapid identification technique was developed for screening these limonoids in the phytochemical extracts through structure-fragment relationships (Fig. 1).

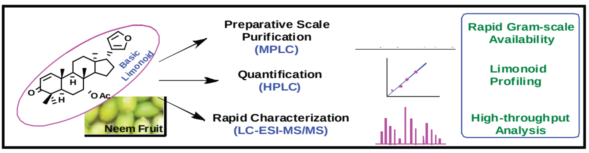


Fig. 1: Basic limonoids from Neem fruits

Fungi mediated biocatalytic transformations of basic limonoids

Rare and synthetically challenging 12β- and 17β-hydroxylation was achieved on the basic limonoid skeleton to produce a series of novel class of hydroxylated limonoids using fungi mediated biocatalysis. The fungal system belonging to the genera of *Mucor* efficiently converted azadiradione, epoxyazadiradione, gedunin and their derivatives into corresponding 12β- and 17β- hydroxy derivatives (Fig. 2). The position and stereo-chemistry of hydroxylation was determined by rigorous spectroscopic and crystallographic studies. This fungal mediated stereo- and regio-selective hydroxylation process was highly efficient and mild enough to sustain chemically sensitive functional groups around basic limonoid skeleton. Modifications of specific functional groups and variation in biocatalyst were shown to bring selectivity among 12β- or 17β-hydroxylation.

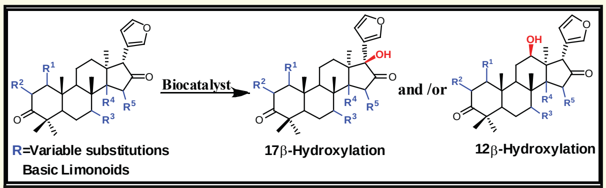


Fig. 2: Bioconversion of basic limonoids

Preparative separation of **α**-and **β**-santalenes and (Z)-**α**- and (Z)-**β**- santalols

The major sesquiterpene constituents of East-Indian sandalwood oil (Z)-a- and (Z)-b-santalols were responsible for most of the biological activities and organoleptic properties of sandalwood oil.

The strategic use of medium pressure liquid chromatography (MPLC) was utilized for the separation of both α- and β-santalenes and (Z)-α-and (Z)-β-santalols. Silver nitrate impregnated silica gel was used as the stationary phase in MPLC for quantitative separation of α- and β-santalenes and (Z)-α- and (Z)-β-santalols with mobile phases hexane and dichloromethane, respectively. The purity of a-santalene and (Z)-α-santalol obtained was >96%; however, β-santalene and (Z)-β-santalol were obtained with their respective inseparable epi-isomers. Limits of quantification (LoQ) relative to the FID detector were measured for important sesquiterpene alcohols of heartwood oil of *S. album* using serial dilutions of the standard stock solutions and demonstrated that the quality of the commercial sandalwood oil can be assessed for the content of individual sesquiterpene alcohols regulated by Australian Standard (AS2112-2003), International Organization for Standardization ISO 3518:2002 (E) and European Union (E. U.).

Sesquiterpene synthases from from ***S. album***

Santalum album santalene synthase (SaSS-WT) was cloned, expressed, purified and functionally characterized with the substrate, (E,E)-FPP to yield 6 sesquiterpene products. These were characterized as α-santalene (41.2%), exo-α-bergamotene (21.6%), epi-β-santalene (4.4%), (E)-β-farnesene (1.1%), β-santalene (29.5%) and exo-β-bergamotene (2.2%) (Fig. 3). Based on the homology modeling with the structurally characterized sesquiterpene cyclase, 'aristolochene synthase', the amino acid sites responsible for governing formation of the products were identified.

Biocatalysis and biosynthesis

Site directed mutageneses of SaSS-WT were performed to achieve 29 functionally characterized mutants. To derive the chemical insights in mechanisms of cyclization of linear substrate, (E,E)-FPP into various cyclic products, deuterium labeled analogues of (E,E)-FPP were synthesized by using a combined approach utilizing chemical and biosynthetic means. Incubation of the labeled substrates with the cyclase proteins generated labeled sesquiterpene products. Tracing the elimination and shift of the labels from GC and GC-MS analyses followed by determination of the deuterium kinetic isotope effects and analyses of the GC-MS spectra, provided mechanistic insights in biosynthesis of the sesequiterpene products.

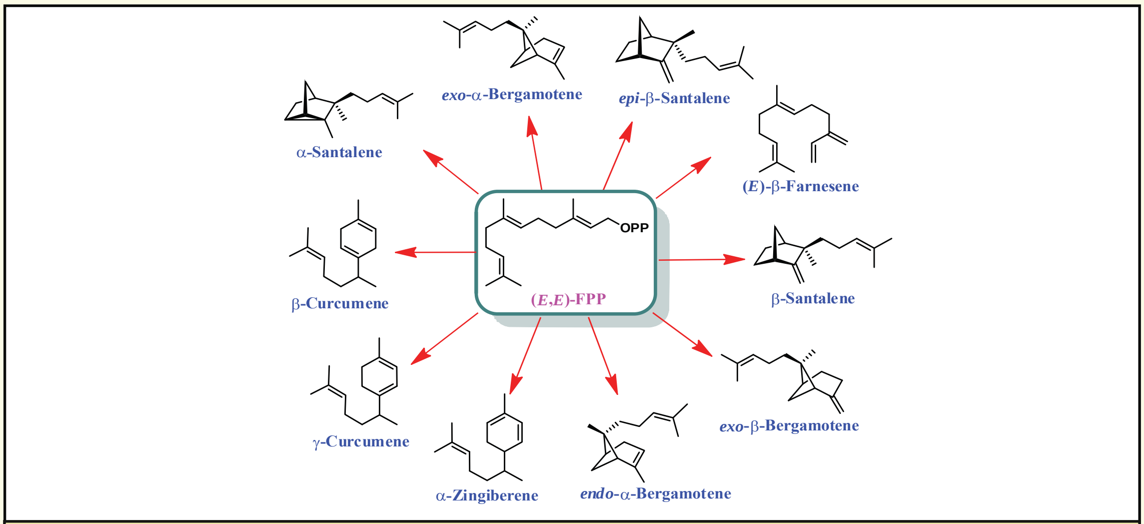


Fig. 3: Biosynthesis of santalenes and analogous sesquiterpenes

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

Vidya Gupta
vs.gupta@ncl.res.in

Publications: Mol. Breeding, 2013, 31, 743; Food Chem., 2013, 136, 585; J. Proteome Res., 2012, 11, 6264; J. Cereal Sci., 2012, 56, 432

Genetic and genotype x environment interactions of end-use quality traits in bread wheat

Molecular marker analysis of bread making quality traits like grain protein content (GPC), sodium dodecyl sulphate sedimentation volume (SV), dough rheological traits (DRT) and LV were performed and also evaluated the genotype x environment interactions (GEI) underlying them. A hexaploid wheat recombinant inbred line population derived from the cross HI977 x HD2329 grown in three agro-climatically diverse locations for two consecutive years was evaluated for GPC, SV, LV and nine DRT by mixograph analysis. Composite interval mapping of QTLs was performed using a linkage map with 202 simple sequence repeat markers.

Additive main effects and multiplicative interaction analysis indicated patterns in GEI in terms of principal components that explained up to 47% of total variation. Pearson correlations estimated individually in each environment showed stable and environmentally influenced correlations and complex trait relationships which were reflected in QTL clusters for four to seven traits and 13 putative pleiotropic regions. Location-specificity in QTLs expressed in single as well as multiple environments depicted marked GEI effects that might necessitate breeding for these traits targeting specific agro-climatic zones.

Seed development and oil accumulation in linseed

Sequence characterization and *in silico* structure prediction of desaturases from the flax varieties:

Sequenced characterization of all the currently known desaturase genes like *SAD (SAD1& SAD2), FAD2 (FAD2&FAD2-2)* and *FAD3 (FAD3A &FAD3B)* from the ten flax varieties was done. The three dimensional models were predicted for all the desaturase proteins (Fig. 1). Structural variations in these genes and the haplotypes due to AA variation were checked.

Further, the functional implications of these changes and their correlation with the final ALA accumulation if any, in flax varieties were analyzed. *FAD3A* gene of TL23 had a premature stop codon which resulted in a truncated protein and consequently very low levels of ALA accumulation. Besides the mutant variety TL23, some of the high ALA group varieties like NL260 and Padmini formed different haplotypes and protein isoforms for both *FAD3A* and *FAD3B*. Further, there were no structural variations observed due to the AA changes in any of the desaturase genes. It suggested the probable involvement of transcriptional control of the desturases for ALA content variation.

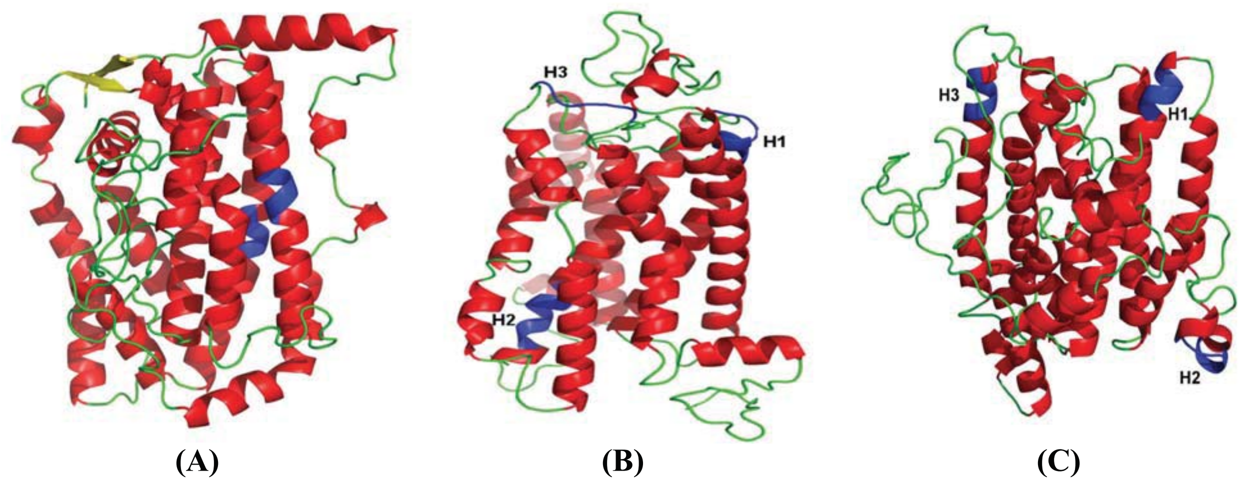


Fig. 1: (A) *SAD1*, (B) *FAD2* and (C) *FAD3A* protein models (helix regionin blue represents conserved di-iron binding motifs)

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

Proteome profiling of flax seed: Characterization of functional metabolic pathways operating during seed development: Proteomic analysis of seven seed developmental stages (4, 8, 12, 16, 22, 30, and 48 days after anthesis) in a flax variety, NL-97 was carried out using a combination of 1D-SDS-PAGE and LC-MSE methods. Total 1716 proteins were identified and their functional annotation revealed that a majority of them were involved in primary metabolism, protein destination, storage and energy. Three carbon assimilatory pathways were appeared to operate in flax seeds. Reverse transcription quantitative PCR of selected 19 genes was carried out to understand their roles during seed development. Besides storage proteins, methionine synthase, RuBisCO and S-adenosylmethionine synthetase were highly expressed transcripts. Further, the identified proteins were mapped onto developmental seed specific expressed sequence tag (EST) libraries of flax to obtain transcriptional evidence and 81% of them had detectable expression at the mRNA level.

Mango flavor biogenesis

The metabolite analysis through various ripening stages of Alphonso was done to know the precursors, metabolic pathway and genes involved in biogenesis of other flavor compounds. Total 24 polar metabolites were identified from mango pulp and skin, which represents 4 major groups of metabolites viz. organic acids, sugars, alcohol and amino acids. This primary analysis explained metabolite diversity of mango and also explained acidic nature of mango due to presence of organic acids and high sugar content during ripe stage. Total seven fatty acids were identified and quantified through various ripening stages of Alphonso mango pulp and skin. Three saturated fatty acids and four unsaturated fatty acids showed dynamic profile during Alphonso ripening. Increased content of unsaturated fatty acids supported the elevated lactone levels during ripening as unsaturated fatty acids are considered to be primary substrates for lactone biogenesis.

DNA barcoding of forest tree species in Western Ghats

The objective was to developed a unique barcode for quick, accurate and reliable species identification using the *Dalbergia* genus as a model system. Ten specied of *Dalbergia* i.e. *Dalbergia melanoxylon, D. rubiginosa, D. paniculata, D. volubilis, D. candenatensis, D. paniculata, D. lanceolaria, D. sissoo, D. horrida* were evaluated for DNA barcoding using *rbcL, trnH-psbA, matK* and nrITS and combination of rbcL with trnH-psbA and matK as well as comination of *matK* and *trnH-psbA*. Among all the above mentioned loci *matK* and *rbcL* were found as the best possible loci for this genus.

Nanobiotechnology

Absar Ahmad
a.ahmad@ncl.res.in

Publications: Colloid. Surface B, 2012, 97, 27; Plos One, 2013, 8, e71805; Chem. Eng. J., 2013, 230, 367; J. Nanomed. Nanotechnol., 2013, 4, 156

The focus was on biological synthesis of inorganic nanomaterials of different sizes, shapes and chemical compositions and their applications. The work also involved conjugation of drugs to nanoparticles for targeted drug delivery applications and fungal mediated biotransformations of organic and inorganic compounds.

Fungus mediated synthesis of biomedically important cerium oxide nanoparticles

Research was done for the bio-inspired synthesis of biomedically important cerium oxide (CeO_2) nanoparticles using the thermophilic fungus *Humicola sp.* The fungus *Humicola sp.* was exposed to aqueous solutions of oxide precursor cerium (III) nitrate hexahydrate (CeN_3O_9_$6H_2O$) resulted in the extracellular formation of CeO_2 nanoparticles containing Ce (III) and Ce (IV) mixed oxidation states, confirmed by X-ray Photoemission Spectroscopy (XPS). The formed nanoparticles were naturally capped by proteins secreted by the fungus and thus did not agglomerate, were highly stable, water dispersible, highly fluorescent and showed anti-microbial activity. These biosynthesized nanoparticles were characterized by standard techniques.

Biosynthesized CeO_2 nanoparticles were used in the preliminary treatment of Parkinson's disease induced rat models. Different concentrations of nanoparticles (10 μM, 100 nM, 10 nM) with distilled water were transplanted stereotaxically in the brain of rats and preliminary behavioral study was carried out. Head swing, forelimb and apomorphine induced rotational behavioral study suggested that 10 nM cerium oxide nanoparticles played a role in reverting the normal activities in rats.

Fungal biotransformation of bulk TiO_2

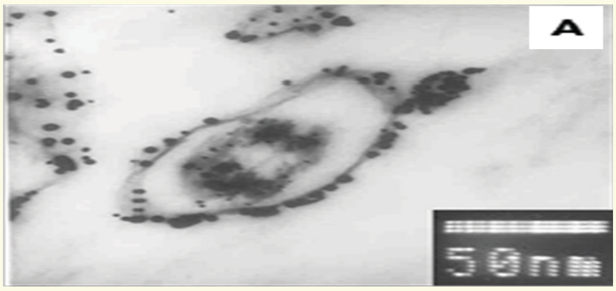
A novel, environmentally friendly top-down approach to nanosynthesis was demonstrated. This method exploited the strength and peculiarities of fungus based bioleaching to extract the radicals from compounds and provided them a reactive capping environment. Thus, protein capped nanoparticles of TiO_2 (2-4 nm, circular and brookite phase) were formed directly from micron size (150-250 nm, disc shape, anatase phase) powder by exposing them to a medium of thermophilic fungus at just 50°C. The fungus was used for the synthesis of nanoparticles and for the transformation of shape, phase and size of TiO_2.

Extracellular biosynthesis of Mn_5O_8 nanoparticles and study of their magnetic behavior

Manganese oxide (Mn_5O_8) at the nanoscale was used in catalysis and as ionic conductors in fuel cells or batteries. The compound Mn5O8 existed in mixed valences of Mn^{2+} and Mn^{4+}. It has drawn an attention due to its antiferromagnetic nature. Extracellular biosynthesis of manganese oxide (Mn5O8) nanoparticles was reported in the size range of 10–11 nm at room temperature by challenging the fungus Fusarium oxysporum with manganese (II) acetate tetrahydrate [(CH_3CO_2_2Mn· $4H_2O$] as precursor. The Mn_5O_8 nanoparticles so formed were characterized by TEM, XRD, FTIR, XPS and TGA. Two mixed manganese ion valencies (Mn^{2+} and Mn^{4+} of Mn_5O_8 were confirmed by XPS studies and antiferromagnetic transitions by magnetic measurements.

Intracellular synthesis of gold nanoparticles using alga *Tetraselmis sp.*

The use of alga *Tetraselmis sp.* was reported in the intracellular synthesis of gold nanoparticles of dimensions 5–35 nm. The particles were more concentrated upon the cell wall than on the cytoplasmic membrane, possibly due to reduction of the metal ions by enzymes present in the cell wall and cytoplasmic membrane. These intracellular nanoparticles may have applications in drug delivery, biomedical applications, catalysis, etc.

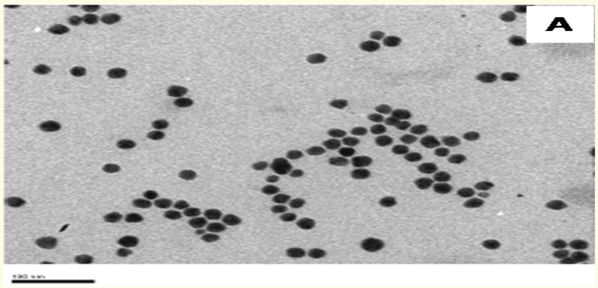


TEM micrograph of thin section of stained *Tetraselmis sp.* cells after reaction with $AuCl_4$– ions for 48 h

Nanobiotechnology

Extracellular biosynthesis of monodispersed gold nanoparticles

Monodispersed gold nanoparticles were produced using a green-synthesis approach. Out of several microorganisms screened, the thermophilic fungus was found to reduce the precursor solution ($HAuCl_4$) at just 50°C and led to the formation of gold nanoparticles of 20-25 nm size with good dispersity, spherical morphology and high stability. These nanoparticles were completely characterized by different standard techniques. The biocompatibility, cytotoxicity and radio labeling studies were carried out. Lastly, these nanoparticles were also conjugated with the anticancer drug Doxorubicin for targeted drug delivery to liver (hepatic) cancer.



TEM micrograph recorded for gold nanoparticles

Vinblastine and Vincristine from endophytic fungus

The endophytic fungi were isolated from *Catharanthus roseus* plant and found a fungus AA-CRL-6 which produced vinblastine and vincristine in appreciable amounts. These drugs were purified by TLC and HPLC and characterized using UV-Vis spectroscopy, ESI-MS, MS/MS and proton NMR. One litre of culture filtrate yielded 76 µg and 67 µg of vinblastine and vincristine respectively. This endophytic fungal strain was identified based upon its cultural and morphological characteristics and internal transcribed spacer (ITS) sequence analysis.

Biotransformation of vinblastine to vincristine by the endophytic fungus

A fungal transformation method for the production of anticancer drug vincristine using the more abundant anticancer drug vinblastine by an endophytic fungus *Fusarium oxysporum* isolated from the plant *Catharanthus roseus* was reported. Vinblastine dissolved in sterile water when incubated with the fungal mycelial mass was transformed into vincristine at room temperature. The biotransformation process was monitored by periodic sampling of aliquots that were extracted with ethyl acetate. The crude transformed compounds were analyzed using TLC where the Rf value of the spot obtained on the 8th day was found to be similar to that of standard vincristine (Rf 0.74). Purification by HPLC using a C 18 symmetry column showed a peak with RT (34.9 min) similar to that of standard vincristine. Further characterization with the help of ESI-MS showed a peak at m/z 825 attributed to the $(M+H)^+$ ion. This indicated that the fungus *Fusarium oxysporum* had converted vinblastine to vincristine.

Penicillin acylases and related Ntn hydrolases

Archana Pundle
av.pundle@ncl.res.in

Publications: Int. J. Biol. Macromol., 2012, 50, 25; Ann. Microbiol., 2012, 62, 1287; Curr. Nanosci., 2012, 8, 130; Acta Cryst. F, 2012, 68, 273

Penicillin V acylases

Penicillin V acylase from *Pectobacterium atrosepticum* was expressed in cytoplasm which was produced in the periplasm of the cells. The enzyme was purified to homogeneity. The protein was found to have high specific activity reaching 400 IU/mg. PaPVA also showed high specificity for its substrate; other beta-lactam antibiotics were hydrolyzed only up to 10% of pen V. The enzyme did not hydrolyze any bile salts. The enzyme exhibited maximum activity at pH 5 and 45°C, with higher stability at acidic pH.

Crystallization screens were set up with 10 mg/ml protein to elucidate the enzyme structure. Needles and microcrystals were observed in a few conditions of Index, PEG Ion (Hampton) and JCSG (Molecular Dimensions) screens. Plate and slab-like crystals (Fig. 1) were obtained with 0.2M sodium potassium tartrate, 0.1M HEPES pH 7.5 and 14% PEG 3350; these diffracted to 3Å. Efforts are being made to further improve the crystal quality and solve the structure, which will help to understand the unique characteristics of such enzymes from Gram-negative bacteria.

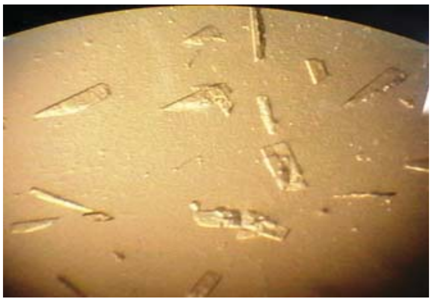


Fig. 1: Plate crystals (PaPVA) formed with tartrate/PEG

Bile salt hydrolases

A marine microorganism producing bile salt hydrolase was isolated from the coastal areas of Arabian Sea near Alibag, India. Media used for isolation of marine strain was Zobell Marine Media (Himedia). This microorganism was identified as *Brevibacterium casei AP9* by *16S* rDNA sequencing. Phylogenetic analysis indicated homology with Marine bacterium.

This is the first report of bile salt hydrolase from a marine source. The isolated strain *Brevibacterium casei AP9* belongs to a group known as Lactic Acid producing Bacteria (LAB). The organism is further classified based on their G+C content of DNA as *Actinomycete* branch (Mol % of G+C >50). The strain was considered as GRAS clear organism and was used in diary product.

Quorum sensing and quorum quenching

Asmita A. Prabhune
aa.prabhune@ncl.res.in

Publications: RSC Adv, 2013, 3, 2288; Appl. Biochem. Biotech., 2013, 169, 1753; Green Chem., 2013, 15, 943; World J. Biol. Biol. Sci., 2013, 1, 10

Component of dental formulations showed the capability to act as a quorum sensing inhibitor in gram negative bacterial systems. Crystalline Xylitol of high purity produced by *Pichia caribbica* isolated by the group inhibited quorum sensing by three distinct molecules namely C6-HSL, C8-HSL and 3-oxo-C6-HSL all serve as important signaling molecules in virulence gene regulation of pathogenic gram-negative bacteria. These findings broadened the scope of eventual application of xylitol in therapeutics. The fore Quorum Quenching ability of *Kluyvera citrophila* Penicillin G acylase was also reported where it can degrade gram negative QS signal molecules- Acyl Homoserine Lactones. AHL degradation capability of Penicillin G acylases was reported. Deamidation of AHLs by KcPGA was validated using biological and chemical assays in addition to in-silico tools and this adds a new facet to the range of activity of this enzyme.

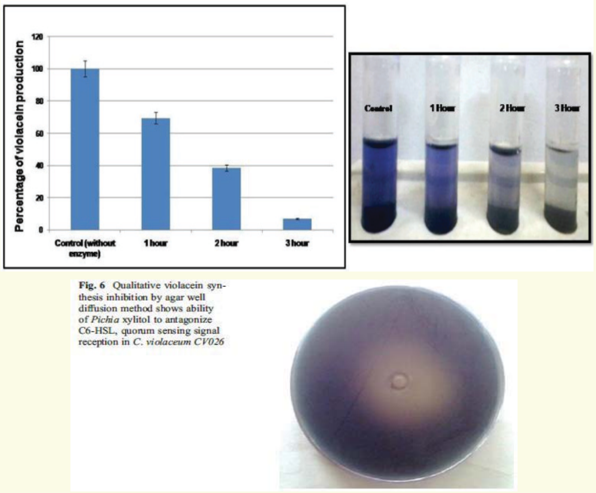
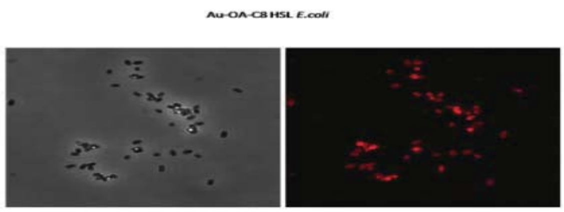


Fig. 6 Qualitative violacein synthesis inhibition by agar well diffusion method shows ability of *Pichia* xylitol to antagonize C6-HSL, quorum sensing signal reception in *C. violaceum CV026*

Violacein Inhibition mediated by the AHL degradative activity of *Kc*PGA

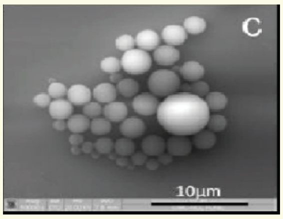
Apart from this, another class of quorum sensing signal molecules known as AI-3 was identified. AI-3 class of signal molecules was shown to mediate their effect via bacterial two component signal transduction pathways. Many important bacterial pathogens have multiple two component signal transduction systems that can simultaneously respond to both host hormone like molecules (Epinephrine and nor-epinephrine) and prokaryotic QS signal molecules like AI-3. These types of two component systems are important determinants in inter-kingdom interaction and successful establishment of infection by the invading pathogens.

Imaging quorum sensing in –vivo was a challenging task. A novel fluorescent Au-nanocluster based imaging system was devised which helped to detect bacteria possessing QS receptors with ease. The system was designed to detect/image AHL mediated quorum sensing and AHL receptors however the Au-cluster based imaging probe was functionalized easily on the surface with other signal molecules.

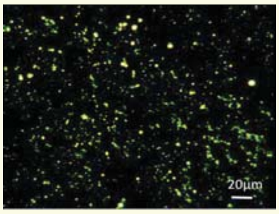


Sophorolipids

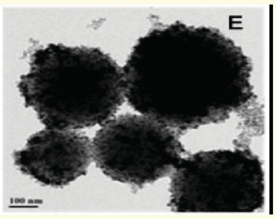
A strong green fluorescence was reported in a fully biocompatible, highly spherical mesoscale molecular assembly of sophorolipid created by pulsed UV laser processing of a water-based dispersion of sophorolipid. The fluorescence property was pulsed laser induced modifications in the molecule and the assembly. The laser synthesized mesostructures were easily redispersed in aqueous medium after being dried and loaded with magnetic nanoparticles (magnetite) for inducing hyperthermia effect.



Sophorolipid mesostructure



Fluorescence image



Fe_3O_4 NP loaded SL assemblies

Mycoinsecticides

M. V. Deshpande
mv.deshpande@ncl.res.in

Publications: Anton. van Leeuwenhoek., 2013, 104, 25; Minirev. Med. Chem., 2013, 13, 222; Biochim. Biophys. Acta., 2013, 1830, 5193; Biotechnol Progr., 2013, 29, 833

Mycoinsecticides based on Metarhizum anisopliae for the control of polyphagous pest *Helicoverpa armigera* were studied. The three identified strains produced 100 g conidia/kg of rice within 10 days. The sugar and sugar alcohols were used for the preservation of conidia. The effects of different components of formulations on the viability and virulence of conidia and their performance in the field to control *H. armigera* infection on pigeon pea and chickpea are being evaluated.

The extracellular cuticle degrading and mycolytic enzyme (CDE/ME) mixture produced by *Myrothecium verrucaria* with and without entomopathogenic fungus was found to be effective against mealy bug and other pathogen control in grapes. The sequential applications of the enzyme mixture, containing mainly chitinase, protease and lipase, followed by *M. anisopliae* conidia were found to be effective (> 70% decrease in mealy bugs in 14 days). Similarly the enzyme mixture was effective in controlling downy and powdery mildews. The bio-control agents were found to be reasonably compatible with chemical pesticides being used in grape fields.

Production and characterization of highly deacetylated chitosan from different fungi

Chitosan was extracted from five different fungi, *Benjaminella poitrasii* (Zygomycetes), *Myrothecium verrucaria* (Deuteromycetes), *Metarhizium anisopliae* (Deuteromycetes), *Saccharomyces cerevesiae* (Ascomycetes) and *Pichia membranifaciens* (Ascomycetes). The maximum yield of chitosan (Degree of deacetylation >90%) was 5.62% in *B. poitrasii*, which was comparatively higher than that of the other fungi. IR spectroscopy showed that the chitosan extracted from *B. poitrasii, P. membranifaciens, M. verrucaria and M. anisopliae* was better than the chitosan extracted from marine waste.

Yeast diversity of wine grapes and effective utilization of winery and vineyard waste

The potential of yeasts isolated from different grape varieties for the production of different enzymes important for aroma and flavour i.e. β-glucosidase, protease, pectinase and β 1, 3 glucanases was studied. Grape pomace obtained from different sources was processed for the isolation of polyphenol-enriched fraction(s). These fractions were analyzed using HPLC technique. The standardized polyphenol-enriched fractions exhibited anticancer and antifungal activities. The residual grape pomace along with chitin was also used as a substrate for SSF production of chitinolytic enzymes like chitinase and N-acetyl-β-D-glucosaminidase using *Myrothecium verrucarria.*

Alkane degradation by ***Yarrowia lipolytica***

Yarrowia lipolytica var. *indica* a marine isolate was found to degrade diesel range n-alkanes up to 70%. Alkane monooxygenase, an enzyme which initiates alkane degradation process, was relatively higher in *var. indica* than a terrestrial strain W29. The cell surface characteristics were studied using cytometric assay microbial adhesion to solvents, contact angle with water and adhesion to polystyrene, showed more hydrophobic nature of *var. indica* than strain W29.

Housekeeping genes in a dimorphic zygomycete ***Benjaminiella poitrasii***

A total of 11 housekeeping genes were involved in different aspects of cellular functions in Benjaminiella poitrasii which included α-tubulin *(Tub-a)*, β-tubulin *(Tub-b)*, β-actin *(ACT)*, translation elongation factors *(eEF1a/b/c)*, Ubiquitin-conjugating enzyme *(Ubc)*, 40s ribosomal protein S3A *(WS-21)*, Tryptophan biosynthetic enzyme *(Try)*, Glyceraldehyde3-phosphate dehydrogenase (GAPDH) and 18s rRNA (18s). Analysis of qRT-PCR data using geNorm software indicated that *WS-21* and *Ubc* were constitutively expressed in 'all life cycle stages', the *eEF1b* and *eEF1c* during 'Y-H dimorphism (vegetative growth)', *Ubc* and *WS-21* in spore formation (asexual stage), while Ubc and *18s* in zygospore formation (Sexual reproduction), in each given subset of RNA samples. These genes were used for comparison with the expressions of NAD- and NADP-glutamate dehdydrogenase genes during morphological transitions.

Characterization of protease inhibitor genes

Ashok P. Giri
ap.giri@ncl.res.in

Publications: BMC Plant Biol., 2013, 12, 217; Insect Mol. Biol., 2013, 22, 258; Biochem. Bioph. Res. Co., 2013, 430, 1060; Biochem. Biophys. Acta , 2013, 1830, 3414, 5087

The clone of selected open reading frames (ORFs) of PIs and mature IRDs were prepared and yeast expression system was applied. The recombinant proteins and peptides were characterized specifically against target proteases. Further, identification and characterization of classical mutants of IRDs was done which lacked the conserved cysteine residues. The mutant showed strong activity against insect proteases by *in vitro* and *in vivo* studies.

The functional significance of evolutionary variations in IRDs and their role in mediating interaction between the inhibitor and cognate proteinase were investigated. IRD-7, 9 and 12 were selected for the further characterization due to variation in their reactive loop, by the difference in number of conserved cystein residues and higher theoretical *ΔGbind* for interation with *Helicoverpaarmigera trypsin*. Inhibition kinetics showed that IRD-9 was more potent protease inhibitor among the three selected IRDs. Molecular dynamic simulations revealed that serine residues in the place of cysteines at 7th and 8th positions of IRD-9 resulted in an increase in the density of intra-molecular Hydrogen-bonds and reactive loop flexibility. Chemical modifications of the above serine residues also supported this observation and provided a possible explanation for the remarkable inhibitory potential of IRD-9. This natural variant among IRDs (IRD-9) showed special attributes like stability to proteolysis and synergistic inhibitory effect on other IRDs. IRDs had co-evolved selective specialization of their structure and function as a response towards specific insect proteases they encountered.

Structural-functional insights of single and multi-domain *Capsicum annuumprotease* inhibitors

Two representative *Capsicum annuum* PI genes (*CanPI-15* and *-7*) comprising one and four inhibitory repeat domains respectively, were expressed and recombinant proteins were characterized. β-sheet and unordered structure was found predominant in CanPI-15 while -7 also displayed the signatures of polyproline fold as revealed by Circular dichroism studies. Inhibition kinetics against bovine trypsin indicated three times higher potency of CanPI-7 (Ki ~57 μM) than -15 (~184 μM). Activity and structural stability of these two CanPIs were revealed under various conditions of pH, temperature and denaturing agent. Structure prediction, docking studies with proteases and mass spectroscopy revealed the organization of multiple reactive site loops of multi domain PIs in space as well as the steric hindrances imposed while binding to proteases due to their close proximity. Cross reactivity in binding of trypsin or chymotrypsin molecules to either TI or CI sites was also observed and suggested that the reactive site loops retain adequate conformational flexibility to allow recognition by a variety of protease molecules. PIs being an innate part of the plant defense strategies protect them from insects, fungi and bacteria have enough variability to interact with a wide range of proteases they come across.

Responses of ***H. armigera*** to plant PIs

The optimal dose of recombinant CanPI-7 (rCanPI-7) for effective antibiosis to *H. armigera* was used to feed and characterize the responses of digestive proteases upon rCanPI-7 ingestion. The gut protease activity was assessed biochemically. Transcript accumulation pattern for selected trypsin and chymotrypsin genes was analyzed by quantitative Real-Time PCR. The growth retardation upon exposure to rCanPI-7 was more pronounced in neonates as compared to third instar larvae. Influence of stage and dosage of rCanPI-7 was conspicuous on the expression and regulation of candidate trypsin and chymotrypsin genes in *H. armigera*. The transcript accumulation pattern was well corroborated with the protease activity in rCanPI-7 exposed larvae. It concludes that early exposure and specific dose of protease inhibitor is essential for effective antibiosis despite the large diversity and plasticity in expression of protease genes in *H. armigera*. Moreover, it is also evident that regulation and expression of *H. armigera* gut proteases is specific to the stage of PI exposure.

Characterization of protease inhibitor genes

Dynamic regulation coupled with a diversity of digestive and detoxifying enzymes played a crucial role in the adaptation of polyphagous insects. An expression of phylogenetically diverse 8 trypsin-like and 4 chymotrypsin-like mRNAs from different life stages of *H. armigera* was profiled reared on nutritionally distinct host plants to investigate the functional intricacy of serine proteases in the development and polyphagy of *H. armigera*. These analyses revealed diet- and stage-specific protease expression patterns. Expressed trypsins showed structural variations, which might result in differential substrate specificity and interaction with inhibitors. Protease profiles in the presence of inhibitors and their mass spectrometric analyses revealed insight in to their differential activity. These findings emphasized the differential expression of serine proteases and their consequences for digestive physiology in promoting polyphagy in *H. armigera*.The identified protease genes are in process for further characterization for their selective interactions with PIs from plants.

Genetic transformation studies in *Casuarina equisetifolia* Forst

S. V. Kendurkar
sv.kendurkar@ncl.res.in

Genetic transformation studies are of great significance in *Casuarina* considering the narrow genetic pool and need for improving biomass, wood quality, insect/disease resistance and nitrogen metabolism.

The research was aimed to develop an efficient *Agrobacterium tumefaciens* mediated transformation protocol for *Casuarina equisetifolia* using young branchlets and nodal explants from 5-year-old tree. For present study *Agrobacterium tumefaciens* strain LBA 4404 harboring plasmid pCAMBIA2301 was used. The plasmid contains chimeric construct having GUS *(uid A)* and Kanamycin *(npt II)* genes driven by CaMV 35S. Parameters such as type of explants, pre-culturing conditions, co-cultivation durations and cell density of *Agrobacterium* were standardized. Kanamycin sensitivity assay for *Casuarina* explants and cefotaxime sensitivity assay for both *Agrobacterium tumefaciens* and *Casuarina* explants were also carried out before co-cultivation studies. Shoot initiation and callusing was obtained from branchlet and nodal explants, which were pre-cultured for two days before co-cultivation with *Agrobacterium tumefaciens* (A_{600} 0.5) for three days. Selection of putative transformants was carried out on callus induction media and shoot initiation media containing kanamycin from lower to higher (0, 25, 50 and 100 mg l^{-1}) dose to avoid the excess stress on explants. The transformations were confirmed by GUS assay of putative transformed tissues.

This study demonstrated that it is possible to transform the branchlet and nodal explants derived from mature trees. The present study helped in standardizing critical parameters affecting transformation of *Casuarina*. This will form the basis for advanced studies on *Agrobacterium tumefaciens* mediated genetic transformation of *C. equisetifolia*.

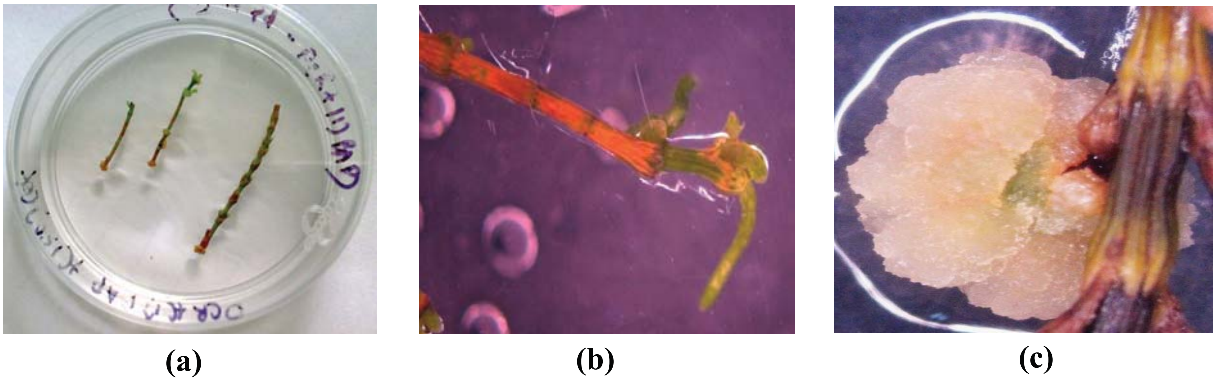

(a) (b) (c)

Fig. 1: *Agrobacterium tumefaciens* mediated transformation of branchlet explant: (a,b) Shoot initiation after 2 weeks on selective SIM; (c) callus formation after 4 weeks on selective CIM

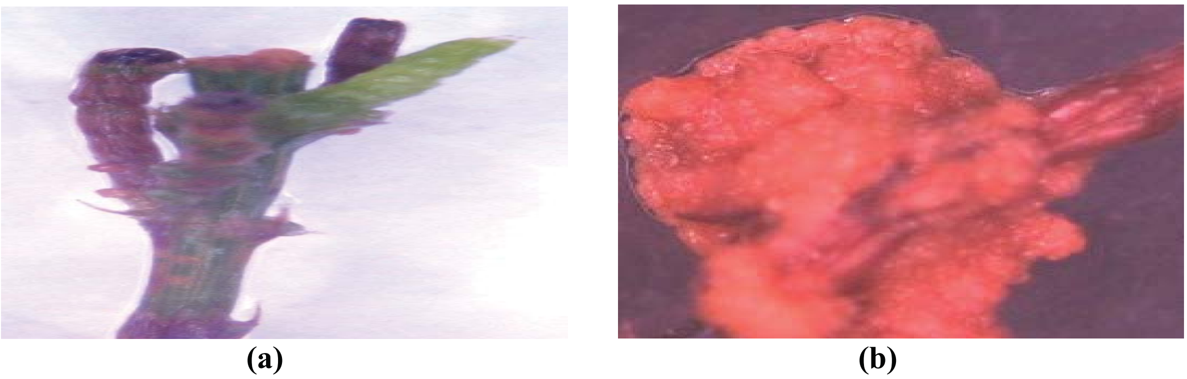

(a) (b)

Fig. 2: *Agrobacterium tumefaciens* mediated transformation of nodal explants:(a) Shoot initiation after 2 weeks on selective SIM; (b) callus formation after 4 weeks on selective CIM

Fungal phytases

J. M. Khire
jm.khire@ncl.res.in

Publications: Process Biochem., 2012, 47, 1066; Appl. Microbiol. Biot., 2013, 97, 673; J. Sci Food Agr., 2013, 93, 2242

The objective was to produce cost effective phytase with fast and economic downstream processing. The traditional approaches had several limitations such as concentration of diluted enzyme; extensive downstream procedures and treatment of generated effluents were employed due to lack of alternative methods.

High activity phytase production from ***Aspergillus niger***

Optimization of culture conditions from parent strain was studied by the Plackett-Burman technique to evaluate the effects of 11 variables for phytase production. The results showed that glucose, $MgSO_4$, KCl, incubation period and $MnSO_4$ were the most significant variables which affect the enzyme production. Further optimization was undergone in variables by using a central composite design technique. It resulted in 3.74 fold increase in the yield of phytase production to 254,500 U/L when compared with the activity observed with basal media (68,000 U/L) in shake flask. It was observed that the phytase from *A. niger* NCIM 563 exhibited desirable activity in simulated gastric fluid conditions with low pH and also improved thermo stability when compared to commercial phytase. The improved yield demonstrated the potential applicability of phytase enzyme as a source of phytase supplement for phosphorus nutrition and environmental protection in animal feed industry. Physical and chemical mutagenesis experiments were carried out in parallel to isolate hyper-secretary mutants that could possibly further enhance the enzyme production. Using optimized media conditions of the parent strain, results showed that mutant strain *A. niger* NCIM 1359 increased the phytase activity by another 1.6 fold to 407,200 U/L.

Down stream processing of phytase using ATPE

Aqueous two-phase extraction (ATPE) application was studied and compared with the traditional procedure involving salt precipitation and column chromatography. High phytase recovery (98.5%) within a short time (3hrs) and improved thermo stability was attained by ATPE. This method is an interesting alternative for simultaneous partitioning and purification of phytase. The influence of system parameters such as phase forming salts, polymer molecular weight and system pH on the partitioning behavior of phytase was evaluated. The ATPE system has the combination of polyethylene glycol (PEG) 6000 and 8000 (10.5%) and sodium citrate (20.5%). It resulted in one-sided partition of phytase in bottom phase with recovery of 98.5% and purification factor 2.5.

Improved plant growth and mineral assimilation by phytase from ***A. niger***

Four yeasts from NCIM resource centre were identified to produce phytase for the first time in the literature. It found to decrease 75-88 % phytic acid from chickpea which is traditional source of protein in Indian food.

Molecular mechanism of anoikis resistance and structural studies of proteins

R. Sureshkumar
s.ramsamy@ncl.res.in

Publications: BiochemBiophys. Res. Commun., 2013, 9, 437; 538
Structure., 2013, 21, 777; ActaCrystallogr F BiolCrystallogr., 2013, 69, 925

The objective was to understand the molecular mechanism by which cancer cells escape signal to die in non-adherant states. The process by which cancer can spread to distant sites away from the primary tumor must be understood to design therapeutics to inhibit the spread of this disease. The secreted protein ANGPTL4 was recently linked to tumor progression. ANGPTL4 was expressed in many cell types such as adipocytes and hepatocytes.

ANGPTL4 with different domain combinations was cloned and co-expressed with some interaction partners. It will be used for the investigation of this complex through Surface Plasmon Resonance (SPR), Isothermal Calorimetry (ITC) and Small angle X-ray scattering (SAXS). The structure determination of ANGPTL4 complex through the X-ray crystallography followed by extensive mutational studies of these complexes was planned.

Protein engineering of industrially important enzymes

Penicillin acylases cleaved the acyl side chain of penicillins and were used in the production of semisynthetic beta-lactam antibiotics. Penicillin V acylases preferentially hydrolyzed phenoxymethyl penicillin (penV). It belongs to the Ntn-hydrolase protein family with cysteine as N-terminal nucleophile. In addition, PVAs showed close sequence and structural homology with bile salt hydrolases (BSHs), forming the choloylglycine hydrolase group. PVAs acted as scavenger enzymes for alternative carbon sources, but their physiological role is relatively unknown. The group aimed to study these enzymes.

A new choloylglycine hydrolase was cloned from the plant pathogenic bacterium *Pectobacteriumatrosepticum* in pET28b with a C-terminal His tag and over-expressed in *E.coli* BL21 star cells. The protein was found to be a penicillin V acylase with high specific activity. Crystallization screens were set up and optimization to improve the crystal quality.

Homology modeling of the active site of the enzyme was also done to study the dynamics of substrate binding and inhibition by bile salts (Fig. 1). The enzyme was highly specific for pen V and did not hydrolyze bile salts. This was observed to be the result of a significant reduction in the size of the substrate binding pocket caused by the lengthening of loop elements that allowed only pen V to bind favourably. Mutagenesis studies could help further to understand the substrate selectivity of the enzyme.

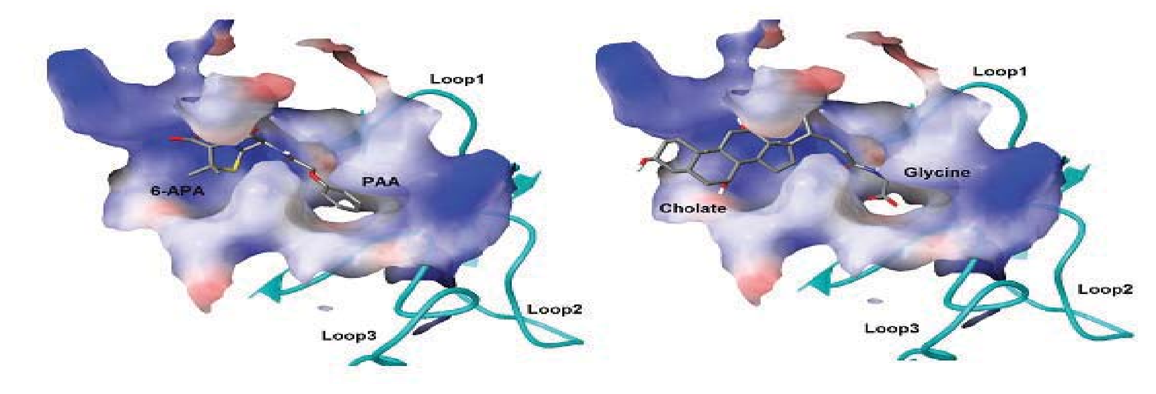


Fig. 1: The mode of binding of penV (left panel) and GCA (right panel) in the active site of PaPVA

Stuctural studies on *Cicer arietinum* lectin

Sushama M. Gaikwad
sm.gaikwad@ncl.res.in

Publications: Int. J. Biol. Macromol., 2013, 56, 149; Biochim. Biophys. Acta, 2013, 1834, 708; Biochem. Biophys. Res. Commun., 2013, 430, 1060; Int. J. Fund. Appl. Sci., 2012, 1, 78

The *Cicer arietinum* seed lectin was cloned and expressed in *Escherichia coli* and purified in active form. Conformational characterization of the recombinant lectin (rCAL) was performed using biophysical and bioinformatics tools. Thermal denaturation of rCAL caused rapid secondary structural rearrangements above 50°C and transient exposure of hydrophobic residues at 55°C, leading to aggregation. Treatment of rCAL with GdnHCl resulted in unfolding followed by dissociation of the dimer. The single tryptophan in rCAL present on the surface of the protein was surrounded by hydrophobic and acidic amino acids and remained as different conformers. The experimental observations correlated well with the structural information revealed from the homology model of rCAL.

Kinetically stable protease

Polyproline II (PPII) fold, an unusual structural element was detected in the serine protease from *Nocardiopsis sp.* NCIM 5124 (NprotI) based on far UV circular dichroism spectrum, structural transitions of the enzyme in presence of GdnHCl and a distinct isodichroic point in chemical and thermal denaturation. The functional activity and conformational transitions of the enzyme were studied under various denaturing conditions. Enzymatic activity of NprotI was stable in the vicinity of GdnHCl upto 6.0 M concentration, organic solvents viz. methanol, ethanol, propanol (all 90% *v/v*), acetonitrile (75% *v/v*) and proteases such as trypsin, chymotrypsin and proteinase K (NprotI:protease 10:1). NprotI seemed to be a kinetically stable protease with a high energy barrier between folded and unfolded states. An enhancement in the activity of the enzyme was observed in 1M GdnHCl upto 8hrs, in organic solvents (75% *v/v*) for 72 h and in presence of proteolytic enzymes. The polyproline fold diminished gradually during thermal denaturation above 60°C. Thermal transition studies by differential scanning calorimetry (DSC) showed scan rate dependence, irreversibility of denaturation and the properties characteristic of kinetically stable proteins.

Structure- function relationship of serine protease from ***Baeveria sp.***

Proteases from *Beauveria sp.* played an important role in insect pathogenesis. The studies involved monitoring functional transitions of the protease as a function of various denaturing agents like guanidine hydrochloride (GdnHCl), proteolytic enzymes, sodium dodecyl sulfate (SDS) and organic solvents. The enzyme showed activation and resistance to 3M GdnHCl and also to proteolytic enzymes like trypsin and chymotrypsin for 12 hours. The enzyme retained activity in organic solvents like methanol and DMSO (50%) for upto 24 hours. The protein showed presence of single tryptophan in partial hydrophobic environment with positive charge density around and contained 20% α-helix, 25% β-sheet, 23.5% turns and 31.5% unordered structure.

Nanobiotechnology and studies on metal tolerance in plants

Urmil J. Mehta
uj.mehta@ncl.res.in

Publications: Mater. Lett., 2013, 102, 5; Curr. Nanosci., 2013, 9,107;
Biotechnol. Appl. Biochem., 2012, 59,47; Biorem. Biodiv. Bioavail., 2013, 7, 54, 49

The aim was to synthesize the extra- and intracellular gold nanoparticles using live peanut callus cells. One of the objectives was to use the peanut hairy root culture as model system for metal tolerance.

The demonstration of the synthesis of gold nanoparticles intra- and extracellularly by living peanut seedlings was done. A novel method for the recovery of intracellular gold nanoparticles without using any toxic chemicals was developed. Phytoremediation is an environmental friendly approach involving various studies pertaining to metal tolerance, metal accumulation and detoxification or decontamination. This aspect of metal tolerance and accumulation offers added value in phytomining and nanoparticles synthesis by using plants.

Synthesis of extra- and intracellular gold nanoparticles using live peanut callus cells

Peanut callus cells when incubated with $HAuCl_4$ solution in ambient conditions led to formation of well dispersed, water soluble extra- and intracellular gold nanoparticles within 24 hours. The extracellular nanoparticles formed showed different shapes and sizes whereas the intracellular nanoparticles were monodispersed. The average particle size was 50 nm for extra- and 31 nm for intracellular gold nanoparticles. The reduction process may occur due to the enzyme secreted by the callus cells into the solution and the nanoparticles may be stabilized by proteins secreted by callus cells. These inorganic nanoparticles may find various applications in targeted drug delivery systems without chances of toxicity as owing to their small size these may easily pass through the kidneys and will be excreted through urine.

Use of peanut hairy root culture as model system for metal tolerance

Studies continue on *Agrobacterium rhizogenes* mediated genetic transformation. The hairy roots technology has potential to become an excellent platform for studying numerous aspects encompassing phytoremediation.

Structure-function studies of some plant and microbial proteins

C. G. Suresh
cg.suresh@ncl.res.in

Publications: Biochem. Physiol., 2013, S2; Acta. Crystallogr. F, 2013, 69, 920; J. Biomol. Struct. Dyn., 2012, 30, 45

Research was done to study the disease proteins which involved four subunits of hydrogenase domain or Q module of Complex-I or NADH-ubiquinone oxidoreductase in human mitochondria. Mainly molecular effects of mutations were reported in these subunits leading to genetic disorders such as Leigh syndrome was studied.

Chitin binding lectins from *Benincasa hispida* and *Datura innoxia* were isolated and characterized. Several Glycosyltransferases (GTs) genes were identified in chickpea genome. The corresponding enzymes were functionally annotated. Molecular modeling and docking studies were carried out to understand the substrate glycosylation group specificity of GTs.

Conjugated Bile Salt Hydrolases (BSH) and Penicillin V Acylases (PVA) were present in bacteria and archaea. The analysis using amino acid sequences showed that CBSH and PVA enzymes were distributed in two clades showing evolutionary divergence, difference in strength of their quaternary association, presence or absence of signal sequence and variations in substrate binding site. It was expected that a better understanding of the evolution of these enzymes and their substrate preferences will improve the current annotation of the family members and provide insights into their biological function. The group has cloned and expressed these enzymes from various organisms for protein engineering to increase stability and efficacy. A novel function of *K. cytrophila* penicillin G acylase related to quorum quenching in bacteria was identified and characterized.

Four core subunits of human mitochondrial Q module were modeled based on the crystal structure of hydrophilic domain of Complex-I from *Thermus thermophilus* to understand the effects of reported pathogenic mutations on the structure and function of Complex-I. The assembly of the subunits in the complex was then modeled based on the prokaryotic crystal structure. *In silico* mutational analysis of individual mutant structures was carried out to understand the effects of the mutations on the individual structures by molecular dynamics simulation analysis using the computer program Gromacs.

All the four core subunits of the Q module were cloned. Out of these NDUFS3 and NDUFS7 subunits were over expressed in soluble form and purified. Biophysical studies on NDUFS3 and its mutants showed that the mutants were more prone to aggregation compared to native protein.

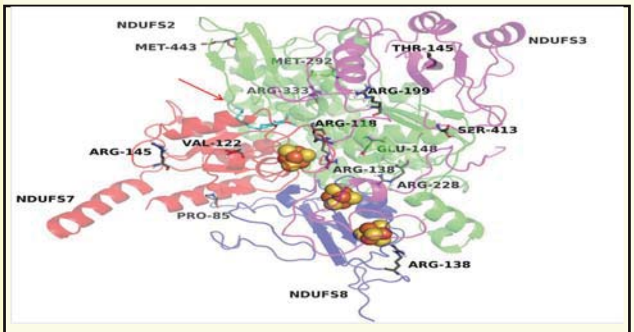


Fig. 1: Molecular model of the Q module is shown with known mutations marked

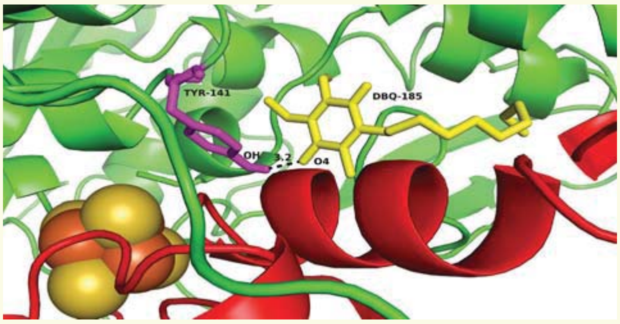


Fig. 2: Docking of DBQ at the interface of NDUFS2 and NDUFS7

Structural Chemistry

Applications of NMR spectroscopy

P. R. Rajamohanan
pr.rajamohanan@ncl.res.in

Publications: J. Am. Chem. Soc., 2013, 135, 11477; ACS Catal., 2013, 3, 303; Eur. J. Org. Chem., 2013, 3529; Macromolecules, 2012, 45, 5967

Methodologies based on solid state and solution state NMR spectroscopy were applied to address various structural problems in area of chemical science and material science for structure-property correlation.

Structural chemistry

Structural features of a number of synthetic peptide oligomers mimicking bio molecular structural architectures resulted from non bonding interactions were brought out by means of modern NMR spectroscopic techniques. Synthetic peptides based on proline –anthranilic acid building blocks possessed a three-dimensional zipper like structure arised from a co-operative interplay of hydrogen bonding, aromatic stacking and backbone chirality. These peptides made use of unusually remote inter-residual hydrogen-bonding and aromatic stacking interactions to attain its shape. Distance constraints derived from NOESY experiments were used for Molecular Dynamics simulations of minimum energy structures.

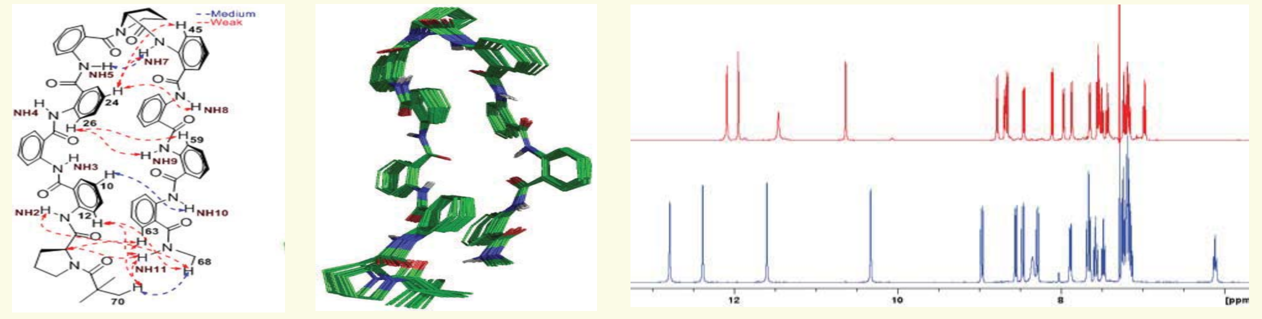
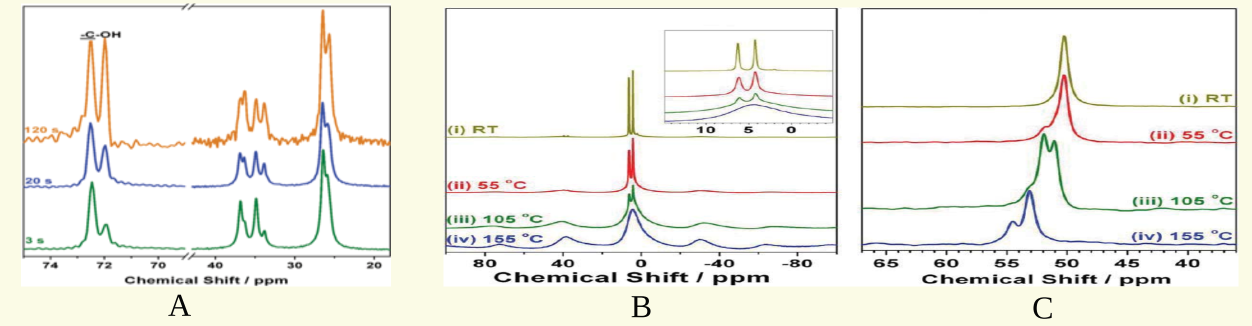


Fig. 1: A- nOe contacts of the peptide, B- Stereo view of superimposed 20 minimum energy structures of the peptide, C-^{1}H NMR spectra of the peptide demonstrating the *pi* stacking effect

Catalysis and surface science

A new single phase molecular adduct of $MgCl_2$ with six cyclohexanol molecules $MgCl_2 \cdot 6C_6H_{11}OH$ (MgCyOH) was prepared and characterized by solid-state NMR. Solid state ^{13}C CPMAS spectrum and single pulse MAS spectra with high power proton decoupling showed the presence of two different sets of magnetically unequal cylcohexanol molecules present around Mg^{2+}(Fig. 2A). The adduct of methanol showed that all six methanol molecules were magnetically equivalent and hence present in a single environment around the Mg^{2+} center in ^{13}C CPMAS NMR. In addition, ^{13}C and ^{1}H NMR measurements made after heat treatment at different temperatures brought out the variations in CH_3OH stoichiometry and coordination of it around Mg^{2+}(Fig. 2 B,C)



A B C

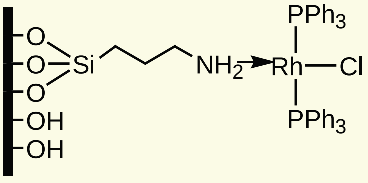
Fig. 2: A-^{13}C HPDEC NMR 75.5 MHz spectrum of MgCyOH, B-^{1}H MAS and C-^{13}C CPMAS NMR spectra

Immobilization of rhodium and ruthenium phosphine complexes

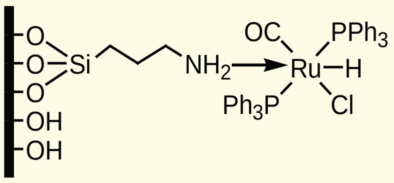
A. P. Singh
ap.singh@ncl.res.in

Highly reactive triphenyl phosphine based rhodium and ruthenium organometallic complexes over PMO_B were synthesized by the immobilization of neat metal complexes like $RhCl(PPh_3)_3$ [Wilkinson catalyst], $RuHCl(CO)(PPh_3)_3$ and $RuCl_2(PPh_3)_3$ over aminofunctionalized PMO_B to get $RhCl(PPh_3)_2$-$PrNH_2PMO_B$, $RuHCl(CO)(PPh_3)_2$-$PrNH_2PMO_B$ and $RuCl_2(PPh_3)_3$-$PrNH_2PMO_B$, respectively. The physico-chemical properties of the functionalized catalyst were analyzed by a series of characterization techniques like elemental analysis, ICP-OES, XRD, N_2 sorption measurement isotherm, FT-IR, solid state ^{13}C, ^{29}Si NMR spectra, XPS, SEM and TEM. XRD and N_2 sorption analyses helped to find out the morphological and textural properties of all synthesized catalysts and confirmed that ordered mesoporous channel structure was retained even after the multistep synthetic procedures. The organic moieties anchored over the surface of PMO_B were demonstrated by solid state ^{13}C NMR and FT-IR spectroscopy.

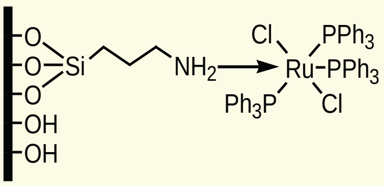
Solid state ^{29}Si NMR spectroscopy provided the information about the degree of functionalization of surface silanol groups with organic moiety. The oxidation state and chemical environment of rhodium and ruthenium metals in heterogeneous complexes were monitored by XPS spectroscopy. Moreover, the morphology and topographic information of synthesized catalysts were confirmed by SEM and TEM microscopy. Catalytic activity and stability of heterogenized complexes were investigated in the liquid phase hydrogenation and sulfoxidation reactions which showed higher activity and selectivity than neat homogeneous complexes and uncatalysed reactions, due to the hydrophobic nature and higher surface area of PMO_B as support. Recycling study of anchored catalysts showed no major deactivation of the catalyst.



$RhCl(PPh_3)_2$-$PrNH_2PMO_B$



$RuHCl(CO)(PPh_3)_2$-$PrNH_2PMO_B$



$RuCl_2(PPh_3)_3$-$PrNH_2PMO_B$

Valorization of agro-waste using heterogeneous catalysts

Paresh L. Dhepe
pl.dhepe@ncl.res.in

Publications: RSC Adv., 2013, 3, 17156, ACS Catal., 2013, 3, 2299

Biomass is considered as a sustainable resource for chemical synthesis by developing environmentally benign methods. Especially the agro-waste (lignocelluloses) and heterogeneous catalysts are precious. A solid acid, solid base and supported metal catalysts for the efficient conversion of agro-waste into value added chemicals were synthesized.

Valorization of hemicelluloses

Hemicelluloses, 2nd most abundantly available plant derived polysaccharide and a component of lignocelluloses was converted into sugars (C5, xylose and arabinose) and furfural in a one-pot method using solid acid catalysts. The SAPO type catalysts were synthesized and showed very nice performance in these reactions when carried out in biphasic medium. At 170°C, within few hours SAPO-44 catalyst could convert >90% of hemicelluloses into xylose and arabinose (5-10%) and furfural (ca.60%). The overall mass balance in these reactions was ca. 90%. The catalysts can be efficiently recycled minimum for eight times. The catalysts were shown to have higher hydrophilic character compared to other known catalysts used in this study and hence SAPO's could remain in aqueous phase and improve the yield of furfural. The XRD, ICP, TPD, NMR data supported the fact that catalysts were stable under reaction conditions.

Hemicelluloses were also subjected to hydrolytic hydrogenation reactions over supported metal catalysts and shown to perform well compared to earlier known catalysts. ca. 60% of sugar alcohols yield was achieved directly from hemicelluloses in a one-pot reaction.

Depolymerization of lignin

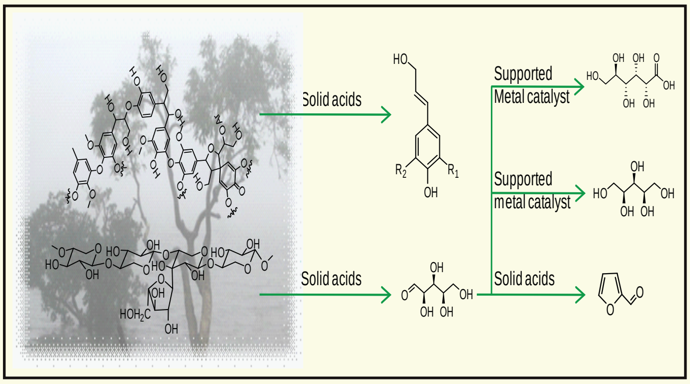
A green method based on solid acid catalysts was developed to obtain aromatic monomers in high yields of 60%. No gas formation was observed in these reactions which in turn enhanced the yields for aromatic monomers. The catalysts were shown to be active for various lignin substrates and can be recycled with loss of 10-15% activity in each run.

Conversion of sugars into value-added sugar derivatives

It was important to develop efficient methods to convert sugars once obtained by hydrolysis of cellulose and hemicelluloses into industrially important chemicals. For this solid acid, solid base and supported metal catalysts were synthesized.

Supported metal catalysts along with solid base were active in the oxidation of glucose and xylose. The products, gluconic acid and xylonic acid are important in pharmaceutical, food, cosmetic and other industries. The presence of solid base avoided the use of mineral base and hence nullified the formation of neutralization waste. Moreover, it was shown that under alkaline conditions sugars were predominantly remained in open chain form which helped to achieve higher activity and yields.

Over solid acid catalysts like SAPO's glucose were efficiently undergone dehydrocyclization reaction to yield 5-hydroxymethyl furfural (HMF). The presence of Lewis acid sites on SAPO's helped to form in fructose from glucose by undergoing isomerization reactions. Further, Brönsted acid sites present on catalyst facilitate dehydrocyclization reactions to yield HMF. ca. 74% HMF yield with very high selectivity (88%) was achieved. The catalysts were shown to be recyclable by obtaining similar activity in each consecutive run. Besides, fructose and glucose catalysts were also capable of converting disaccharides (maltose, cellobiose) and polysaccharide (starch) into HMF at around 150-170°C within few hours.



Regenerable metal oxide adsorbents for CO_2 capture

A. G. Gaikwad
ag.gaikwad@ncl.res.in

Publications: J. Anal. Sci. Technol., 2012, 3,182; Maced. J. Chem. Eng., 2012, 31, 255; Ads. Sci. Technol., 2012, 30, 817; Water Air Soil Poll., 2013, 224, 1569

The objective was to develop the mixed oxide adsorbents to capture CO_2 at high temperature and utilize the CO_2 adsorbents to convert the methane to syn-gas.

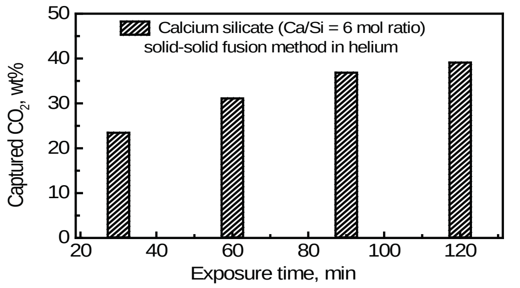
Development and characterization of regenerable metal oxide adsorbents for CO_2 capture

Carbon, zeolites, amines, and ionic liquids are not suitable adsorbents for CO_2 due to a decline in their capturing capacity at high temperatures (>450°C). The captured CO_2 by the mixed metal oxides at higher temperatures involved carbonate formation and adsorption in the pores and on the surface. The mixed metal oxides are thermally stable at post- and pre-combustion temperatures. Mixed metal oxides are good candidates for the capture of CO_2 at high temperatures, 500 to 1000°C.

Adsorbents, calcium silicate and calcium zirconate, copper aluminate and Zinc aluminate were prepared by different methods such as solid-solid fusion, sol gel, molten salt and templates (CTAB, cetyltrimethyl ammonium bromide or Aliquat-336, tricaprylmethyl ammonium chloride).These adsorbents were obtained by calcining in air or helium atmosphere at 900℃. These adsorbents were characterized by surface area, alkalinity, SEM images and XRD patterns.

The calcium zirconate, calcium silicate, copper aluminate and zinc aluminate were screened for the capture of CO_2 and then conversion of CO_2 by methane to syn-gas at the post and pre-combustion conditions. The adsorbents showed high capture capacity towards the CO_2. The obtained results were compared to the well established catalyst such as Ni-Mg, supported noble metal catalyst for the conversion of CO_2 to syn-gas. It was observed that the explored adsorbents showed the conversion of CO_2 by methane to syn-gas at higher temperatures. The conversion and utilization of methane and carbon dioxide are the important issues in the context of global warming effect from the two greenhouse gases. The adsorbents were used to capture the CO_2 and then converted the CO_2 to syn-gas. The syn-gas was converted into fuel. These are the important aspects behind exploring the adsorbents to capture the CO_2.

The following figure illustrates the captured CO_2 by calcium silicate with respect to time.



Captured CO_2 at 550 °C by calcium silicate (Ca/Si = 6 mol ratio) prepared by solid-solid fusion method and calcined in helium for 10 h at 900 °C.

Research & Development Reports

Catalysts for polymerization, steam reforming and solar energy water splitting

C. S. Gopinath
cs.gopinath@ncl.res.in

Publications: ACS Catal., 2013, 3, 303; Appl. Catal. A, 2013, 452, 132;
J. Phys. Chem. C., 2012, 116, 24115; Dalton Trans., 2012, 41, 11311

Molecular adducts as support materials for polyolefin synthesis

Method of preparing the support for polyolefin catalyst drastically influences the catalytic activity through porosity. Molecular adducts made from $MgCl_2$ with different alcohols provided an excellent route to vary the porosity and hence surface and electronic structure. Indeed number and nature of alcohol molecules in the support helps to generate different porosity. Polyolefin catalyst support was prepared by treating $MgCl_2$ with different alcohols, such as methanol, isobutanol, cyclohexanol and evaluated for polymerization activity.

Influence of $MgCl_2.6CH_3OH$ support on polyolefin synthesis: A single phase molecular adduct, $MgCl_2.6CH_3OH$ was synthesized using $MgCl_2$ and methanol. Detailed studies were carried out for a better understanding of single phase $MgCl_2.6CH_3OH$ adduct. ^{13}C CP-MAS solid state NMR and Raman spectral studies support an octahedral coordination of six CH_3OH molecules around Mg^{2+}. Titanated active catalyst, $TiCl_4$ on $MgCl_2.6CH_3OH$ (Figure 1), was synthesized and subjected to detailed characterizations. Active catalyst shows high surface area (102 m^2/gm) and mesoporosity. Titanated catalyst was screened for ethylene polymerization reactions using different co-catalyst (R_3Al; R= $-CH_3$, $-CH_2CH_3$ and $-CH_2CH(CH_3)_2$). 7.25 kg of polyethylene per gram of catalyst was obtained with Me_3Al co-catalyst, which is six times higher in activity compared to commercial $Me_3Al/TiCl_4/MgCl_2.6EtOH$ supported catalyst. Though porosity influences the catalytic activity, other factors also seem to contribute to the total catalytic activity.

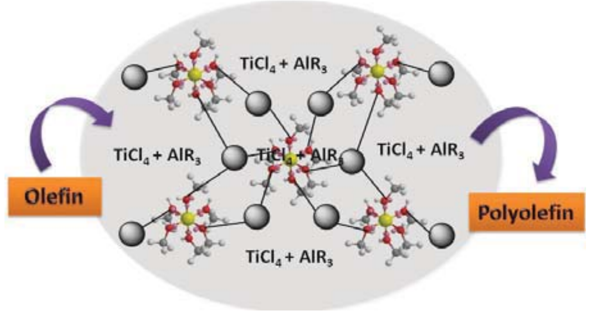


Fig. 1: A schematic representation of polyolefin synthesis from TiClx incorporated $MgCl_2$, prepared from $MgCl_2.6CH_3OH$ adduct

Influence of $MgCl_2.6C_6H_{11}OH$ (MgCyOH) support on polyolefin synthesis: A new and single phase molecular adduct of $MgCl_2$ with six cyclohexanol molecules $MgCl_2.6C_6H_{11}OH$ (MgCyOH) was synthesized. Structural insight to this adduct was obtained by a variety of physico-chemical methods. NMR studies showed the presence of two different sets of magnetically unequal cylcohexanol molecules present around Mg^{2+}. Raman feature of MgCyOH at 712 cm^{-1} confirms that cylcohexanol molecules are present around Mg^{2+} in an octahedral environment. MgCyOH was used as support material to prepare Ziegler-Natta (Z-N) active catalyst. Textural property of above Z-N catalyst exhibits high surface area (236 m^2/g) with high porosity. Above active catalyst was screened for ethylene polymerization. Depending on the co-catalyst employed (Me_3Al, Et_3Al and iso-Bu_3Al) and ethylene pressure, polyethylene yield varies an order of magnitude, from 378 to 3570 g/g catalyst, indicating a possible creation of different active sites and different interaction between co-catalyst and catalyst.

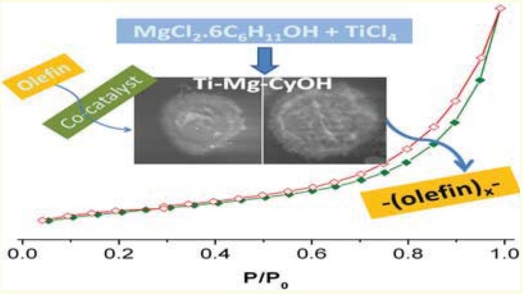


Fig. 2: Polyolefin synthesis from high surface area and TiClx incorporated $MgCl_2$, prepared from $MgCl_2.6C_6H_{11}OH$ adduct

Influence of $MgCl_2.4(CH_3)2CHCH_2OH)$ support on polyolefin synthesis: A new molecular adduct of $MgCl_2$ with isobutanol namely, $MgCl_2.4((CH_3)_2CHCH_2OH)$ (MgiBOH) was prepared as a precursor to supporting material for olefin polymerization catalyst. MgiBOH adduct and final titanated Z-N catalysts were thoroughly characterized for structural and spectroscopy aspects. Peak was observed at 712 cm^{-1} in the Raman spectra of MgiBOH indicate the characteristic $Mg-O_6$ breathing mode and the formation of adduct. Diffraction feature at $2\theta = 7.8^{\circ}$ (d = 11.223 Å) in the XRD confirm the adduct formation and the layered structure. Thus, the presence of isobutanol, in the initial molecular adduct, influences the final Z-N catalyst properties and its activity.

Catalysts for polymerization, steam reforming and solar energy water splitting

Steam reforming over metal doped mesoporous alumina

γ-$Al_{2-x}M_xO_{3\pm y}$ (M = Ti^{4+} through Ga^{3+}): Potential 3D mesoporous material: A simple and highly efficient surfactant-free sol-gel process was developed to obtain nanocrystalline mesoporous γ-Al_2O_3 and metal ion incorporated mesoporous γ-Al_2O_3 with general formula γ-$Al_{2-x}M_xO_{3\pm y}$ (where M = Ti^{4+} through Ga^{3+}). Disordered mesoporosity makes the material as pseudo-3D with a pore diameter of <10 nm and surface area of 200-400 m^2/g. Metal ions in γ-Al_2O_3 resulted changes in the acidity and electronic environment. The efficacy of these materials in catalysis was evaluated successfully for steam reforming of dimethylether; Ni, Cu and Zn containing Al_9GaTM oxides showed high activity and stability. This preparation method is versatile enough to be used for a reproducible synthesis of metal ion incorporated mesoporous γ-Al_2O_3 by varying the metal content and their combinations, and it is expected that many other metal ions could be introduced into the lattice framework for a variety of applications by tuning acidity and electronic structure.

Fig. 3: Photographto show the color associated with different Al_9GaTM oxides (TM = V, Cr, Mn, Fe, Co, Ni and Cu), Al10Ga oxide (Ga), and the mesoporous γAl_2O_3 (center).

Disordered mesoporous V/TiO_2 system for ambient oxidation of sulfides to sulfoxides: High sulfide conversion and predominant sulfoxide yield was observed with 0.1% vanadium doped disordered mesoporous $Ti_{1-x}V_xO_2$ material at ambient and sub ambient temperatures using environmentally green H_2O_2 oxidant. $Ti_{1-x}V_xO_2$ materials were prepared by one-pot solution combustion method in less than 15 min. and thoroughly characterised by x-ray diffraction, HRTEM, Raman spectra and other physicochemical techniques. Different sulfides, such as, phenylsulfide, methyl p-tolylsulfide, ethylsulfide, thioanisole, were converted into the corresponding sulfoxide. Isolated V^{5+} incorporated in the TiO_2 lattice is likely to be the active species for the sulfide oxidation reaction. Catalyst recycling studies indicates the robustness of the catalyst.

Solar energy conversion and storage

The Research was aimed to tap the solar energy for storage as well as to utilize it for chemical conversion, such as water splitting to hydrogen.

Solid solutions of ZnO with nitrides for water splitting: Water splitting to produce hydrogen using abundantly available solar energy and water is a process of importance due to exponentially increasing global energy requirement, over-consumption and drying up of fossil fuels, as well as economic and environmental issues. No breakthrough result is reported yet in terms of quantum efficiency more than 10% in visible light and sustainable activity without any sacrificial agent. Solid solution between an oxide or nitride are emerging as promising materials. These solid solutions show electronic structural changes and the same play a significant role in reducing the band gap to induce visible light absorption. Above solid solutions also demonstrate significant visible light driven photocatalytic activity and exhibiting high potential towards that.

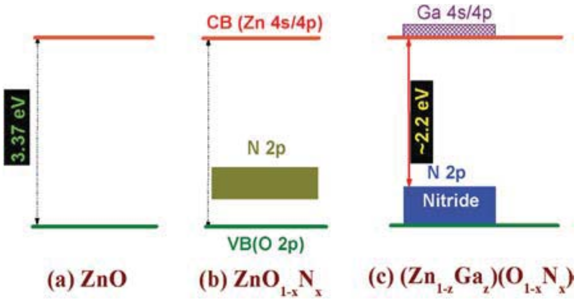


Fig. 4: Schematic representation of band gap measured from optical absorption spectra for (a) ZnO, (b) $ZnO_{1-x}N_x$, and (c) $(Zn_{1-z}Ga_z)(O_{1-x}N_x)$. $(Zn_{1-z}In_z)(O_{1-x}N_x)$ is also similar to that of c

Gold for sunlight absorption and hydrogen generation: Nanogold clusters are electronically integrated with multifunctional, nanocrystalline and mesoporous $TiO_{2-x}N_x$ (Au-NT) by one pot tandem solution combustion method. Au-NT nanocomposite materials exhibit visible light photocatalytic activity and solar H_2 generation (1.5 mmol h^{-1} g^{-1}) from aqueous methanol was demonstrated. Water splitting activity of these materials was attributed to (a) surface plasmon resonance (SPR) of Au for visible light absorption between 500 and 800 nm, (b) pseudo three dimensional (p3D) mesoporosity of $TiO_{2-x}N_x$ for better/faster transport of electrons towards nano Au clusters, and (c) charge separation, and better utilization of electrons by electronically integrated (and hence defects-less) Au with $TiO_{2-x}N_x$ for H_2 production.

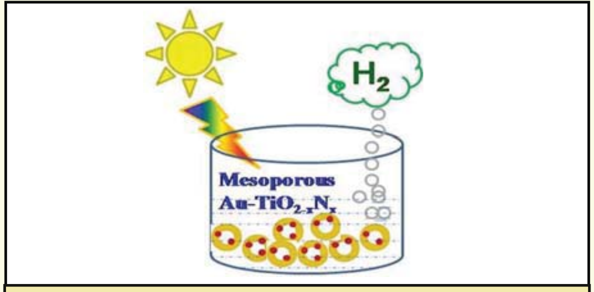


Fig. 5: Dream reaction of water splitting to hydrogen under solar light with a suitable catalyst, such as Au-$TiO_{2-x}N_x$

Heterogeneous catalysts

P.N. Joshi/ V.V.Bokade
pn.joshi@ncl.res.in/vv.bokade@ncl.res.in

Publications: Catal. Today, 2012, 190, 31; 198, 321; Chem. Phys. Lett., 2012, 548, 51; Appl. Surf. Sci., 2013, 264, 574; AIChE Proceedings 2, 2012, 263, 375

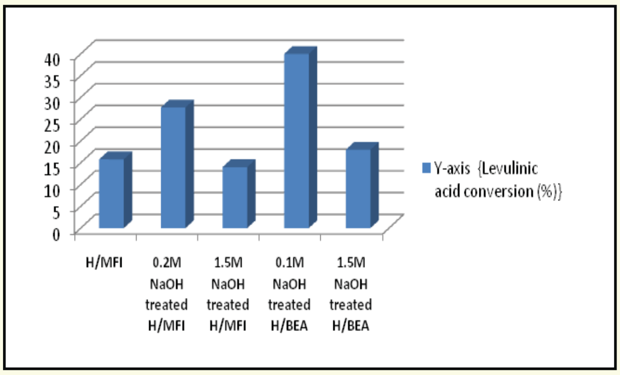
The research was focused on the synthesis, characterization, scale-up, post-synthesis modification and formulation of zeolite based adsorbent and proprietary catalyst for glycerol hydrogenolysis at Catalyst Pilot Plant (CPP). It was focused to build and maintain a balanced portfolio of CPP and the R & D activities which lead to create and sustain the specialized knowledge competencies.

Heterogeneous catalysts for utilization of renewable feedstocks

The coal fly ash was modified by two methods such as solid state fusion with alkali metal hydroxide and acid treatment. The Cu deposition was carried out either by impregnation or precipitation method. These Cu modified coal fly ash catalysts were characterized by different spectroscopy techniques and evaluated for the hydrogenolysis of glycerol to 1,2 - propanediol (1,2-PDO) in a batch reactor under 52 bar H_2 pressure in the temperature range of 473–513 K conditions. Among these two methods, solid state fusion of coal fly ash with alkali metal hydroxide followed by impregnation of Cu (Al:Cu=1:1) showed the highest glycerol conversion, 1,2-PDO selectivity and stability in glycerol hydrogenolysis.

In another approach, Cu/Al_2O_3 catalysts were prepared by co-precipitation, alkali fusion followed by precipitation and direct solid state fusion methods. The effect of preparation method on catalytic performance in glycerol hydrogenolysis to 1,2-PDO was investigated. The catalyst prepared by co-precipitation using Na_2CO_3 showed the predominant presence of metallic Cu phase with a crystallite size of 5 nm, well segregated spherical morphology and highest acidity in the activated sample. These intrinsic properties contributed to achieve the highest glycerol conversion and 1, 2-PDO selectivity in glycerol hydrogenolysis.

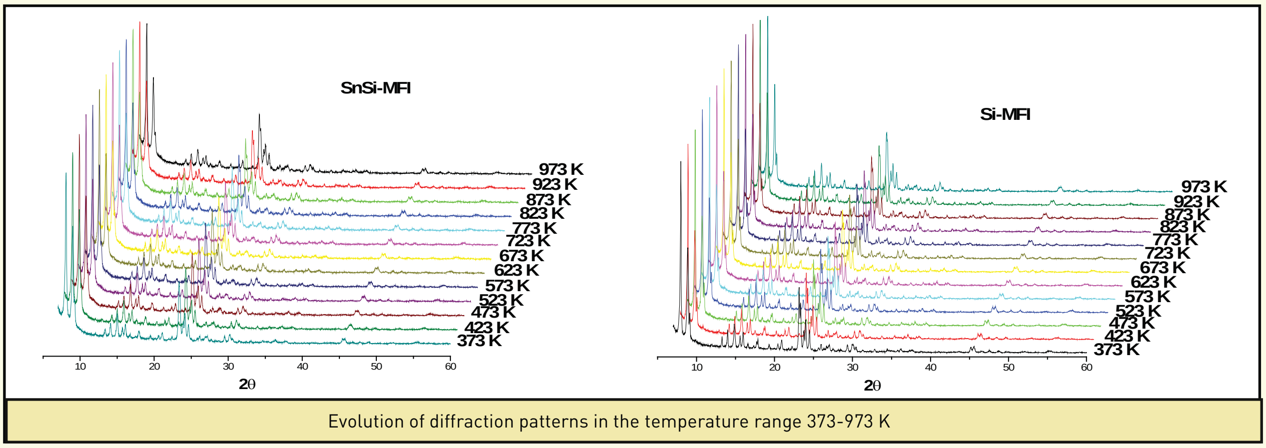
In order to overcome the disadvantages of microporous MFI, BEA and LTL zeolites, i.e, to improve the accessibility and molecular transport, a strategy of post synthesis modification viz. alkali treatment was employed for the creation of mesopores within the zeolite crystals. The XRD crystallinity, chemical composition, textural and acidic properties of these resultant bimodal micro/ meso-porous composites were found to depend on the characteristics of individual zeolite and the concentration of alkali used. The effectiveness of mesoporosity introduction in H/MFI and H/BEA zeolites was investigated in esterification of levulinic acid (LA) with ethanol as this green process produces novel energy chemical i.e. ethyl levulinate (EL) which can be used as diesel miscible biofuel. A recyclable and most efficient 0.1 M NaOH treated H/BEA catalyst exhibited 40% LA conversion with 98% EL selectivity using LA.



Characterization of perovskites and Sn-MFI molecular sieves

The characterization of bulk and surface structures of nanoscopic lanthanum chromite and silver doped lanthanum chromite synthesized by microwave combustion method was carried using XRD, TEM and XPS. X-ray diffraction analysis revealed crystalline nature of sample with hexagonal lattice structure and metallic state of silver. The particle size distribution observed for $LaCrO_3$ was relatively broad; ~20–100 nm and ~30–100 nm for samples synthesized by chromium nitrate and chromic acetate respectively, while the silver doped samples have a finer particle size of ~7–12 nm and ~20–14 nm respectively for A and B site doping. The results revealed the presence of La in +3 oxidation state, chromium ions in two different i.e. +3 and +6 oxidation states, oxygen anions as −2 state while, silver exist in metallic state in the lattice. The atomic ratio of constituent elements showed charge compensation with role of precursors such as chromium nitrate and acetate. Silver as a crystal dopant influenced the bulk as well as surface composition of the sample.

The thermal expansion properties and structural changes occurring in Si-MFI and SnSi-MFI molecular sieves as a function of temperature were studied by *in situ* high temperature X-ray diffraction technique. An isomorphous substitution of Si^{4+} by Sn^{4+} possessing higher ionic radii in the MFI framework found to expand the unit cell. At all the temperatures, ranging from 373 to 973 K, both the samples showed the trend in the values of unit cell parameters as: a > c > b. The isomorphous substitution of Sn^{4+} in MFI framework seemed to be operative in enhancing the strength of the NTE coefficient which may be partly attributed to the transverse thermal vibrations of two fold coordinated oxygen and the intrinsic property of the framework.



Evolution of diffraction patterns in the temperature range 373-973 K

Fractionation and characterization of lignin extractives from E-AFEX™

Pretreatment process: Extractive AFEXTM (E-AFEX™) is a novel pretreatment technology that converts cellulose I to cellulose III simultaneously and partially extract lignin from lignocellulosic biomass. As a result, pretreated feedstocks contain highly digestible carbohydrate content and significantly reduced lignin content. Depending on the pretreatment conditions, it is possible to obtain variations in the selectivity towards lignin solubilization. Temperature, ammonia concentration and co-solvent type are the major factors that contribute to a selective lignin solubilization and subsequent fractionation. Some pretreatment conditions tend to solubilize ash and hemicellulose residues along with lignin. However, since most applications for lignin require low ash and carbohydrate contents, these extractives have been further fractionated to obtain varying purity lignin fractions. For this purpose, solvent precipitation and filtration based methods were developed to fractionate lignin. In this work, multiple fractions generated from the E-AFEX™ extractives generated from pretreated corn stover were characterized by several techniques, which include GPC, TGA, ^{13}C-NMR, ^{1}H-NMR and 2D NMR.

E-AFEXTM Lignin Fractionation

Ultra small nanoclusters for bioimaging and fabrication of sinter resistant nanoreactors

R. Nandini Devi
nr.devi@ncl.res.in

Publications: ChemCatChem, 2013, 5, 1911; Dalton T., 2014, 43, 2120

Ultra small noble metal nanoclusters < 2 nm in diameter have attracted much attention in the past decade due to their unique physicochemical properties. The intense fluorescence emission property renders them ideal for biolabelling and bioimaging application, provided they are water dispersible. Ultra fine size and biocompatibility as a consequence of appropriate functionalization also make them more applicable compared to quantum dots. The research group has designed a novel thiol ligand with ionic head groups facilitating water dispersibility. Various noble metal nanoclusters with size < 2 nm were synthesised using this ligand. Au nanoclusters were found to have emission in NIR region peaking at 820 nm which is advantageous for biological systems. These nanoclusters were also found to be stable against further functionalisation.

Pd ultra small clusters were encapsulated in silica to fabricate nanoreactors. Abundance of organic ligands in the system helps in creating porosity in the silica matrix and encapsulation within the silica ensures protection against agglomeration and sintering. These Pd@SiO_2 systems were found to control sintering with Pd nanoparticle size maintained at 3 nm even at temperature of the order of 700°C.

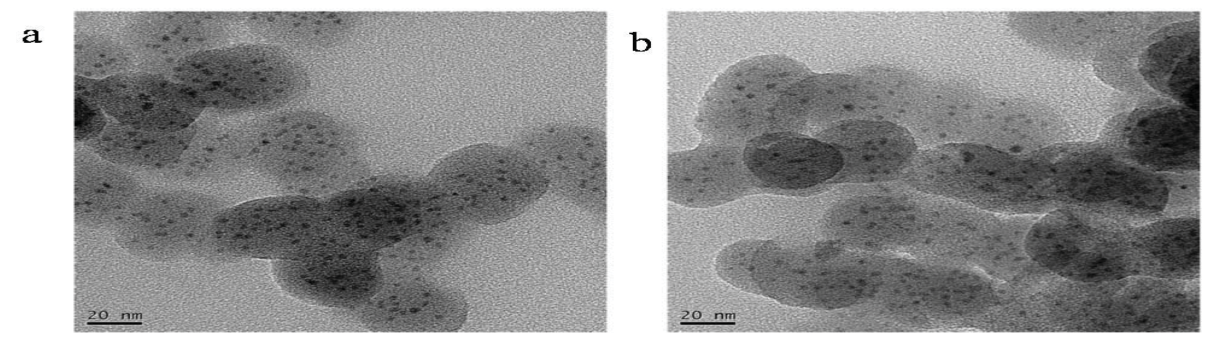


Fig. 1: HRTEM images of calcined Pd@p-SiO_2 nanoreactor at different temperatures; (a) 550°C and (b) 750°C

Keep away for better conduction

Layered structures with well-defined conduction pathways separated from photo generation sites can be envisaged to address the problem of recombination effectively. $InMO_3(ZnO)_m$ series of oxides form one such family of compounds which were conventionally studied for their excellent thermoelectric properties as well as transparent conducting oxides. The enhanced conductivity was suggested to be due to a spatial separation of the carrier donors located in insulating layers and the conducting layers which transfer the carriers effectively. The spatial separation in $InMO_3(ZnO)_m$ was found to be much higher compared to contemporary semiconductors. Most interestingly, this was manifested in the anisotropic nature of the electrical conductivity. This was reflected in hydrogen evolution activity as given in the figure below.

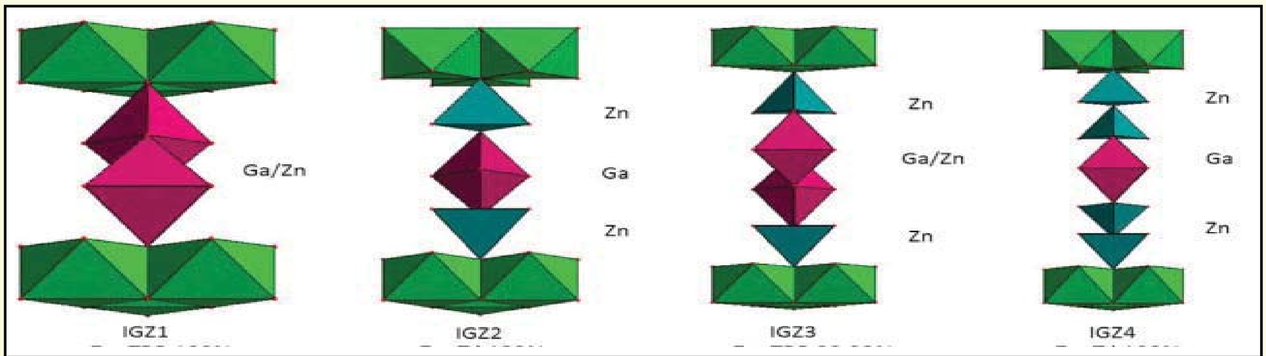


Fig. 2: Structural details of a typical $InMO_3(ZnO)_m$ series which changes with increase in ZnO layer numbers

Selective oxidation and reduction of hydrocarbons using solid catalysts

T.Raja
t.raja@ncl.res.in

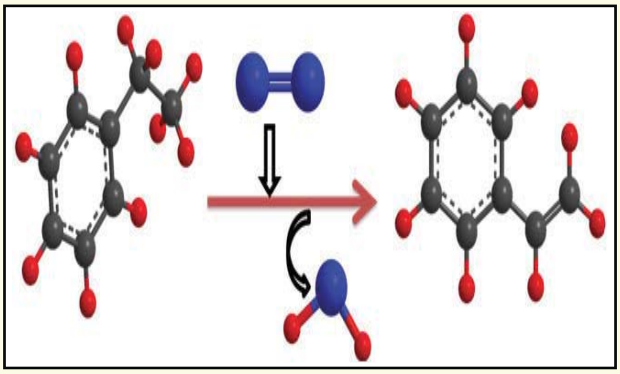
Publication: Green Chem., 2013, DOI: 10.1039/C3GC41321G

Oxidative dehydrogenation (ODH) of ethyl benzene (EB) to styrene (ST) is one of the commercially important transformations. Potassium promoted hematite catalysts were used commercially at very high endothermic reaction conditions. The energy required for this process was too high and was around 15.9 x 10^8 cal per tonne of styrene. The energy consumption in a modified process in presence of CO_2 was also high because of the usage of steam (1.9×10^8 cal per tonne of styrene). ODH is a thermodynamically favourable exothermic pathway which can be carried out at lower temperatures compared to commercial dehydrogenation process. It can be carried out with various oxidants like oxygen, air, N_2O, carbon dioxide, etc. Heterogeneous catalyst was synthesized along with basic support for the above said reaction for giving high yield of ST.

ODH of ethylbenzene to styrene

Styrene "an important monomer" was obtained from ODH of EB using cerium containing mixed oxides (Mg, Al) as catalyst employing oxygen as oxidant. The catalyst showed a stable activity when compared to pure ceria which showed a decrease in activity at long time on stream conditions. The catalyst with 0.3 mol % of cerium showed a better activity than other catalysts prepared. The maximum conversion of EB obtained was 49.4% with 97% selectivity towards styrene. This activity was more or less stable for 72 hours of time on stream (TOS) reaction conditions.

The spent catalyst analysis proved the stability of the catalyst where there was no significant difference in catalyst characteristics even after the reaction. Interestingly there was no sintering or aggregation of ceria in spite of exothermic nature of the reaction



Furfural to furfuryl alohol

Hemicellulosic fraction of biomass was used as feedstock to produce many important chemicals, such as furfural, furfurylalcohol, THFA, furan, and THF. Furfuryl alcohol (FOL) is another essential starting material in various industries due to its application in the production of synthetic fibers, rubbers, resins, and agricultural chemicals. It is normally prepared from furfural (FAL) by hydrogenation and this reduction reaction is carried out either in the gas phase or in the liquid phase. Various amount of nickel containing mixed metal oxide was derived from hydrotalcites it was prepared by co-precipitation followed by hydrothermal treatment was used as catalyst. The maximum conversion of 74% and selectivity 83% towards furfuryl alcohol was observed at optimised conditions. TOS studies were carried up to 48 hours for monitoring the catalytic stability. The catalyst was stable for long run and the spent catalyst was subjected to various physico-chemical analyses.

Oxidation of cyclohexane

Cyclohexene and KA oil (cyclohexanol and cyclohexanone) are important intermediates in production of adipic acid which has a high commercial use. Cobalt containing mixed oxide with different Co ratio ($Co_xMg_{3-x}Al_1$, x= 0.3,0.5,1.0) were synthesized by different synthesis methods like co-precipitation, sol-gel method and combustion method. Physico-chemical characterizations showed a good dispersion of cobalt in the mixed oxide matrix. Oxygen was used as oxidant to carry out the oxidation as oxidative dehydrogenation to form cyclohexene. Some test reactions were carried out in which cyclohexene was the main product and other products like benzene, cyclohexadiene and CO_x.

Catalytic transformation of biomass derived platform molecules for biorefinery application

C. V. Rode
cv.rode@ncl.res.in

Publications: Green Chem., 2012, 14, 2780; Catal. Today, 2012, 190, 31, 321; Catal. Lett., 2012, 142, 779

Simultaneous glycerol dehydration and in-situ hydrogenolysis

Catalytic hydrogenolysis of glycerol to 1,2-PDO has a potential of its commercialization. The use of high pressure fossil derived hydrogen limits the commercial prospective of processes. A non-noble metal Cu-Al was developed for *in-situ* glycerol hydrogenolysis utilizing H_2 generated by glycerol APR under inert conditions (Fig. 1). Distinct spinel $CuAl_2O_4$ phase formation was identified even at low calcination temperature (400°C) due to Cu-Al formulation prepared by simultaneous co-precipitation and digestion technique. Multifunctional characteristics of this catalyst were found to be responsible for its uninterrupted *in-situ* hydrogenolysis performance of 450 h using refined glycerol as well as bio-glycerol feed directly without any pretreatment.

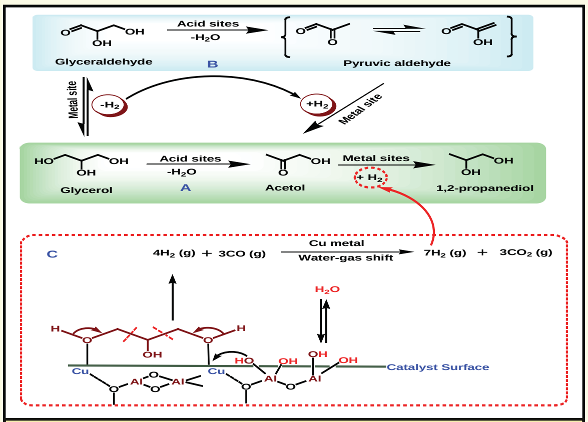
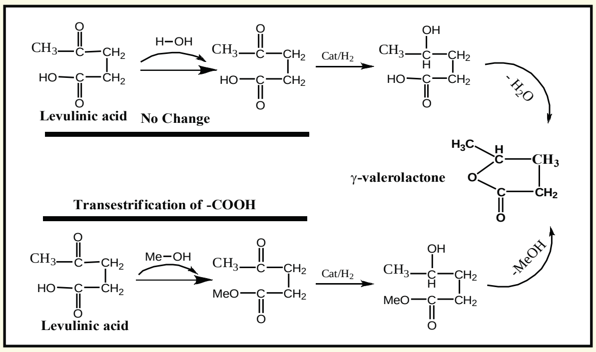


Fig.1: Autogeneous hydrogenolysis of aqueous glycerol to 1,2-PDO

Copper based catalysts prepared by co-precipitation, alkali fusion followed by precipitation and direct solid state fusion methods. The catalyst prepared by co-precipitation using Na_2CO_3 showed the predominant metallic Cu phase with a crystallite size of 5 nm, well segregated spherical morphology and highest acidity in the activated sample. These intrinsic properties contributed to achieve the highest glycerol conversion of 62% and 1,2-PDO selectivity of 88% in glycerol hydrogenolysis.

Cu-ZrO2 nanocomposite catalyst for selective hydrogenation of levulinic acid and its ester to γ-valerolactone

Hydrolysis of cellulose in presence of aqueous as well as alcoholic solutions gives levulinic acid (LA) and esters. Processes were developed starting from wood and agro wastes. Catalytic hydrogenation of LA gives γ-valerolactone (GVL) which is a sustainable commodity chemical having great commercial applications as a solvent in lacquers, as a food additive and also a potential fuel additive for replacing ethanol in gasoline-ethanol blends. It can be converted to a variety of monomers.



Non-leachable and non-noble metal nanocomposite catalysts were developed by incorporating Zr and Al with copper for selective hydrogenation of levulinic acid and its methyl ester to GVL. HRTEM revealed the particle size of copper in a range of 10-14nm. Both XRD and Raman spectroscopy confirmed the formation of $Cu-ZrO_2$ nanocomposite and also the presence of mixed oxide phases along with Cu^0. Both the catalysts showed complete conversion of LA and its ester with >90% selectivity to GVL.

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

Acid functionalized ionic liquids were found too efficient (99% conversion) to catalyze the alcoholysis of furfuryl alcohol (FAL) in presence of various alcohols to the corresponding levulinic acid esters under mild temperature (90-130°C) conditions. The Bronsted acidity of ILs could be tailored by extending the alkyl chain length using 1, 4-butane sultone resulting into highest selectivity of > 95% to Me-LA. Using a combination of suitable IL and Ru catalyst, direct conversion of FAL to γ-valerolactone (GVL) was reported for the first time. A complete conversion of FAL with the highest selectivity of 68% to GVL could be achieved under optimum conditions. The catalyst system could be efficiently recycled for five uses retaining the original activity and selectivity profiles.

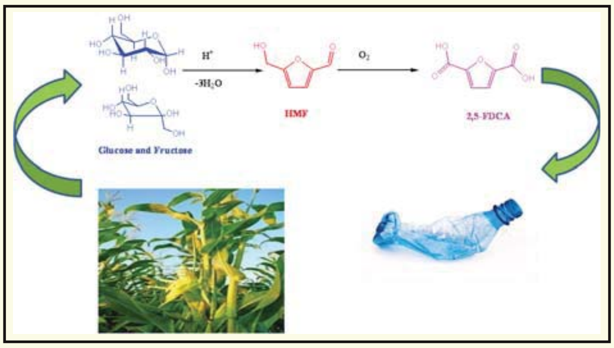
Green processes for platform chemicals and fuels from biomass

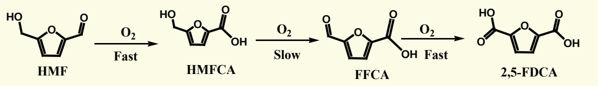
C. V. V. Satyanarayana
sv.chilukuri@ncl.res.in

Publications: Micropor. Mesopor. Mater., 2012, 181, 38; Catal. Sci. Technol., 2012, 2, 1852

Preparation of hydroxymethylfurfural and furandicarboxylic acid from C6 sugars

Reported processes used the homogeneous base (1–20 equiv. NaOH) and high oxygen pressure (10–20 bar) to produce FDCA. This new catalytic process developed overcame these limitations, making it suitable for industrial-scale applications. The Ru exchanged Manganese containing octahedral molecular sieves (OMS) were used for the oxidation of HMF to FDCA without addition of homogeneous base.



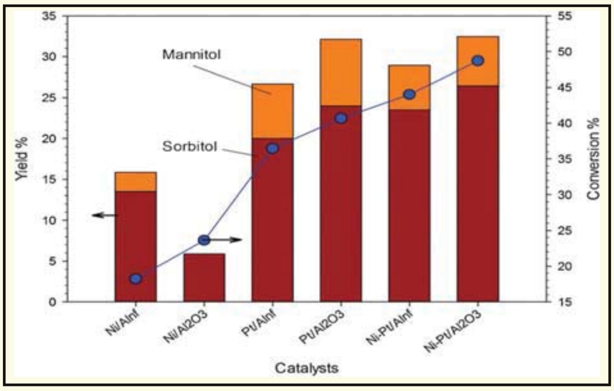


Reaction pathway for the oxidation of HMF to FDCA

The FDCA yield increased during the oxidation of HMF due to the rise in the temperature from 90-110°C. But, beyond 110°C, the FDCA yield falls after reaching a maximum because of the condensation of acid (FDCA) and alcohol (HMFCA), catalyzed by acidic Mn^{4+} ion. Oxygen pressure has a marked effect on the yield of FDCA, as higher pressure led to loss in FDCA yield. The catalyst was successfully recycled with only minimal loss in activity. Even Ru or Mg did not leach out under reaction conditions. The catalyst can be scaled up and applied for commercial exploitation.

Conversion of cellulose to polyols

Sorbitol is a key platform chemical that has uses in several industrial applications, including bio-fuels and hydrogen production. Presently there is no commercial heterogeneous catalytic process to produce sorbitol from cellulose due to low yield and high cost of noble metals required for good conversion of cellulose. The reported process which is an aqueous phase hydrolysis–hydrogenation process converted cellulose to sorbitol using a cheap Ni based catalyst.



Though monometallic Ni catalysts showed little activity, with the addition of a small amount of Pt to the Ni catalyst (Ni : Pt = 22 : 1 atom ratio), the activity was greatly enhanced. Results showed that the bimetallic Ni–Pt catalysts supported on mesoporous alumina gave a hexitol (sorbitol + mannitol) yield of 32.4% compared to only 5% with a Ni catalyst. Whereas, Ni–Pt supported on a mesoporous beta zeolite support provided even higher yield of 36.6%. These results were obtained after only 6 hours of reaction at 200°C and 50 bar H_2 pressure.

Aqueous phase reforming of glycerol

Nitrogen doped mesoporous carbons were synthesized with variable nitrogen content via a colloidal silica nanocasting method using melamine, phenol and formaldehyde as precursors. These mesocarbons were used as support for the preparation of 5% Ru and 5% Pt containing catalysts. Glycerol conversion was increased initially with time on stream, which later stabilized at around 80%. Hydrogen selectivity was also quite good around 90%, gave yield of H_2 around 72%. It clearly showed that formation of other lower hydrocarbons (C_2-C_4) through hydrogenation of CO was low on these catalysts. Moreover, there was hardly any deactivation of the catalysts with time on stream. The study of spent catalysts with TEM, minimal segregation of Ru was reported which showed that nitrogen doping helped to arrest sintering of the catalysts under the hydrothermal conditions employed for APR.

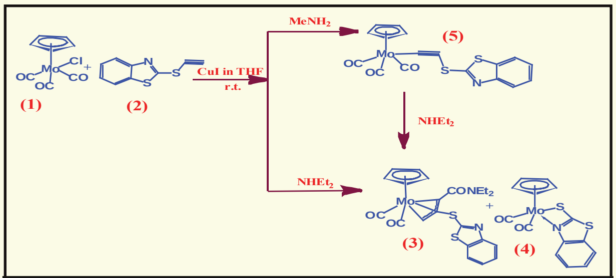
Catalyst for organic transformations and environmental application

S. B. Umbarkar/A. V. Biradar
sb.umbarkar@ncl.res.in

Publications: Green Chem., 2013, 15, 1211; Chem. Eur. J., 2013, 19, 2030

Homogenous Catalysis

Synthesis of molybdenum based organometallic complex: The objective was to synthesize molybdenum based organometallic complexes. Targets were achieved by using alkynyl ligands which showed good catalytic activity. An alternative route was developed for the preparation of CpMoO$_2$(-C≡CPh) from MoO$_3$ precursor which involved less number of steps and very simple work up procedure. Mo-carbonyl complex was prepared with propargylated benzthioazole thiol using a method developed for synthesis of Mo-acetylide complex. A product Moη^3-allyl complex was obtained where η^1-propargyl group was rearranged to η^3-allyl group with migration of CO ligand from Mo center to the organic moiety with participation of the amine solvent (Scheme 1, Fig. 1).



Scheme 1: Represents the synthesis of Mo S-propargyl (5) and S-allyl (3) complexes

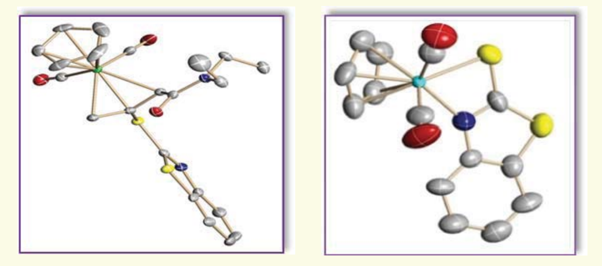
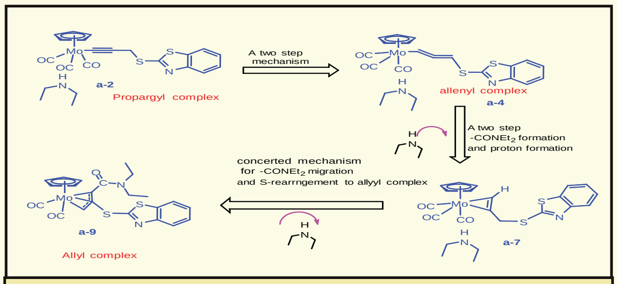


Fig. 1: Single crystal X-ray structures of 3 and 4

The detailed mechanism of this rearrangement was studied by DFT calculations (Scheme 2). The catalytic activity of the allylic and propargyl complexes was evaluated for oxidation of cyclohexene as model substrate using organic t-butyl hydrogen peroxide. Allylic complex gave 100% cyclohexene conversion whereas propargyl complex gave only 37% conversion under identical condition. However both the complexes gave very high selectivity of 98% for epoxide product.



Scheme 2: Mechanism of rearrangement of propargyl complex to allyl complex

The catalytic activity of the dichlorodioxomolybdenum complex was investigated for selective oxidation of aromatic alcohols to corresponding aldehydes using dimethyl sulfoxide (DMSO) as an oxidant. The catalyst showed high conversion for range of aromatic alcohols; though the catalyst is homogenous in nature, it was efficiently recycled even up to five cycles without appreciable loss in the activity.

Oxidation of allylic alcohols was investigated using various Schiff base dioxomolybdenum complexes and molybdenum carbonyl complexes as catalysts and aq. H$_2$O$_2$ as an oxidant. All the catalysts showed 100% conversion with very high selectivity for epoxy alcohol (99%). Under identical conditions benzylic alcohol showed 99% conversion and 50% selectivity favoring α, β unsaturated carbonyl compound instead of epoxy alcohol suggesting the influence of double bond position on selectivity of oxidation to either epoxidation or alcohol oxidation. This work was carried out in collaboration with Prof. Francine Agbossou, UCCS, France.

Heterogeneous catalysts for valorization of renewable

Conversion of lactic acid to acrylic acid with sodium modified calcium pyrophosphate: An improved catalyst was developed to convert lactic acid to acrylic acid which is an important raw material for polymer industry. This continuous down flow process gave 100% lactic acid conversion with 75% selectivity for acrylic acid with acetaldehyde as the only by-product using sodium modified calcium pyrophosphate catalysts.

Catalyst for organic transformations and environmental application

Palladium nanoparticle supported on barium hydroxyl fluorides: Palladium supported on alkaline earth metal hydroxyl fluorides catalysts were prepared in one pot by fluorolytic sol-gel method in collaboration with Prof. Kemnitz, Humboldt University Berlin. The catalyst showed very high benzyl alcohol conversion upto 99% with 100% selectivity for aldehyde. The catalyst was efficiently recycled up to five cycles without appreciable loss in catalytic activity. There was no Pd leaching during the reaction as confirmed by AAS analysis.

Catalyst for removal of NOx from automobile exhaust engines: Objective was to develop a modified benchmark catalyst 2%Ag/Al_2O_3. Hence bimetallic catalyst with 1% Au and 1% Ag loading on high surface area alumina were prepared by different methods and extensively characterised by various physico-chemical techniques and tested for SCR activity under lean burn engine exhaust condition. Ag-Au/Al_2O_3 catalyst showed very high (100%) NO conversion to N_2 at 367°C compared to 1Ag/Al_2O_3 (96%) and 1Au/Al_2O_3 (70%). Aging of the Ag-Au/Al_2O_3 catalyst in the reaction feed at 500°C for 12 h has considerably improved low temperature activity with ~40% NO conversion at 200°C.

Template free synthesis of high surface area mesoporous solid acid catalysts for nitration of aromatics: Preparation of high surface area silica without using template (BET SA ~900 m^2/g) was carried out. A series of molybdenum and tungsten based solid acid catalysts were prepared and used for acid catalysed reactions like esterification and nitration of aromatics. Spectroscopic investigations of nature of catalytically active species were done on the catalyst surface while acid catalyzed esterification was done using sol gel synthesized MoO_3/SiO_2 catalyst. It revealed the formation of silicomolybdic acid as catalytically active species in presence of water. Additionally, preparation of series of WO_3/SiO_2 catalyst by varying WO_3 loading and precursors was carried out and their catalytic activity was evaluated for the liquid and vapour phase nitration of aromatics using varying concentration (30-98%) of HNO_3 as nitrating agent, without using any sulfuric acid. Very high conversion (upto 92%) was achieved in liquid phase nitration using 30-70% nitric acid as nitrating agent without using any sulfuric acid.

Silica microspheres as catalyst: Silica microspheres were prepared and further modified by etching with KOH (Fig. 2). These silica microspheres were used for olefin oxidation using H_2O_2 as an oxidant. Very high cyclohexene conversion (70%) with 92% selectivity for epoxide was obtained. This catalyst has been used for oxidation of variety of olefins.

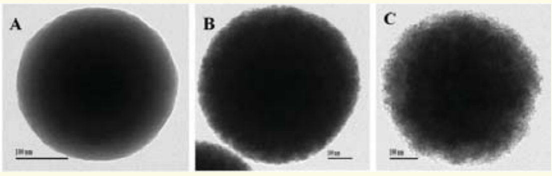


Fig. 2: TEM images of silica microspheres etched with 0.02 M KOH for (a) 2 h (b) 3h and (c) 4 h

Molybdenum oxide nanoparticles as catalyst: Ultrasmall molybdenum oxide (MoO_3) nanoparticles supported on various metal oxides nanospheres (SiO_2, TiO_2 or ZrO_2) were synthesized. Catalysts showed excellent catalytic activity for cyclohexene epoxidation giving >90% conversion and 93% epoxide selectivity. The catalyst was successfully recycled up to five cycles without losing much activity and selectivity.

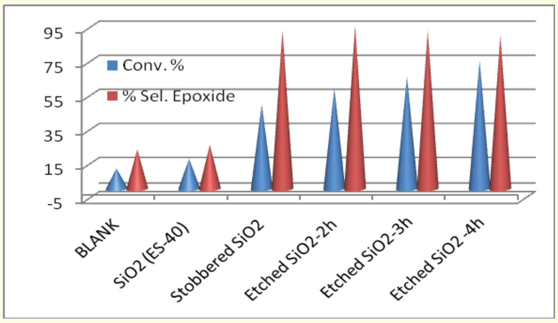


Fig. 3: Epoxidation of cyclohexene using different silica as catalysts

Novel mesoporous catalysts for fine chemicals

D. Srinivas
d.srinivas@ncl.res.in

Publications: Catal. Today, 2012, 198, 59; J. Catal., 2012, 293, 126; J. Mol. Catal. A-Chem., 2013, 65, 112, 368, 377; Catal. Commun., 2013, 37, 36

Catalysis by nanoporous solid catalysts plays an important role in sustainable development and environmental protection. A new class of mesoporous, M = Ti, Mn, Fe and V-incorporated silicas (M-SBA-12 and M-SBA-16) was prepared for a variety of oxidation and acid-catalyzed reactions that can find applications in fine chemical manufacturing. The three-dimensional pore architecture of these mesoporous silica materials enable facile access and diffusion of bulky reactant molecules of pharmaceutical interest to the active sites inside the pores. These new catalysts are reusable and more hydrophobic than the known porous silica catalysts. These catalysts were prepared in highly acidic conditions. Heteroatom incorporation in the framework is challenging under those reaction conditions.

Epoxidation

Titanium silicate (TS-1) is known for its excellent catalytic oxidation and epoxidation activity at mild conditions using aqueous H_2O_2 as oxidant. However, its application was confined only to smaller molecules of dimension < 0.5 nm due to its microporous nature. Ti-containing mesoporous MCM-41 catalysts are relatively less stable and exhibit lower intrinsic catalytic activity than TS-1. The three-dimensional mesoporous titanosilicates (Ti-SBA-12 and Ti-SBA-16) were prepared and are superior to both TS-1 and Ti-MCM-41 in the epoxidation of cyclic olefins (cyclohexene and cyclooctene, for example) using tert-butyl hydroxide as catalyst. Epoxide selectivity of 100% and olefin conversion greater than 92% could be obtained in just one pass at 40°C over these catalysts.

Hydroxylation

Hydroxylation of phenol is an industrially important reaction as the product diphenols, viz., catechol and hydroquinone. There are few commercial processes for this transformation which use homogeneous catalysts. Hydroxylation of phenol with H_2O_2 catalyzed by TS-1 or TS-2 was created an environmentally benign route for the production of catechol and hydroquinone. It was found that Ti-SBA-12 and Ti-SBA-16 are more efficient catalysts for this transformation. The selectivity for hydroquinone in this process over these new catalysts and the life of the catalyst is higher than TS-1. If H_2O_2 efficiency is ~ 90 mol%.

Oxidation of amines to amides

Methacrylamide and caprolactum are two industrially important amides used in polymer manufacturing. Several approaches reported to synthesize it use expensive metal catalysts. Development of a greener approach which doesn't generate waste and uses cheaper metal catalysts is desired. Manganese incorporated mesoporous silica (Mn-SBA-12 and Mn-SBA-16) are efficient catalysts for preparing amides from primary amines by direct reaction with aerial oxygen and ammonia solution. Benzamide yield as high as 50 mol% could be obtained with these catalysts in the reactions at 150 °C. It is found that weak acidity and Mn in +3 oxidation state are the key parameters enable the synthesis of amide in high yields.

Aminolysis of epoxide (β - Aminoalcohol synthesis)

Oxycontin, Coreg and Toprol-XL are a few examples of active pharmaceutical ingredients (APIs) that contain a β-amino alcohol unit in their structure. Zyvox and Skelaxin are a few others that can be formed through β-amino alcohol precursors. Several Lewis and Brönsted acid catalysts catalyze this transformation. The Ti-SBA-12 and Ti-SBA-16 with three-dimensional mesopore architecture are reusable, solid catalysts for the synthesis of a range of β-amino alcohols in high yields and selectivity through ring-opening of epoxides with amines at ambient and solvent-free conditions.

Esterification

Biodiesel, a sustainable and biodegradable diesel fuel extender is a synonym for fatty acid methyl or ethyl esters, produced through esterification / transesterification of vegetable oils or animal fat with alcohol. The conventional technology of its production using homogeneous alkali base or mineral acid catalysts has environmental issues. Use of solid catalysts in these processes lead to eco-friendly processes. Ti-SBA-16 exhibits high catalytic activity for esterification of oleic acid with methanol producing biodiesel and with polyols producing bio-lubricant base stocks. These catalysts are reusable.

This novel class of highly efficient, mesoporous titanosilicates opens up a new avenue for their application in oxidation and Lewis acid-catalyzed transformations of industrial relevance.

Nanoengineered materials for catalytic applications

C. P. Vinod
cp.vinod @ncl.res.in

Publications: Catal. Sci. Technol., 2013, 3, 1190;
Part. Part. Syst. Char., 2013 DOI: 10.1002/ppsc.201300195

Core-Shell Au@SiO_2 catalyst for oxidation reactions

One of the main challenges in gold based catalysis was to resist sintering which is considered as the root cause for deactivation. Since gold (Au) nanoparticles are found to be active in a narrow size window of 5-10 nm, attaching dual functionality, viz. reactivity and stability, amounts to synthesizing monodisperse gold nanoparticles of small size which are resistant to any morphology changes under thermal or chemical treatments during the reaction. Attempts in this direction have led to the synthesis of sinter resistant gold nanocatalysts, which involve confining gold in catalytically relevant mesoporous oxide materials. To this end synthesizing porous core–shell nanostructures, with gold core and porous SiO_2 shell was demonstrated with good room temperature CO oxidation activity and stability.

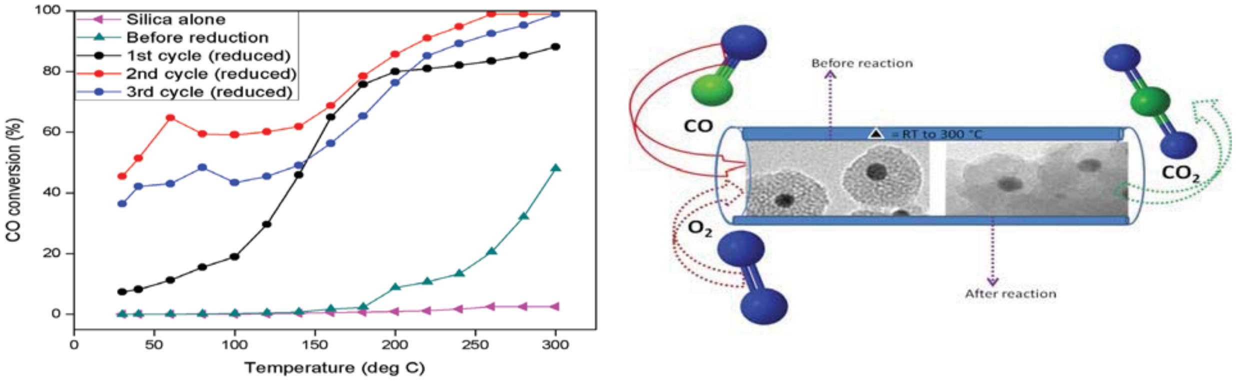


Fig. 1: CO oxidation profile for Au@meso-SiO_2 core-shell catalyst from RT to 300^{0}C. The schematic shows the stability of the catalyst retaining its size even after three cycles of reaction

Oxidation resistant Au@Ni bimetallic nanostructures

Electronic and geometric factors are considered to play a crucial role in defining the overall chemical and physical properties of bimetallic nanostructures. By carefully choosing the individual component in the bimetallic nanostructure the property of the other metal can be modulated. It was showed that Ni which is a very valuable metal in catalysis and which undergoes surface oxidation rapidly can be made oxidation resistant by introducing Au core. Such Au@Ni bimetallic nanostructures of approximate size 8-10 nm can be synthesized both in magnetic and non-magnetic form and are found to be oxidation resistant until 150^{0}C showing very good reduction properties in the conversion of *p*-nitrophenol to *p*-aminophenol.

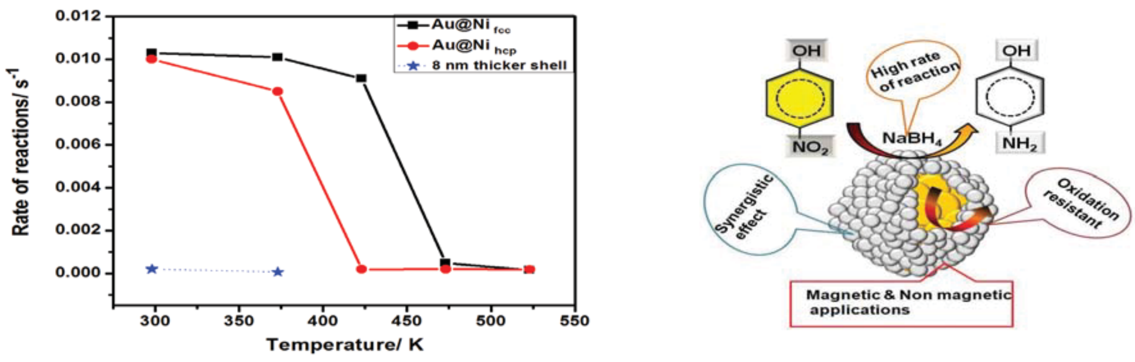


Fig. 2: The rate of *p*-nitrophenol reduction reaction on the as synthesized and annealed Au@Ni catalyst (both fcc and hcp). The schematic shows the diverse properties exhibited by the bimetallic nanostructures

Supercritical fluid technology

Sunil S. Joshi
ss.joshi@ncl.res.in

Efforts were made to develop a novel heterogeneous catalyst system for hydrogenation of CO_2 to formic acid and its derivatives with a process technology to meet the economic efficiency.

Hydrothermal conversion of biomass to industrially useful chemicals

Research was done to exploit the special properties of the supercritical water (scH_2O) to breakdown lignin and cellulose into industrially useful chemicals. De-polymerization of the lignin derived from sugarcane bagasse was carried out in two stages in a continuous mode. In the first stage, hydrolysis of the complex biopolymer was done while in the second stage catalytic oxidation resulted into substituted phenols. Reactions were carried out under different sets of conditions sub-critical and super critical of water. The de-polymerization of cellulose to monomer was catalyzed by acid. A solid acid catalyst system for cellulose conversion into platform chemicals was successfully developed.

An assessment of various process parameters like the impact of the feedstock on the conversion and product distribution was done. The results were quite encouraging and further studies on the role of various homogenous and heterogeneous catalysts on product distribution are being investigated.

Lanthanide doped nanomaterials and its applications

Meitram Niraj Luwang
mn.luwang@ncl.res.in

Publications: New J. Chem., 2014, 38, 115; Appl. Surf. Sci., 2014, 290, 332

Lanthanide doped nanomaterials

Research was aimed to find lanthanide doped nanomaterials having prospect in white light LEDs applications. The application of lanthanide doped nanomaterials as a bioimaging agent, drug delivery, gas sensing and photocatalysis was taken up. A novel approach utilising the photoluminescence properties of the lanthanide doped nanomaterials for the detection and separation of hazardous materials from aqueous medium is also under investigation.

Arsenic detection and removal: A novel approach

Highly crystalline Eu^{3+} (5%) doped YPO_4 nanorods were synthesized in a very simple co-precipitation method and characterized them with different instrumental techniques like XRD, SEM, TEM, XPS etc. These nanoparticles were used for the first time to detect arsenic in water. These nanoparticles adsorbed both arsenic and arsenious acids in presence of excess of chloride ions. The effect of arsenic adsorption on the luminescence behavior of the nanoparticles was studied. Arsenic acid enhanced the luminescence intensity whereas arsenious acid quenched the luminescence (Fig. 1). This relation of luminescence property with concentration of arsenic can be used to detect arsenic in industrial waste. This novel technique of detecting Arsenic ion in aqueous solution utilizing the luminescence properties of lanthanide doped nanomaterials might have a potential application in the detection and removal of hazardous materials from wastewater.

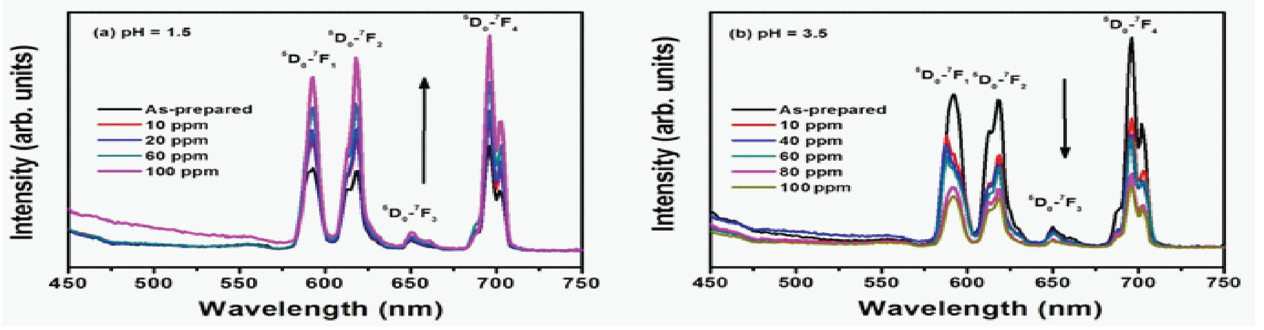


Fig. 1: Photoluminescence spectra of YPO4:Eu^{3+} at varying concentration of Arsenic at different pH

Treatment of industrial wastewater

Sanjay P. Kamble / S. N. Shintre
sp.kamble@ncl.res.in

Treatment of industrial wastewater by using advanced oxidation processes

The objective was to develop modified photo-catalyst and semi-continuous/ continuous pilot scale photocatalytic reactor for the treatment of industrial wastewater using solar radiation.

Initially, a batch type photocatalytic reactor was developed for the treatment of pharmaceuticals wastewater using solar and artificial radiation. The effect of various operating parameters such as initial concentration of pollutants, photocatalyst loading, pH of solution and effect of presence of co-existing ions on photocatalytic oxidation of pollutants was studied in order to establish the optimum process parameters. Industrial effluents contain pollutants apart from different salts at different levels of concentration. The salts are generally ionized under the condition of photocatalytic degradation. It was found that the rate of CFN degradation in presence of the sodium carbonate has a substantially detrimental effect on the photocatalytic degradation, however in the absence of salt almost complete degradation of CFN was achieved within 30 min. The pronounced effect of carbonate is due to their effect on adsorption of substrate on the photocatalyst and their ability to act as hydroxyl radical scavengers. The kinetics of photocatalytic oxidation was also studied. It was found that the photocatalytic oxidation of model pollutants like paracetamol, CFN etc. using solar radiation showed much promising results as compared to artificial radiation. Based on these results a pilot scale photocatalytic reactor was setup (Fig. 1) as a part of XII five-year plan network project and pilot trail for the treatment of the simulated and actual wastewater will be performed soon. During the course of project combination of photocatalytic /hydrodynamic cavitations or the Fenton process will be attempted for the treatment of pharmaceuticals wastewater using solar radiation.

Fig. 1: Pilot scale photocatalytic reactor assembly for the treatment of industrial wastewater

Development of low temperature demulsifier

The stability of water in oil emulsions is attributed to the presence of surface active materials, such as asphaltenes, resins, naphthenic acids and clays. These materials form a rigid interfacial film at the oil/water interface, which hinders the coalescence of emulsified water droplets. In terms of cost, safety and general ease, a low molecular weight carboxylic acid was chosen such as acrylic acid/ modified acrylic acid. It was preferred for the synthesis of demulsifier in this project. From manufacturing point of view, acrylic acid and its monomers are far better in terms of synthesis, handling and storage. Other chemicals based demulsifiers were also developed. The developed demulsifiers were tested for demulsification of actual ONGC crude oil and results were encouraging. Based on these results offshore demulsification of actual ONGC crude oil was performed at Bombay high ONGC platform. The results are very promising and further work is going on.

Solvent extraction of carboxylic acid in continuous mode

Shashank G. Gaikwad
sg.gaikwad@ncl.res.in

The investigations were done for (Liquid + liquid) equilibrium (LLE) of the ternary (water + acetic acid + toluene) system. Since this chemical system was frequently used in liquid–liquid extraction investigations, published LLE data was compared with the experimental data. The present experimental data was found to be in good agreement with published literature data. Attempt was made to extract acetic acid from aqueous phase with toluene in continuous mode with packed extraction column. It was found out that extraction factor is inversely proportional to continuous phase flow rate and directly proportional to dispersed phase flow rate.

Separation of fine chemical from reaction mixture by solvent extraction

Experiments were carried out with synthetic mixture of p-aminophenol, aniline and sulphuric acid. This study was carried out for 80% selectivity for p-aminophenol. 95-96% p-aminophenol was extracted in precipitated form from the mixture and 97-98 % aniline was extracted with toluene.

Real time performance improvement for a thermal power plant using artificial intelligence techniques

Sanjeev S. Tambe
ss.tambe@ncl.res.in

Publications: J. Therm. Anal Calorim., 2012, 112 , 805; Int. J. Comput. Biol., 2012, 1, 67

Coal-based thermal power plant processes incorporates certain complexities which aggravates further owing to variations in the coal quality and power demand, high ash content of the coal, grid instability, etc. These issues posed serious challenges in maintaining the design efficiency of the plant. Online plant optimization systems tackled this complexity by simultaneous optimization of parameters, resulted in the real-time performance improvement through effective plant operation. Such an improvement was achieved via data-driven modeling and optimization using relatively recent Artificial Intelligence (AI) techniques.

Accordingly, an adaptive AI-based modeling and optimization system (AIMOS) was developed based on the quality data with a wide variation in it, collected from a 500 MW thermal power plant. This model cum optimizer recommended set-points of various boiler controllable parameters viz. excess air, burner tilt, air distribution, etc., in real-time for an optimized plant operation. The AI-based system maximized plant performance while satisfying strictly defined constraints pertaining to steam and metal temperatures. The developed system lies in the regime of "grey" box modeling methods borrowing both from data-driven and phenomenological models. It was customized according to the specific needs of the plant and was least affected by external disturbances, thus being flexible and at the same time robust in performance.

Kinetic modeling of photopolymerization of bis-aromatic and alicyclic based solid urethane acrylate macromonomer

Detailed kinetic modeling was performed for the reaction involving photopolymerization of bis-aromatic and alicyclic based solid urethane acrylate macromonomer in presence of large excess of reactive diluent.

Prediction of reactivity ratios in free-radical copolymerization from Q-e parameters: Genetic programming based models

In free radical copolymerization prediction of reactivity ratios of co-monomers assumed significant importance since it assists in gaining knowledge about polymer composition. The principal deficiency of the commonly utilized Alfrey-Price (AP) scheme for computing comonomer reactivity ratios in the widely used free radical copolymerization is that its reactivity ratio predictions are often inaccurate. Accordingly, exclusively data-driven, Q-e parameters based new models were developed for the reactivity ratio prediction in free radical copolymerization. A novel artificial intelligence formalism known as "genetic programming (GP)" was employed for this development. The GP-based models possessed very different functional form than the AP model. A comparison of the AP, GP and artificial neural network (ANN) based models indicated that the GP models exhibit superior reactivity ratio prediction accuracy and generalization performance when compared with the AP and ANN models. The GP-based reactivity ratio prediction models have the potential of replacing the widely used AP models.

Physical chemistry of organic reactions in environmental benign media

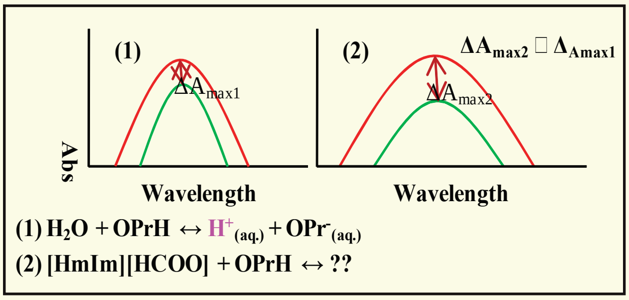
Anil Kumar
a.kumar@ncl.res.in

Publications: J. Org. Chem., 2012, 77, 8775; J. Phys. Chem. B, 2013, 117, 2456; Phys. Chem. Chem. Phys., 2013, 15, 8050; J. Phys. Chem. A, 2013, 117, 2446

The objective was to decipher the nonbonding interactions of ionic liquids to reveal the molecular origin of their effect in different chemical reactions. It was aimed to investigate the structure property relationship in ionic liquid systems involving microemulsions. Also the focus was on the mechanism of organic reactions at "on water" condition and the hydrophobic effects in the chemistry of carbohydrates used as renewable organic raw materials.

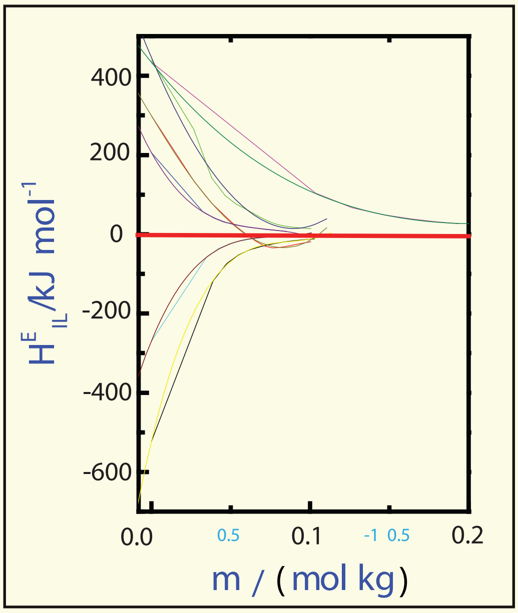
Acidity of the binary mixture of the ionic liquids

Acidity functions were used to express the ability of a solvent/solution to donate/accept a proton to a solute. This work accounts for the acidity in the alkylimidazolium-based protic ionic liquids (PILs), incorporated with carboxylate anion, water and in a binary mixture of PIL and water using the Hammett acidity function, H_0. A reversal in the acidity trend was observed, when organic acids were transferred from water to PIL. It was emphasized that an increased stabilization offered by PIL cation toward the more basic conjugate anion of organic acid was responsible for this anomalous change in acidity order in PILs, which was absent in water. The greater stabilization of a basic organic anion by PIL cation is discussed in terms of the stable hard–soft acid base (HSAB) pairing. The H_0 function in binary mixtures points to the involvement of pseudosolvent, its behavior changes with the nature and concentration of acid. The presence of the maxima/minima in the H_0 function is discussed in terms of the synergetic behavior of the pseudosolvent composed of the mixtures of aqueous PILs.



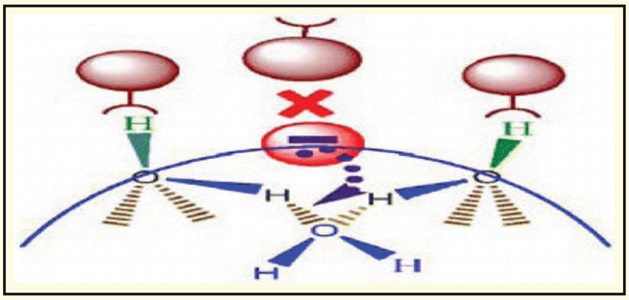
Probing enthalpic variation in ionic liquids

The present communication divulges interesting thermal behavior of different protic ionic liquids arising due to the hydrophobicity modifications in their parent cationic ring structures. This work assisted to differentiate between protic ionic liquids, their aprotic counterparts and common electrolytes in water. The thermal signatures produced by protic ionic liquids, aprotic ionic liquids and electrolytes emerge as individual fingerprints for them.



The 'on water' organic reaction mechanism

An exhaustive kinetic analysis was carried out to offer the convincing evidence of the involvement of the oil–water interface in guiding "on water organic reaction" mechanism. Sensitive techniques were established for the preferential solvation of polarizable ions at the water surface. The experimental methods were developed to control the molecular structure of oil–water interface in situ. Both the kinetic and thermodynamic outcomes have univocally established that the hydrogen-bonding ability of the surface water molecules plays a critical role in deciding the on water organic reaction mechanism.



Physical chemistry of organic reactions in environmental benign media

Mechanistic aspects of baylis-hillman reaction

The kinetic data for a Baylis-Hillman reaction in certain ionic liquids possessing ethylsulfate anion [$EtSO_4$]–demonstrated that the rate determining step (RDS) was second order in aldehyde, but first order in acrylate and DABCO.

Anomalous viscous behavior of ionic liquids

The salting behavior in water can be altered in the presence of ionic liquids. It was confirmed that the salting-in agents in the presence of the ionic liquids with higher alkyl chain can display unusual fall and rise in the viscosity of the systems.

Deep eutectic solvent with sustainable properties

A new family of deep eutectic solvent (DES) based on unique combination of carbohydrates and organic salts were introduced and characterized to replace ILs as solvents for organic reactions and separation technologies. The DES provided better perspective in each process carried out in organic reactions and was likely to be effective in separation technologies as compared to other solvents.

Theory and Computational Science

Theoretical chemistry

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. 107 - 110

Publications: J. Phys. Chem. C, 2012, 116, 17336 ; J. Chem. Phys., 2013, 138, 94108 ; Catal. Today, 2012, 198, 106

Sourav Pal
s.pal@ncl.res.in

Thermal stability of gold fullerene Au_{32} cluster using density functional theory

Structural, electronic and catalytic properties of Au_{32} cluster were analyzed by using relativistic density functional theory (DFT) based methods. DFT based molecular dynamical (MD) simulations were also performed on Au_{32} golden fullerene to understand its thermal stability at various working temperatures. Various conformations were populated and analyzed at different temperatures of a cluster. The study showed that the ground state icosahedral conformation is stable only up to 300 K and structure remained in a hollow conformation only up to 400 K. This was the reason for the failure in trapping the unique fullerene conformation in spite of the stable theoretical predictions. The study also showed that the bare fullerene Au_{32} cluster can be used without any stabilizing ligands for potential catalytic applications only around room temperatures.

Decorated MOF-5 for improved hydrogen storage

The effect of light transition metal decoration of Scandium on metal-organic framework -5 (MOF-5) was studied for the reversible storage of hydrogen using density functional theory. The studies of periodic DFT showed that Ti atoms cluster strongly among themselves. However, Sc atoms do not cluster among themselves while decorating MOF-5, thus significant improvement in hydrogen adsorption. Substitution of Boron on metal decorated MOF-5 enhanced the interaction energy of the metal with MOF-5. Sc-decorated MOF-5 showed a hydrogen storage capacity of 5.81 wt %. This can be used for hydrogen storage at room temperature.

Transition dipole moment and dipole oscillator strengths

Fock-space multi-reference coupled cluster method was used to evaluate transition dipole moments and oscillator strengths. This was obtained as the matrix element between the ground state and the excited state. Two different approaches were used, one was expectation value approach and the second a Lagrangian formulation using a linearized left vector. The excitation energies and dipole moments of the few excited states along with the oscillator strength were computed for small test molecules.

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

Aluminum clusters are recognized as technologically important due to their high catalytic activity. Identification of reactive sites to understand catalytic behavior is extremely important. The present study on the small-sized aluminum clusters used density functional theory (DFT) based reactivity descriptors to achieve this purpose. The study involved how the size, shape, and charge of the cluster influenced the number of available sites for an electrophilic and nucleophilic attack. Depending on symmetry, susceptibility of various types of reactive sites within a cluster toward an impending electrophilic or nucleophilic attack was predicted by using the reactivity descriptors. The predictions by reactivity descriptors were tested by performing an explicit adsorption of water molecule on Al clusters with four atoms. This demonstrated an interesting result that the most stable water-cluster complex was obtained when the molecule was adsorbed through an oxygen atom on the site with the highest relative electrophilicity.

A lagrange multiplier approach for excited state properties

A formulation based on Lagrange multiplier approach for efficient evaluation of excited state energy derivatives in Fock space coupled cluster theory within the intermediate Hamiltonian framework was presented. The formulation was used to derive the explicit generic expressions up to second order energy derivatives for [1, 1] sector of Fock space with singles and doubles approximation. Comparison with the Lagrange multiplier approach in standard formulation of Fock space, which is built on the concept of Bloch equation based effective Hamiltonian was discussed.

Calculation of molecular properties using coupled cluster method

Nayana Vaval
np.vaval@ncl.res.in

Publications: J. Chem. Phys., 2012, 136, 234110; Chem. Phys. Lett, 2013, 568, 170; Int. J. Quantum Chem., 2013, 113, 1690

The extended coupled cluster method was used for the calculation of dipole quadrupole polarizabilities of the molecules. Effect of electron correlation was studied. For the calculation of dipole moments of the doublet radicals the intermediate Hamiltonian based response approach was used. Fock space multi-reference coupled cluster method takes care of nondynamic correlation very accurately. Method was used for difference energy calculations. However, it suffered from the convergence problem due to presence of intruder states. Intermediate Hamiltonian theory was implemented to avoid the problem of intruders. Study of life time of the metastable states was very interesting task. This involved simultaneous treatment of electron correlation and continuum effect. Equation of motion coupled cluster method was used for the study of position and width of shape resonance.

Study of quadrupole based properties using extended coupled cluster method

Analytic response approach within variational coupled cluster framework was used for the study of quadrupole moments, dipole–quadrupole polarizabilities and dipole polarizabilities. Extended coupled cluster functional was used which included all the double linked terms within (CCSD) approximation. These terms will be important for the accurate description of properties at the stretched geometries. The properties for carbon monoxide and hydrogen fluoride molecules, methane, tetrafluoromethane, acetylene, difluoroacetylene, water and ammonia were studied.

Constrained variational response approach for properties of doublet radical

Fock-space multi-reference coupled cluster theory takes care of non dynamic correlation efficiently which arises due to nearly degenerate states. However, it suffered from the intruder state problem for large model space. The intermediate Hamiltonian formulation eliminated the intruder state problem and helped in the convergence of equations. Intermediate Hamiltonian approach in Fock-space coupled cluster method was used for the response properties. Dipole moments of doublet radicals of CN, SF and NS radicals were calculated by using this approach.

Study of shape resonance: Equation of motion coupled cluster

The equation-of-motion coupled-cluster method (EOM-CC) in augmentation with complex absorbing potential was used for the study of shape resonance. The shape resonance in e –N2, e –CO and e–C_2H_2 were studied along with the potential curves for N_2 and CO.

Ultrafast structural and conformational dynamics of biomolecules

Sayan Bagchi
s.bagchi@ncl.res.in

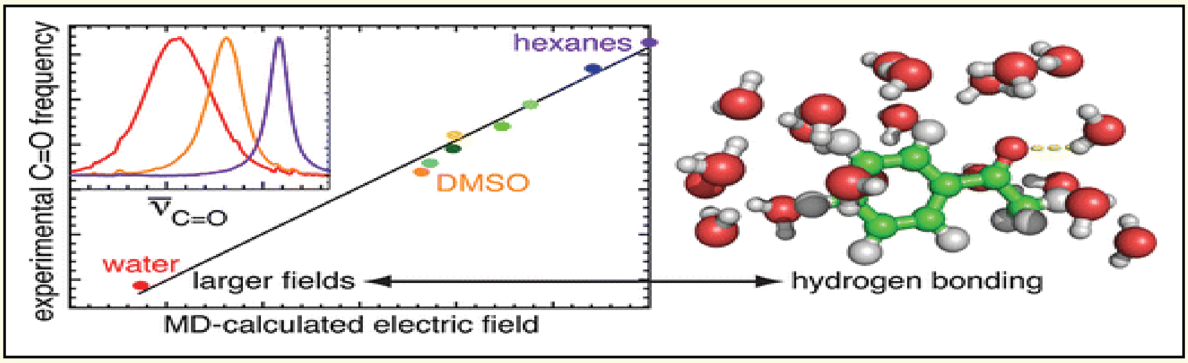
Publication: JACS, 2013, DOI: 10.1021/ja403917z

The goal was to understand how functions are intimately related to the molecule's ability to undergo structural and conformational changes (dynamics) and the variations in the magnitude and direction of electric fields experienced by them (electrostatic interactions).

Measuring electrostatic fields in hydrogen-bonding and nonhydrogen-bonding environments

Vibrational probes provided a direct readout of the local electrostatic field in complex molecular environments, such as protein binding sites and enzyme active sites. This information provided an experimental method to explore the underlying physical causes of important biomolecular processes such as binding and catalysis. However, specific chemical interactions such as hydrogen bonds can have complicated effects on vibrational probes and confound simple electrostatic interpretations of their frequency shifts. Vibrational Stark spectroscopy and infrared spectroscopy of carbonyl probes in different solvent environments and in ribonuclease S were employed to understand the sensitivity of carbonyl frequencies to electrostatic fields, including those due to hydrogen bonds.

Additionally, molecular dynamics simulations were carried out to calculate ensemble-averaged electric fields in solvents and in ribonuclease S and found excellent correlation between calculated fields and vibrational frequencies. This data enabled the construction of a robust field–frequency calibration curve for the CO vibration. The results suggested that carbonyl probes are capable of quantitatively assessing the electrostatics of hydrogen bonding, making them promising for future study of protein function.



The molecular mechanism and competing reaction pathways in enzymatic reactions

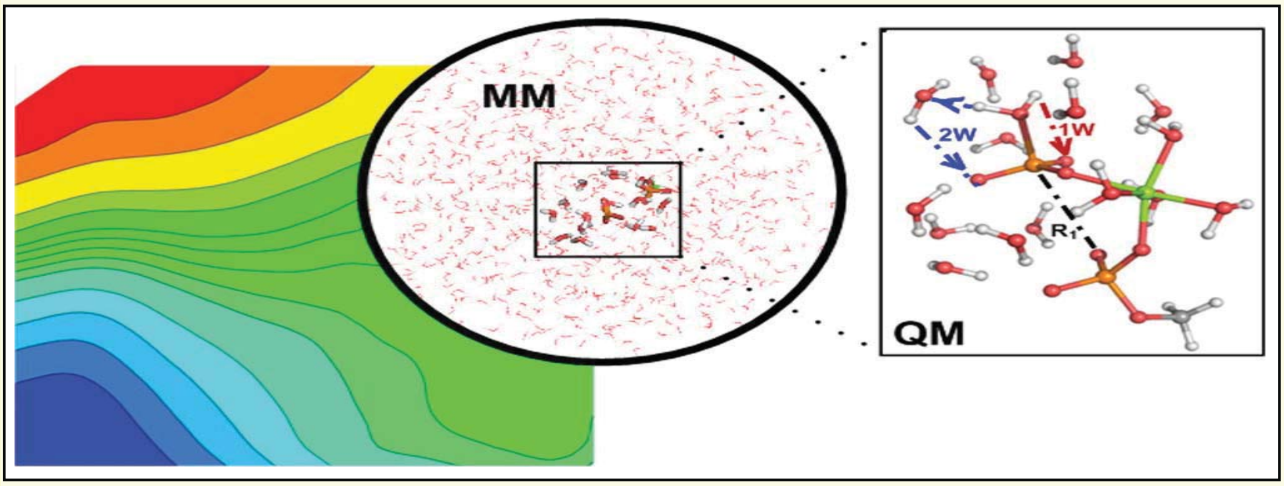
Suman Chakrabarty
s.chakrabarty@ncl.res.in

Publication: J. Phys. Chem. B, 2013 DOI: 10.1021/jp4020146

The objective was to develop and apply efficient computational methodologies that can be used in realistic and quantitative estimation of free energy surfaces of enzymatic/catalytic reactions. The primary focus was on the identification of the molecular mechanism and possible pathways in a complex catalytic cycle.

Quantification of the mechanism of phosphate monoester hydrolysis in aqueous solution

Phosphate hydrolysis (e.g. ATP hydrolysis) is considered one of the most biologically important catalytic reactions. Quantitative understanding of the nature of the underlying free energy surfaces of such processes is challenging as obtaining converging results using *ab-initio* QM/MM free energy calculation is computationally highly expensive. The focus was on obtaining the free energy surfaces of phosphate monoester hydrolysis for two possible pathways, involving one (1W) and two water molecules (2W) at the proton-transfer step. It was found that the 1W path can have 6-9kcal/mol higher barrier than the 2W pathway in specific cases. The effect of presence of Mg^{2+} ions in the system and the effect of proton tunneling by incorporating a nuclear quantum mechanical correction was estimated simultaneously.



Scientific Computing

This chapter and Theoretical Chemistry have interrelation and for the sake of brevity, the content is not repeated. Please also refer the chapter on Theoretical Chemistry: p. 103 - 106

Publication: J. Comput. Chem., 2013, 34, 1060

Debashree Ghosh
debashree.ghosh@ncl.res.in

A multi-scale simulation and modeling approach to design smart functional materials

The objective of this project was to develop the electronic structure methods within the QM/MM framework. It dealt with the development of sophisticated and empirical parameter free MM methods such as effective fragment potential (EFP) and its extension to treat protein environments.

Development and extension of effective fragment potential method

Effective fragment potential (EFP) was implemented in the quantum chemistry package Q-Chem. It was interfaced with various QM methods to treat ground and excited states, so that spectroscopic properties of solutes in solvents with accuracy were understood easily. A library of commonly used solvents was also developed for the users. Additionally, a "fragment only" or "EFP only" feature was used to calculate the non-covalent interactions between fragments as well as the decomposition of the energy components.

Publication: J. Chem. Phys., 2013, 138, 14303

Kavita Joshi
k.joshi@ncl.res.in

Correlation between the variations in observed melting temperatures

The correlation between the variation in the melting temperature and the growth pattern of small positively charged gallium clusters was investigated. Significant shift in the melting temperatures was observed for a change of only few atoms in the size of the cluster. Clusters with size between 31-42 atoms melt between 500—600~K whereas those with 46-48 atoms melt around 800~K. Density functional theory based first principles simulations were carried out on Ga^+_n clusters with n=31,...,48. At least 150 geometry optimizations were performed towards the search for the global minima for each size resulting in about 3000 geometry optimizations. For gallium clusters in this size range, emergence of spherical structures as the ground state led to higher melting temperature. The well separated core and surface shells in these clusters delayed the isomerization which resulted in the enhanced stability of these clusters at elevated temperatures. The observed variation in the melting temperature of these clusters therefore has a structural origin.

Rationalizing role of the structural motif and the underlying electronic structure

In spite of having identical structural motif 36 atom clusters of aluminium and gallium have substantially different melting temperatures. T_m was measured experimentally for Al_{36} and Ga_{36} was found to be 834K and 525K respectively. The identical structural motif of the ground state along with considerably different T_m has provided a unique opportunity to rationalize the role of structural motif and the underlying electronic structure in the melting transition of small clusters. The most important features in a heat capacity curve are position of the peak which was identified as the melting temperature of the cluster and its shape. These extensive *ab initio* molecular dynamics simulations demonstrated that the melting temperatures depended on the bond strength and coordination of atoms within the cluster, whereas the shape of the heat capacity curve was governed by the ground state structure. Similar structural motif for the ground state of these two clusters was responsible for comparable isomerization pattern. It resulted into identical shape of the heat capacity curve. In short, the shape of the heat capacity curve was governed by the ground state structure whereas the melting temperatures depend on the bond strength and coordination of atoms.

Scientific Computing

Publications: Dalton T., 2013, DOI: 10.1039/C3DT51677F; ACS Catal., 2013, 3, 920; Inorg. Chem., 2013, 52, 4238; Comput. Theor. Chem., 2012, 992, 18

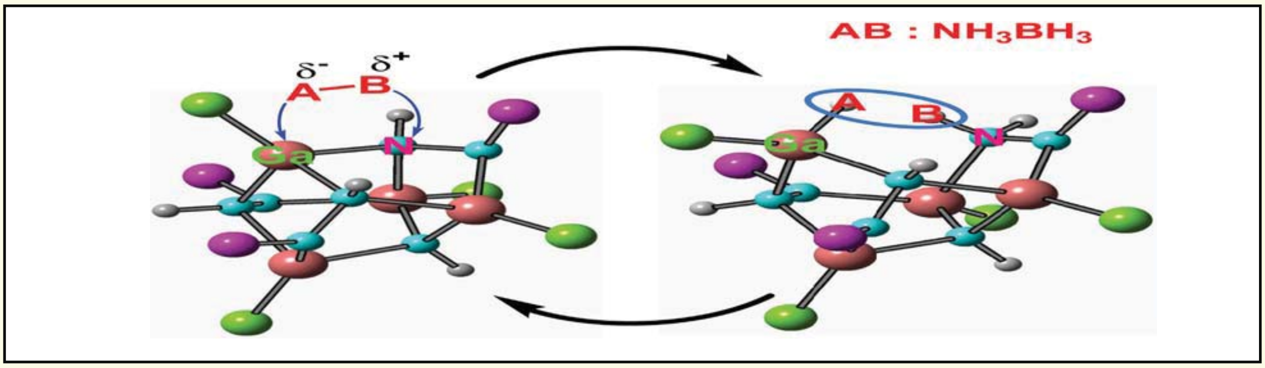
Kumar Vanka
k.vanka@ncl.res.in

Computational studies into small molecule activation

The objective was to design and develope new systems based on the transition metal and the main group for the activation of small molecules. This was achieved with the aid of computational tools, employing density functional theory (DFT), stochastic simulations and the energetic span model (ESM). New methods were developed in order to study the kinetics and thermodynamics of the systems. New important metal and non-metal systems for small molecule activation were predicted and strategies were also developed for its synthesis.

Small molecule activation using metal and non-metal based catalysts

Novel ideas were explored in the field of small molecule activation. In non-metal systems, caged structures showed enormous potential for the catalysis of important reactions such as the dehydrogenation of ammonia borane. For transition metal systems, innovative changes were suggested to pincer ligated transition metal systems.



Publications: Eur. Biophys. J. Biophy., 2013, 42, 487

Neelanjana Sengupta
n.sengupta@ncl.res.in

A multi-scale simulation and modeling approach to design smart functional materials

The objective behind this work was to undergo the simulations of the intrinsic behavior of proteins, especially amyloidogenic proteins, and their adsorption behavior of biomolecules at various interfaces. The research was motivated to find the novel strategies that may help to counteract the neurodegenerative effects of amyloids.

Structural response and collapse propensities of monomeric amyloid beta

The full-length amyloidogenic peptide Aβ who's self-assembly is strongly correlated with the onset of Alzheimer's disease was simulated in the vicinity of a model hydrophilic surface of rutile TiO_2. A strong beta-sheet propensity was found to be induced by hydrophilic surface in a distance dependent manner and the peptide was failed to achieve the collapsed state which was essential for seeding the self-assembly mechanism. The results had the ramifications in the design of nanomaterials that were used for blocking the amyloidogenic pathways and were potentially utilized in therapeutic strategies.

It illustrated the peptide residues in the systems A, B, C and F were over the last 10 ns of the simulated trajectories. The protein was most proximal to the rutile surface in 'A' and proximity decreases from 'B' to 'C'. The peptide tends to be a free monomer in 'F'. Enhanced beta-sheet propensity showed the increased proximity.

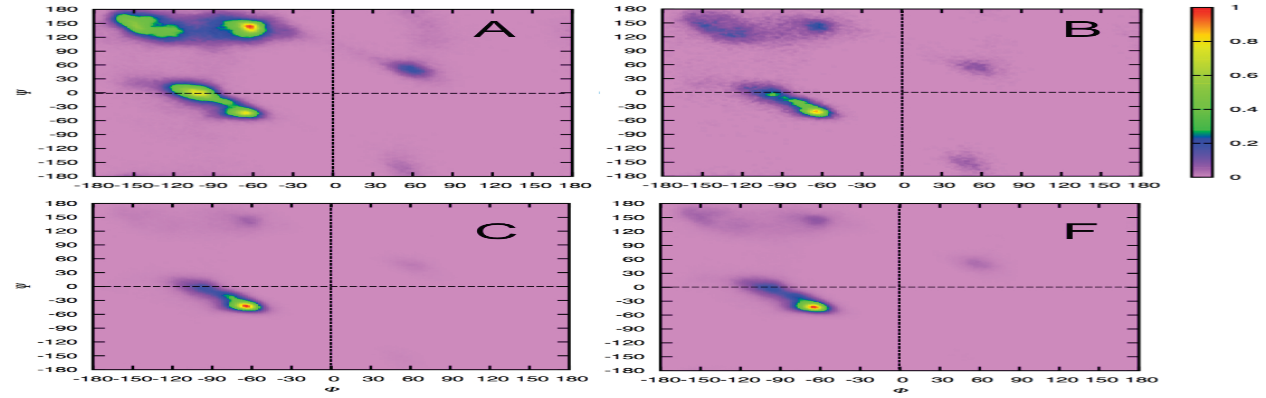


Fig. 1: Distributions of the (ø, Ψ) torsional angles (in degrees), or the Ramachandran diagram

It illustrated the peptide residues in the systems A, B, C and F were over the last 10 ns of the simulated trajectories. The protein was most proximal to the rutile surface in 'A' and proximity decreases from 'B' to 'C'. The peptide tends to be a free monomer in 'F'. Enhanced beta-sheet propensity showed the increased proximity.

Publications: Soft Matter, 2013, 9, 2269; Macromolecules, 2013, 46, 363; J.Phys.Chem. C, 2013, 117, 12172; J. Phys. Chem. B, 2012, 116, 4731, 7357; 2013, 116, 3083

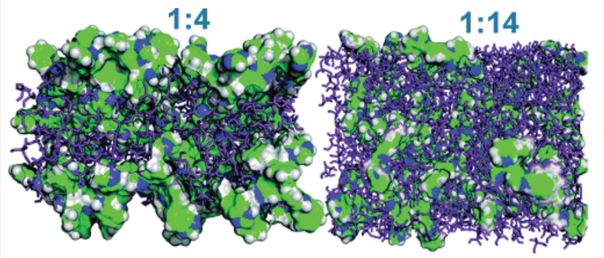
Sudip Roy
s.roy@ncl.res.in

Theory and simulation of soft matters

The group aimed to address various phenomena of soft matters, which occur in higher length and time scales. But at the same time atomic/molecular details of any component of the soft matter is also important to elucidate structure property relation at atomistic scale. The objective was to develop and apply multiscale molecular modeling approach which will handle such systems from atomic scale to mesoscale and establish connections between different scale phenomena.

Proton conductance mechanism in benzimidazole based fuel cell electrolytic membrane

Phosphoric acid doped Polybenzimidazole (PBI) membranes are promising electrolyte membranes for high temperature (100°C and above) fuel cells. Molecular dynamics simulations on phosphoric acid doped 2-phenyl-1H,1'H-5,5'-bibenzo[d]imidazole (monomer unit of polybenzimidazole) were performed to characterize the structural and dynamical properties at varying phosphoric acid content and temperature. From the structural analysis, the arrangement of the phosphoric acids, formation of H-bonds in the system and the contribution of different atoms towards H-bonding were predicted. These H-bonds formed a network of H-bonds which percolates through the membrane. Prediction of the diffusion of phosphoric acid to understand the nature of the proton conductivity by diffusion of the whole phosphoric acid molecule was done at different temperature and phosphoric acid doping level.. Snapshots of the phosphoric acid doped PBI systems are shown below.

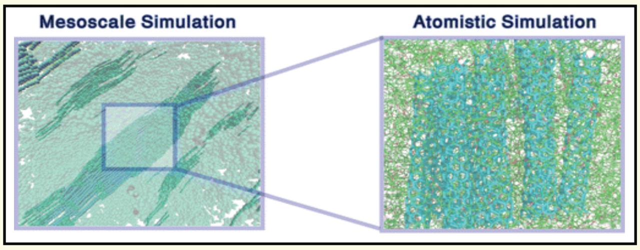


Scientific Computing

Morphology and dynamics of carbon nanotube in polymer matrix

Particle based multiscale simulations were performed on pure monomer, trimer and polymer of polycarbonate and their mixtures with different molecular weight percentages of embedded single walled CNT at different temperatures. The diffusion behaviors of monomer, trimer of polycarbonate and carbon nanotubes in composite matrices were investigated and compared with pure PC. Both structural and dynamical properties indicated the weak interaction between the nanotubes and matrix PC molecules.

There was high tendency of nanotubes to form bundles which was observed during simulations. The bundle formation free energies were calculated from the potential of mean force calculations. The mechanism and energetics of bundle formation were explored in the atomistic scale. The formation of the CNT bundle was a favorable process in the oligomeric PC matrix. Percolation pathway formation by CNT in the polymeric matrix at larger time and length scales was explored in details from mesoscale dissipative particle dynamics simulations. Calculations of the CNT bundle size distribution and their diffusion in the matrix were done with the help of mesoscale simulations. The figure below represents the morphology of the polymer CNT composite in atomistic and mesoscopic length scale.



Decomposition, formation and CO_2 sequestration of gas hydrate by molecular dynamics simulation

The gas hydrates are crystalline, ice like solids in which water molecules are arranged in a three dimensional hydrogen bonded network (cages) which are stabilized by entrapped gas molecules. The methane gas in the solid hydrate phase present under the permafrost or in the oceanic sediments can be recovered by disturbing the thermodynamic equilibrium, thus decomposing the solid methane hydrate. However, uncontrolled decomposition of gas hydrates has the potential to assist natural disasters, like global warming, earthquakes, tsunamis etc.

Solar Energy

Publications: Energy & Environ. Sci., 2013, 6, 1249 ; J. Mater. Chem., 2012, 22, 19694
2013, 22, 17302; Green Chem., 2013, 15, 943; ChemSusChem., 2012, 5, 2159

S. B. Ogale
sb.ogale@ncl.res.in

From dead leaves to high energy density supercapacitor

Functional microporous conducting carbon with high surface area of about 1230 m^2g^{-1} was synthesized by a single step pyrolysis of plant dead leaves (Neem) without any activation. The process is clearly generic and applicable to most forms of dead leaves. Synthesized functional carbon exhibited very high specific capacitance of 400 Fg^{-1} and enengy density of 55 Wh kg^{-1} at a current density of 0.5 Ag^{-1} in aqueous 1M H_2SO_4. The areal capacitance value of the carbon derived was significantly high (32 μF cm^{-2}). In an organic electrolyte the material showed a specific capacitance of 88Fg^{-1} at a current density of 2Ag^{-1}.

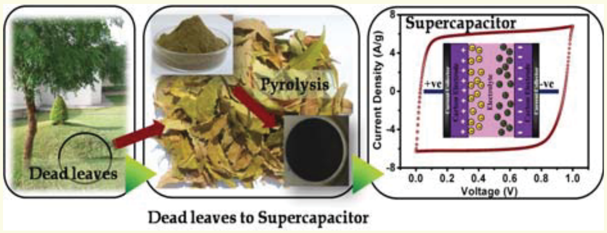


Fig. 1: Schematic Diagram for the process from dead leaves to high energy density supercapacitor

Concurrent synthesis of control of dopent (Nitrogen) and defect complexes

A facile solution based synthesis protocol to incorporate nitrogen within zinc oxide nanorods with substantially improved visible light harvesting via broadband absorption stretching from UV to deep visible wavelengths (650 nm) was performed. A peculiar visible region of maximum around 470 nm was reported. Raman and X-ray photoelectron spectroscopy confirmed the incorporation of nitrogen along with other complex defects such as zinc interstitials and oxygen vacancies. It exhibited a significant superior photoelectrochemical performance over undoped ZnO. Under monochromatic green light illumination (530 nm) N:ZnO showed a photocurrent density of 3.2 mA cm^{-2}, whereas pristine ZnO failed to show any photo-response. The IPCE spectrum of N:ZnO followed the broadband absorption spectrum extending up to an unprecedented value of 650 nm, potentially expanding the scope for using this material in other solar energy harvesting applications.

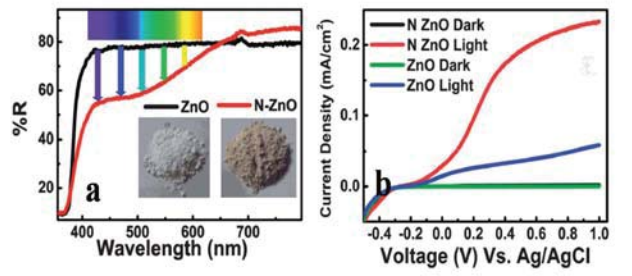


Fig. 2: a) Diffused reflectance spectra for ZnO and N:ZnO nanorod samples.; b) Linear sweep voltagrams for ZnO and N:ZnO samples in the dark and with AM1.5 radiation

Fluorescent sophorolipid molecular assembly and its magnetic nanoparticle loading

Strong green fluorescence in a fully biocompatible highly spherical mesoscale molecular assembly of sophorolipid by pulsed UV laser processing of a water-based dispersion of sophorolipid was reported. The pulsed laser property induced the modifications in the molecule and the assembly. This fluorescence character was driven by the oleic acid component while the assembly process was assisted by the glucose component. The laser synthesized mesostructures were easily redispersed in an aqueous medium after being dried and loaded with magnetic nanoparticles (magnetite) for inducing the hyperthermia effect.

Single-layer-graphene-assembled 3D hexaporous carbon for high performance supercapitor

Hierarchical porous graphene with hexagonal nanopores was synthesized. The catalyst-free synthesis led to single-layer-graphene-assembled carbon without use of any template. The as-synthesized sample exhibited a high surface area of about 1720 m^2g^{-1} and showed a bulk specific conductivity of 23 Sm^{-1}. The material showed excellent supercapacitance performance in aqueous medium with maximum specific capacitance of 154 Fg^{-1} at a current density of 0.5 Ag^{-1}. Due to specific pore size distribution the power density was found as high as 17485 Wkg^{-1}. The material showed good stability at higher current densities and after 1000 charge discharge cycles without any apparent sign of decay even for further cycling.

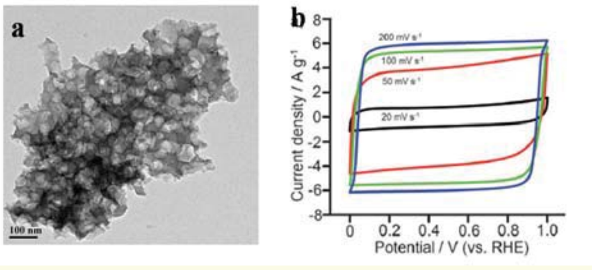


Fig. 3: a)TEM image of polymer derived carbon; b) Cyclic Voltametry Curve for polymer derived carbon at different scan rate from 10-100mvs^{-1}

Dye sensitized solar cell by a novel fully room temperature process

A protocol for making room temperature curable titania-nanoparticle-based paint for easy application on hard as well as flexible substrates using a simple paint brush or other facile application methods was developed. A conversion efficiency of 5% was obtained on FTO/glass substrates without any heat treatment or even an added light harvesting layer. Further optimization including use of a light harvesting layer will push this efficiency higher. An efficiency of 2.4% on semi-transparent flexible ITO/PET substrate amenable to roll-to-roll processing was achieved.

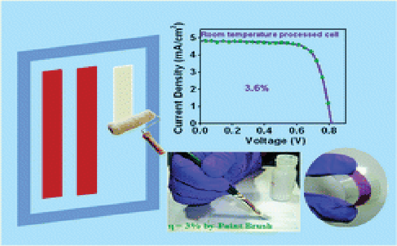


Fig. 4: Titania-nanoparticle-based solar paint with 3.6% conversion efficiency

A quasi-liquid iontronic–electronic light-harvesting hybrid photodetector

An interface between a quasi-liquid ionic conductor and light-harvesting configuration of quasi-1D functional metal oxide yielded a highly efficient photodetector which showed strong photoresponse in the UV and partial visible range. Impedance spectroscopy was used to bring out a significant decrease in the charge transfer resistance and the capacitance of this interface controlled device upon illumination. This work showed that the gel layer improved the response time and IPCE of ZnO–gel–Pt system in comparison to bare ZnO–Pt system.

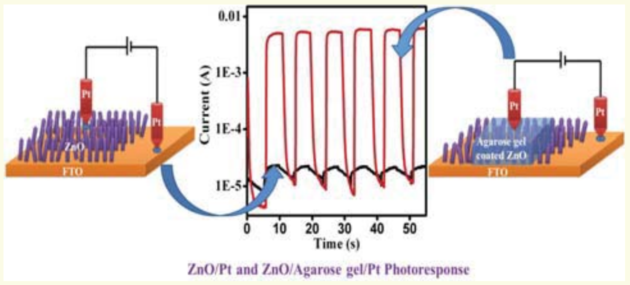


Fig. 5: Photoresponse of ZnO/Pt and ZnO/ Agarose gel/Pt device

MOF derived porous carbon–Fe_3O_4 nanocomposite as superadsorbent

An interface between a quasi-liquid ionic conductor and light-harvesting configuration of quasi-1D functional metal oxide yielded a highly efficient photodetector which showed strong photoresponse in the UV and partial visible range. Impedance spectroscopy was used to bring out a significant decrease in the charge transfer resistance and the capacitance of this interface controlled device upon illumination. This work showed that the gel layer improved the response time and IPCE of ZnO–gel–Pt system in comparison to bare ZnO–Pt system.

A high surface area carbon composite with Fe_3O_4 nanoparticles was synthesized by pyrolysis of an iron containing Metal Organic Framework (MOF). The composite was prepared by annealing the MOF at different temperatures (500°C and 600°C), each case exhibited unique property in terms of the hydrophobic behaviour and surface area resulted in specific applicability domains. This work has highlighted the exceptional behaviour of this material as a magnetically separable and recyclable superadsorbent for removal and recovery of environmental pollutants.

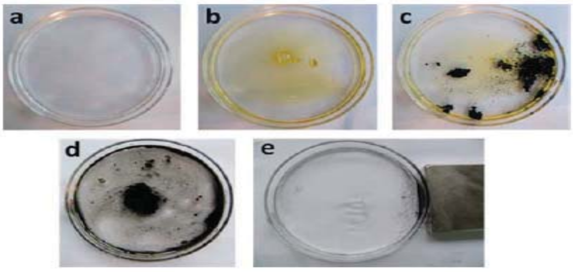


Fig. 6: Images of the oil removal experiment

Solar Energy

Plasmonic functionalization for efficient solar photoelectrochemical water splitting

A strong enhancing effect of plasmonic Au nanoparticles on the photoelectrochemical (PEC) performance of ZnFe2O4 /ZnO nanostructured hetero-junction was used as photoanode for water splitting application. This work demonstrated that use of an ultrathin layer of a suitable material to coat a light harvesting nanostructure helped to enhance the benefits of Au NP near-field plasmonic functionalization in the context of PEC water splitting.

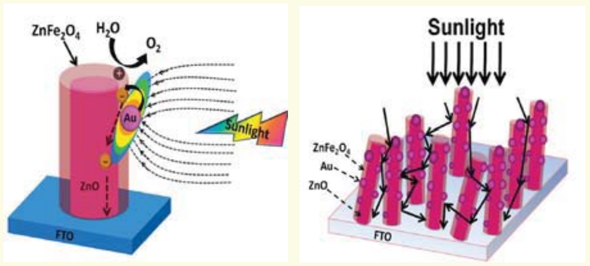


Fig. 7: Au NP plasmonics functionalization

Publication: Microfluid. Nanofluid., 2012, DOI 10.1007/s10404-012-1119-z

Manjusha V. Shelke
mv.shelke@ncl.res.in

Antireflective micropatterned materials

Hierarchical assemblies of nanostructured building blocks on conducting substrates are significant for construction of functional devices like photovoltaic cells. Microfluidics is powerful but less exploited tool for spatial organization or growth of functionally sophisticated nanostructures with precise control. Synthesis of patterned antireflective nanomaterials via microfluidics was done successfully.

Microfluidic spatial growth of vertically aligned ZnO nanostructures for antireflective patterning

Efforts were put to integrate ZnO nanostructures into a more regular form to enhance the performance of the nanodevices. A variety of techniques were employed to fabricate patterned vertically aligned ZnO nanostructure arrays including photolithography, nanosphere lithography, interference lithography, laser writing, electron beam lithography (EBL) and nanoimprinting. Mostly a seed layer is patterned with these techniques and then used to grow patterned arrays of ZnO nanostructures separately. These require clean rooms and expensive equipments and are low throughput techniques. Soft lithography is a low cost and experimentally convenient technology for patterning micro or nanoscale structures. Micropatterned seedless vertical growth of functional ZnO nanostructures by means of soft microfluidic channels was achieved. The photoluminescence and antireflection characteristics of the hierarchically structured ZnO nanowire arrays were studied. This technique facilitated fabrication of complex device architectures.

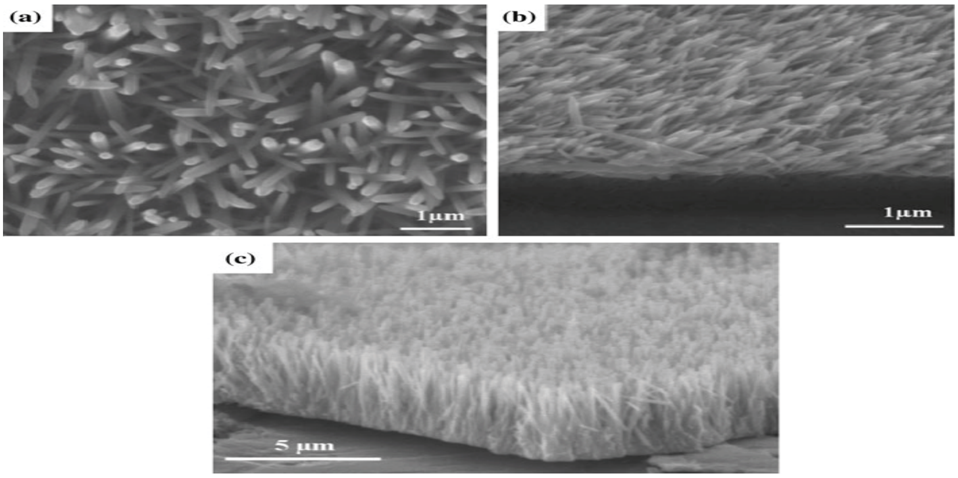


Fig.1: SEM images of selective growth of ZnO nanostructures inside microfluidic channels

Solar Energy

Vincent Paul
vpaulpreeti@ncl.res.in

The synthesis of two organic dyes V12 and V13 was reported. The backbone of the dye was the 2-(methylthio)-10H-phenothiazine unit which itself was a strong electron donor containing electron rich sulfur and nitrogen atoms. The spacer was an auxiliary donor containing methoxy-substituted oligophenylenevinylene and cyanoacrylic acid worked as an acceptor moiety and also the anchoring group. This auxiliary donor was used to avoid π- π stacking which was a major problem with π conjugated systems. An auxiliary donor containing spacer enhanced the electron donating ability and broadened the absorption range of the sensitizer. S-methyl phenothiazine based molecules as dye sensitizers for DSSC were also developed. Power conversion efficiency (η), efficiency of η =4.3-5% (68-79% wrt N719) dye was achieved.

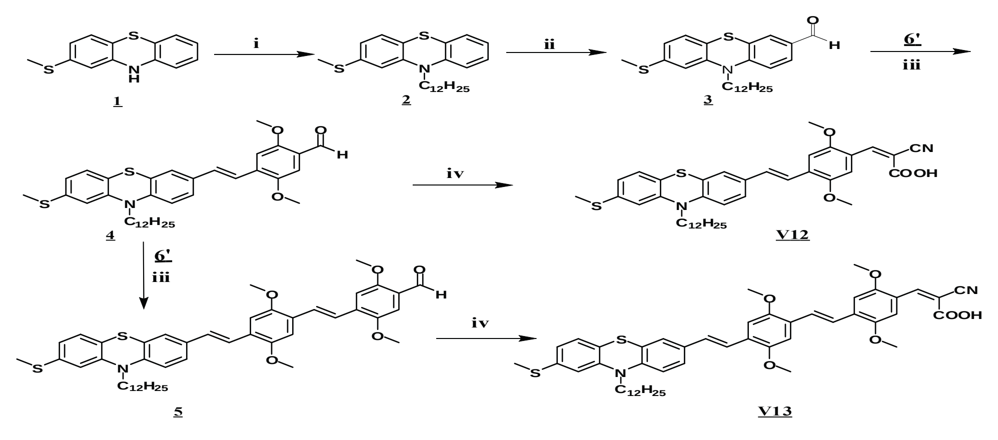


Fig. 1: Synthetic approach for the formation of V12 and V13

Sustanable Polymer Industry through Research Innovation and Training

Publications: Rheol. Acta., 2013, DOI: 10.1007/s00397-013-0739-x; J. Rheol., 2013, 57, 559; Macromolecules, 2013, 9, 46, 3631; J. Chem. Phys., 2013, 138, 124505; Eur. Biophys. J., 2013, 42, 487

Ashish K. Lele
ak.lele@ncl.res.in

Fundamental research was carried out on polymer extrusion film casting (EFC) process which involved computational molecular modeling of Ziegler-Natta polymerization catalysts; synthesis of Cr-based polymerization catalysts and novel PLA-based materials. It aimed to study the effects of donor on the insertion and termination processes of polymerization via the route of binding to the titanium metal center, with the titanium supported on the (110) $MgCl_2$ surface. CoE-SPIRIT aimed to develop a new series of catalysts for the synthesis of high molecular weight polyethylene.

Center of excellence in polymers: CoE-SPIRIT©

Industrial extrusion film casting (EFC) process was beset with two interrelated defects, necking and edge-beading. In the EFC research program, considerable understanding on the influence of polymer architecture on these defects was developed. The experiments showed that high polydispersity and presence of considerable amounts of LCB reduces the necking tendency. Predictions of non-isothermal CFD simulations of EFC incorporating "molecular" constitutive equations which relate polymer architecture to rheology were found to be in semi-quantitative agreement with our experimental data. Computational modeling results on Z-N catalysts suggested that the internal and external donors bound to the (110) lateral cuts of $MgCl_2$, thereby provided more stereospecific sites. Moreover, it was also possible that the donors could be bound directly to the active catalyst. The titanium complex bound to the $MgCl_2$ surface, thereby influencing the catalysis by modulating the barriers for the insertion and termination processes occurred at the catalyst center.

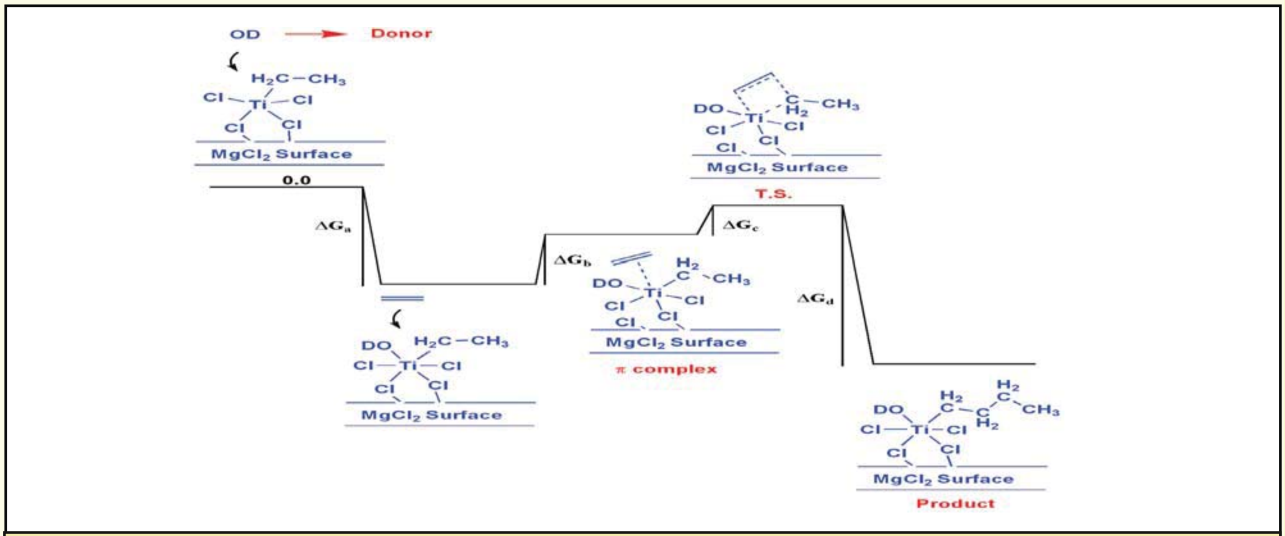


Fig. 1: The energy profile for the insertion of ethylene into the Ti-C_2H_5 bond with the donor (OD) coordinated to the titanium center

Surface Science

Publication: J. Phys. Chem. C, 2013, 117, 4717

C. S. Gopinath
cs.gopinath@ncl.res.in

The Centre of Excellence on Surface Science (CoESS) was established to avail the major surface science equipments and setup facility to carry out *in-situ* reactions/ measurements related to physics and chemistry of material interfaces and biology. The first equipment added to CoESS is the laboratory version of Ambient Pressure Photoelectron Spectrometer (Lab-APPES), which significantly bridges the vacuum gap that exists between high vacuum measurement conditions in surface science equipments and real-world applications at ambient pressure. This unique facility acquired by CoESS on 2012 is one of the few such installations around the world and second in Asia that can do *in-situ* measurements at pressures up to 1 mbar and 1000 K. The facilities are expected to shed more insights into material properties, reaction mechanism and in turn help to design futuristic tailor-made materials for various areas, such as catalysis, nanomaterials and sensor.

Ambient Pressure photoelectron spectrometer (APPES) was setup to explore the materials surfaces under actual working conditions.

APPES is a custom-built photoelectron spectrometer with provided design aspects provided from the group and the machine was fabricated in a compact and elegant manner by Prevac, Poland. Conventionally, XPS or ESCA facility works under ultra-high vacuum (<10-9 mbar) and hence it was not possible to explore the electronic structure of materials under actual working conditions, which is usually ambient conditions or even severe. With present APPES, it is possible to explore the surface science and electronic structure aspects of materials up to 1 mbar pressure of reactants and 1000°C. This was possible due to the advancement in electronics and design aspects of electron energy analyzer and the mechanical design of APPES as a whole unit.

Fig. 1: APPES at CSIR-NCL

Interaction of molecular oxygen with catalytically relevant Cu, Ag and Au surfaces

The interaction of O_2 with polycrystalline foils of Cu, Ag, and Au from UHV to 1 mbar and up to 773 K was studied. APPES results showed that Au is totally inert, Ag can be mildly oxidized and Cu can be totally oxidized. Diffusion of oxygen into subsurfaces of Ag occurs, which is a precursor towards oxidation. No oxide formation was observed with Au. Silver behaved mildly; formation of subsurface oxide species at 600 K and 1mbar O_2 pressure demonstrated this fact. However, Cu is prone to react with oxygen and complete surface oxidation to CuO was observed at 1 mbar O_2 and $\geq$ 600 K. Indeed there was a systematic oxidation of Cu metal to Cu_2O, to CuO with increasing temperature at 1 mbar O_2 pressure. This study showed the capability of equipment to understand a material surface and the undergoing changes during reactions at working conditions.

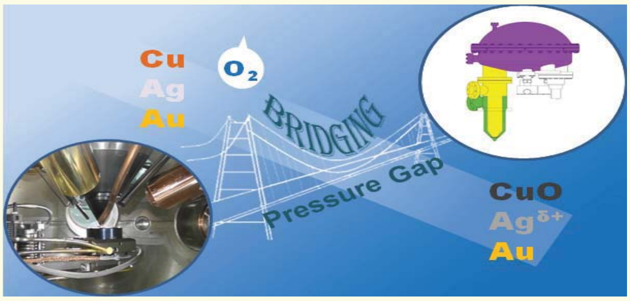


Fig. 2: APPES helps to bridge the large pressure gap that exists between actual working condition of materials and XPS measurements under high vacuum conditions

NMITLI

Design, development and demonstration of high performance parabolic trough based 300 kW solar thermal power plants

S. B. Ogale
sb.ogale@ncl.res.in

This work involved optimization and design of different parts of solar thermal power plant like parabolic trough collector, solar selective absorber receiver, glass to metal sealing etc. The developement of solar selective absorber coatings on stainless steel substrate using Multitarget Magnetron Sputtering System was done.

Multitarger magnetron MILMAN sputtering system

Some of the cermet systems optimized on MILMAN sputter coating system were W-Al_2O_3, Mo-Al_2O_3, W-AlN and W-TiAlN. The best optimised coatings were found as W-Al_2O_3 and W-AlN. The optical and high temperature (400°C) thermal emissivity properties for the W-Al_2O_3 and W-AlN are shown in the following Fig. 1 and Fig. 2 respectively.

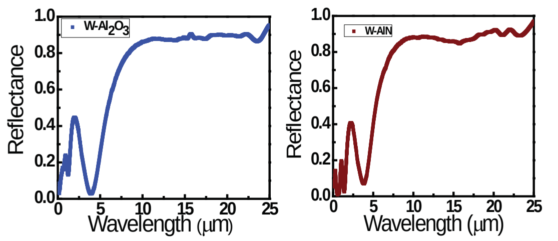


Fig 1: Diffused refelectance spectra of (a) W-AlN and (b) W-Al_2O_3 cermet coating

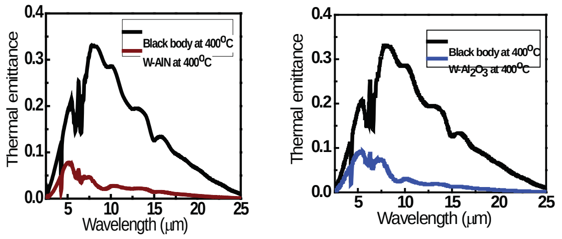


Fig 2: Thermal emittance of (c) W-AlN and (d) W-Al_2O_3 cermet coating

The table provides the diffused reflectance, absorptance and thermal emissivity at 400°C for the best two cermet coatings.

Sample	Type of cermet	Reflectance (200-800 nm)	Absorptance (α) (200-800 nm)	Thermal emissivity at 400°C (ε)
W-Al_2O_3	Normal	0.10	0.90	0.17
W-AlN	Graded	0.04	0.96	0.14

Thermal stability of the samples in air and vacuum

The thermal stability of the W-Al_2O_3 and W-AlN samples in air and vacuum at 500°C was studied. Both the W-Al_2O_3 and W-AlN samples were heated in air and vacuum at 500°C for different time intervals. It was concluded that the W-Al_2O_3 was unstable in air at 500°C but was stable in vacuum whereas W-AlN was stable in air as well as in vacuum at 500°C.

Polymer electrolyte fuel cells: Durability and round-robin testing of stacks

Ashish Lele
ak.lele@ncl.res.in

Objective behind this activity was to build multiple PEFC stacks and test them for durability in a round-robin format. This was accomplished recently. Six stacks of low temperature PEFCs of power rating 200–500 W were assembled and tested at three locations. The durability of the stacks was found to be acceptable as per global standards.

Stack details

Six low temperature fuel cell NAF stacks were assembled recently. The components of the stacks were manufactured either in the labs or at local vendors based on CSIR design. The main component i.e. membrane electrode assembly was developed in requisite numbers for the six stacks as per the optimized formulation and standard operating protocols. The flow channels and other features on the bipolar plates were machined at different vendors. The graphite plates were either purchased from Schunk GmbH or compression molded in CSIR-NPL. The porous carbon papers were either purchased from SGL, GmbH or were prepared by CSIR-NPL. The other ancillary components such as gaskets, end plates, collector plates, tie rods, nuts-bolts, heater, air ducts and blowers/pumps were purchased from local vendors or OEMs as per CSIR design. The stacks were tested for peripheral leaks and cross flow. Only after leak testing of the stacks was completed, it was taken to test-stations for PEFC testing.

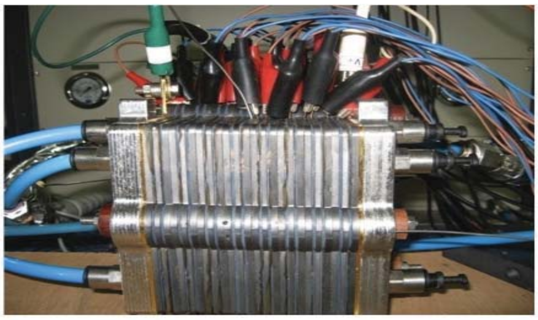


Fig. 1: NAF Stack

Stack testing

Stacks were tested for the durability under constant current conditions. The current was determined based on polarization data such that the voltage was between 0.6-0.7 V per cell. The drop in voltage was monitored as a function of time. Testing was carried out at 60-65°C in intermittent mode i.e., shutting down after every 12-16 h of continuous testing for a period of 12-8 h and then again restarting. The OCV and polarization of each cell of the stack and for the whole stack were monitored during durability testing. The stacks were conditioned and then tested for 50 h with H_2-O_2. After completing 50 h testing, the oxidant was changed to air and the stack was tested for 500 h with H_2-air. Fig 1 shows a representative NAF stack. Fig 2 shows the durability data for all six NAF stacks.

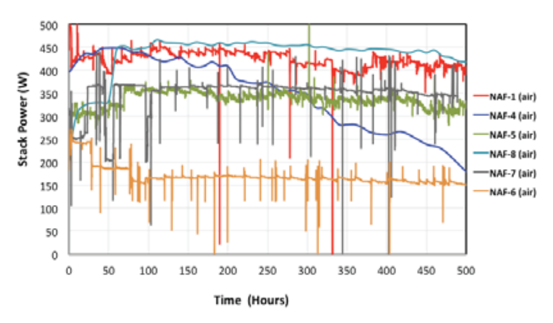


Fig. 2: Durability of NAF stacks

Scale-up of selective hydrogenolysis of glycerol to 1,2-propanediol

C. V. Rode
cv.rode@ncl.res.in

Publications: Org. Process. Res. Dev., 2012, 16, 1043; WO 2011/138643 A2, 2011

Research was aimed to design a high pressure pilot plant for continuous hydrogenolysis of glycerol with a scale of operation of ~1 kg of catalyst. Focus was on developing and establishing the strategy for effective separation and recovery of pure 1,2-PDO.

Catalyst preparation scale-up and continuous hydrogenation trials

A method for the preparation of a non-noble metal (Cu-Al) catalyst was developed at lab level which was scaled up to 1 kg successfully. Reproducibility of the catalyst preparation scale-up at various stages ranging from 6g lab scale to maximum 1 kg pilot scale was established by the repeated activity testing experiments for batch glycerol hydrogenolysis. In order to formulate the catalyst powder into tablets suitable for pilot scale trials, systematic experimental plan was executed by varying the binders in different compositions so as to obtain the tablets with the desired crushing strength. This tableted catalyst (5 × 5 mm) was then tested for continuous glycerol hydrogenation (50h), with 60% glycerol loading gave an average conversion of ~68% with ~92% selectivity to 1,2-PDO. In-situ activation under optimized conditions gave the performance results similar to previous bench mark experiment.

RESOURCE CENTERS

Central NMR Facility

The NMR facility provides support to all 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 four Bruker Avance NMR spectrometers at 200, 300, 400 and 500 MHz and a JEOL ECX 400 spectrometer. Bruker AV300 is a wide bore spectrometer dedicated to solid state NMR while the standard bore Bruker AV500 and JEOL ECX 400 spectrometers are equipped with solid state accessories.

During the year, the NMR facility analysed about 35,000 samples including 350 samples from industry and 25 samples from R&D and academic institutes generated the ECF of ₹ 53.2 lakhs.

Catalyst Pilot Plant

The activities at Catalyst Pilot Plant (CPP) focus on optimization and upgradation of the processes for the preparation of solid catalysts, adsorbents and supports such as zeolites, metal oxides, spinels, mesoporous molecular sieves and composites. CPP is equipped for the process optimization of petrochemicals, petroleum reactions and value addition to renewable feedstock such as alternative fuels and energy. alternative fuels and energy. The research work was also done in the areas viz. heterogeneous catalysts for utilization of renewable resource, characterization of perovskites and Sn-MFI molecular sieves and fractionation and characterization of lignin extractives from E-AFEX^{TM} pretreatment process.

Digital Information and Knowledge Resource Centre

Digital Information and Knowledge Resource Centre (DIKRC) comprises of Network Administration Unit and Knowledge Resource Centre. It brings together information, knowledge, tools and systems to support the R & D activities of the laboratory.

Network Administration Unit is responsible for planning, installation, operation, enhancement and maintenance of IT infrastructure of the laboratory. It provides the essential IT services and maintains a Tire-II type Data Centre. The unit maintains 'Centre of Excellence of Computational Chemistry' for the high performance computational work.

The unit has created Data Centre infrastructure, needed for CSIR-ERP and its proposed Disaster Recovery System initiative. It manages an National Knowledge Network Bandwidth (NKN BW) to enable WAN-based research collaboration across all the research institutes; interconnected over (NKN BW).

KRC provides information support using both archival print resources and contemporary digital resources. To fulfill the objective KRC subscribed to various Print & Electronic resources.

KRC has a collection of 1.43 lakh documents, including books and bound volumes of journals. 173 Books were purchased and 200 journals (Foreign & Indian; Print +E) were subscribed this year. 69 PhD theses were archived in Institutional Repository. KRC being part of CSIR-NISCAIR's National Knowledge Resource Consortium (NKRC) project got the access to more than 1500 journals of about eight well known publishers.

During the year 101 students, 14 corporate members and 73 casual visitors availed the services of KRC.

Center for Materials Characterization

Center for Materials Characterization (CMC) houses some of the most sophisticated equipments utilized for R & D projects of the Laboratory. The Resource Center is equipped with facilities such as X-ray diffractometry, Scanning electron microscopy, Environmental scanning electron microscopy, High resolution transmission electron microscopy, Transmission electron microscopy, Electron spectroscopy, Mass spectrometry and Magnetic measurements.

More than twelve thousand samples were analysed out of which 176 samples were from outside CSIR-NCL generating the ECF of about ₹ 27 lakhs.

National Collection of Industrial Microorganisms

NCIM Resource Center offers services to educational/ research institutes and industries. It is a unique nonprofit resource dedicated to the isolation, collection, preservation and distribution of authentic cultures of industrially important microorganisms. NCIM holds about 4000 microbial strains of bacteria, yeast, fungi and algae. NCIM acts as depository of patent strains and retains the important microflora in the country. NCIM has the expertise in the isolation and development of industrially important strains needed for microbial-based technologies. Many novel bacterial species were identified using polyphasic approach.

Summary of the highlights are listed below:

- ECF generation by supply of cultures was ₹ 110 lakhs.
- 34 Industrially important strains were deposited and authenticated using molecular identification methods.
- Around 200 microbial strains were lyophilized.
- DNA extraction and PCR amplification protocols for bacteria, fungi, yeasts and algae was standardized.
- For fungi and yeast non-liquid nitrogen based highly reproducible method involving CTAB and βmercaptoethanol, Harju heat and quick chill lysis metod was used.
- For bacteria fast and reliable simple lysis method like SDS-Proteinase K method, phenol chloroform method and quick colony PCR method was used.
- For algae: Physical disruption using glass beads followed by CTAB with lysozyme method yielded efficient and amplifiable DNA.
- Modern microbial identification methods rely on nucleic acids like DNA, RNA and Proteins as these are rapid, reliable and economic.
- Sequence based authentication and cataloging of 75 fungal and yeast strains in NCIM collection.

National Repository of Molecules

A national repository of small molecules was created at CSIR-NCL to acquire and maintain an inventory for biologically active molecules. The library is reshaped with NRM ID, sdf formatting of structures, donors name, analytical data, physical properties, toxicity; related literature etc. A library has the collection of about 2650 compounds, besides about 2300 natural product extracts and fractions. It has adapted the screening protocol for antiTB activity of compounds using XTT-Menadione assay.

S & T

SUPPORT SERVICES

Business Development

Business Development Division (BDD) plays a technology facilitation role through discussions related to research proposals, business negotiation, research valuation, IP ownership and contracts management. MIS Group activities involve 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 development, operation and management of various IT applications.

Human Resource Management

Project Training: More than 370 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 did their Summer/Winter projects at CSIR-NCL.

Guest workers: Total number of seventy-five guest-workers worked at CSIR-NCL during the year including fellows of various Indian sciences and engineering academies. Three students from abroad were also trained at CSIR-NCL.

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

CSIR-UGC NET Examination: The tests were conducted at Pune Centre on June 17, 2012 and Dec 23, 2012 for 18671 and 21699 registered candidates, respectively.

The Combined Administrative Services Examination was conducted on March 31, 2013 for 3516 candidates at Pune Centre.

Publication and Science Communication

Publication and Science Communication (PSC) Unit carries the responsibility to establish the communication between the laboratory and its stakeholders. It also renders facilities like web, print and electronic media. The unit manages video conference facility, external and internal websites and prepares annual reports and brochures. It communicates 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. The unit provides support to organize conferences and manages CSIR-NCL publications using publication databases and participates in exhibitions. It organizes press interviews with scientists for reporters and also manages institutional repository and open access.

Instrumentation and Communication

Instrumentation Development

Wireless Instrumentation development work was carried out using LabVIEW developer suite; one for heat exchanger and another for variable frequency drive available at Chemical Engineering Division. Wireless interface design and development for Zigbee, Probee and Bluetooth were done and tested for the range prescribed. Wireless Sensor Network was developed for all types of wireless interfaces and tested between various floors and across the width of the main building. This work of prototyping is being done for Indus magic. Initial work on embedded Ethernet module development was done. Further wireless developments using LabVIEW Real Time and WiFi are being carried out.

Wireless instrumentation for heat exchanger

Wireless instrumentation for variable frequency drive

Communication System

Alcatel Omni PCX Enterprise system has proven its advantage in design and single platform implementations. Major work of rerouting of one to one cables over optic fiber was done in the Main Distribution Frame boxes of communication system room in main building and in other communication room where system redundancy is established. Initiative is taken to launch different Session Initiation protocols.

Research Planning and Audit

The Unit co-ordinates five-year plan projects of chemical clusters and its review, in-house projects and its review. The unit also deals with the committee for disbursing funds to CSIR-NCL scientists for attending conferences abroad. The unit co-ordinates Research Council meetings

With the initiation of the 12th plan (2012-17), more than 60 proposals were sent to CSIR under the Chemical clusters and Biology clusters. Review meetings were also held at CSIR-NCL and with other laboratories for finalization of the proposals. Finally, more than 45 projects were approved for CSIR-NCL with being the nodal lab for 10 of those.

The unit provided supporting information to two audit teams stationed at CSIR-NCL and for the local audit team at New Delhi.

Lab Safety Management

The activity of running safety awareness and orientation courses initiated in the previous year picked up the momentum during the year when 16 such courses were organized. Generally, the courses are run with a frequency of at least once a month and round the year with 4 hours duration involving lectures, video shows and discussions on several aspects of lab safety. However, with the new batch of research students joined during January & July, the scope of the orientation was broadened and the duration was extended to almost 10 hours. During the past one year more than 400 students, project assistant and trainees attended the course work.

Invited seminars and training sessions were conducted outside CSIR-NCL to several organizations (colleges, university departments and chemical and pharma research labs), in addition to a full day training session with participation of several safety professionals from all over India. Taking a clue from the safety culture, facilities and infrastructure in CSIR-NCL, several other academic and industrial establishments in western India, have also initiated programmes for ensuring safety compliance and for better storage of flammable solvents and for its disposal. Such actions are an acknowledgment of the leading and responsible role that CSIR-NCL plays.

The hazardous waste generated in the lab is disposed off as per the standard procedures wastes and in line with the guidelines of Maharashtra Pollution Control Board. During the year, approximately 50KL of waste solvents were disposed.

The laboratory infrastructure was strengthened with the provision of antidotes for toxic and corrosive chemicals, fire safety cabinets and other personal protective equipments to all staff including fire retardant aprons. New guidelines were implemented for the issue of flammable solvents.

Engineering Services

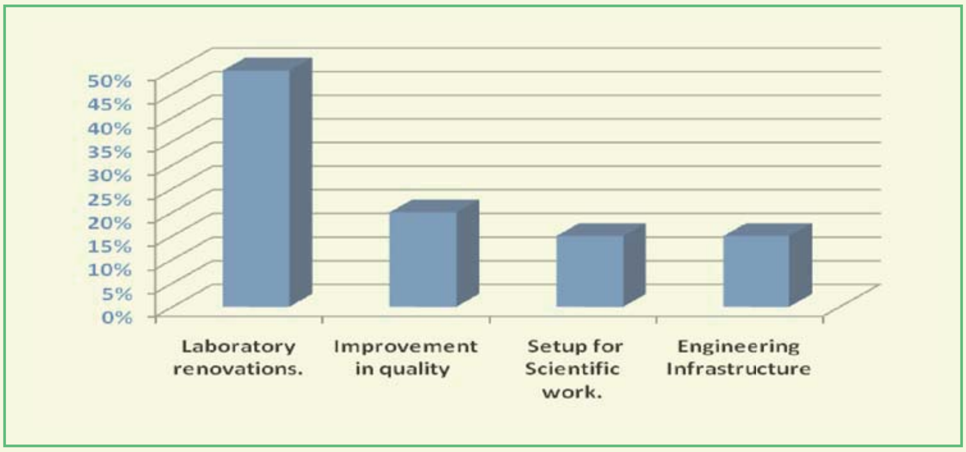
Engineering Services Unit plays an important role in smooth functioning of CSIR-NCL's research activities. It provides basic infrastructural facilities related to Civil, Electrical, Mechanical engineering and Glass blowing.

Glass Blowing

Various kinds of glass wares are fabricated as per the requirement of set up of experiments; it also maintains the glass wares by its routine inspection and fixation. The activity includes fabrication of distillation units, Filtration units etc.

Some of the major works carried out by engineering services during the year were:

- Major construction work of Hall of Residence IV.
- Completion of first phase of Indus magic project of chemical engineering.
- Architectural work related to PAM building first floor.
- Major repairs of D-II type quarters.



वित्त एवं लेखा

1	**निधि की उपयोगिता 2012-13**	
	सीएसआईआर अनुदान राशि	
	परियोजनाएँ	**राशि (रु. लाखों में)**
	नेटवर्क (सी/एफ सहित)	3765.999
	गैर-नेटवर्क	11381.441
	निमिटली परियोजनाएँ	422.042
	ईएमआर एवं वैज्ञानिक पूल	905.498
	प्रयोगशाला आरक्षित निधि	482.999
	बाहरी वित्तपोषित परियोजनाएँ	1934.838
	विविध जमा राशि	54.247
	बाहरी निकायों की ओर से भुगतान	326.388
	प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	48.434
	कुल	**19321.886**
2.	**प्रयोगशाला आरक्षित निधि का अर्जन**	**(रु. लाख में)**
	वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर से भिन्न) के निवेश पर अर्जित व्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	275. 571
	अन्य लेखाशीर्षों से	428.939
	कुल	**704.510**
3.	**31.3.2013 को अतिरिक्त निधि का निवेश (रु. लाख में)**	**2700.000**
4.	**आपत्ति-पुस्तिका मदों का निपटारा**	
	वर्ष के दौरान किए गए समायोजन	(रु. लाख में)
	निजी	2746.206
	यात्रा भत्ता/छुट्टी यात्रा रियायत	81.242
	स्थानीय	92.175
	कुल	**2919.623**
5.	**निम्न प्रकार के वाउचर तैयार किए गए**	
	भुगतान	20096
	प्राप्त राशि	4231
	टी.ई.	169
	कुल	**24496**

Finance and Accounts

1.	Funds Utilization 2012-13	
	CSIR Grant	
	Projects	(₹ in lakh)
	Network (including C/F)	3765.999
	Non – network	11381.441
	NMITLI Projects	422.042
	EMR & Scientist Pool	905.498
	Laboratory Reserve	482.999
	Externally Funded Projects	1934.838
	Misc. Deposits	54.247
	Payment on behalf of outside bodies	326.388
	Deposits for Sponsored conf. / seminars	48.434
	Total	19321.886
2.	Generation of Lab Reserve	(₹ in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	275.571
	From other heads	428.939
	Total	704.510
3.	Investment of surplus funds as on 31.3.2013 (₹ in lakh)	2700.000
4.	Clearance of OB items	
	Adj. made during the year	(₹ in lakh)
	Private	2746.206
	TA/LTC	81.242
	Local	92.175
	Total	2919.623
5.	Following types of vouchers were generated	
	Payment	20096
	Receipt	4231
	TE	169
	Total	24496

भण्डार एवं क्रय

सम्पादित किए गए कार्य/गतिविधियों के संख्यात्मक संकेतक

मद	संख्या		मूल्य (रु. करोड़ में)	
	2011-12	**2012-13**	**2011-12**	**2012-13**
कुल प्राप्त एवं निष्पादित माँगपत्र	1595	1519	113.17	64.22
कुल दिए गए ऑर्डर (आयातित)	223	290	37.00	34.42
कुल दिए गए ऑर्डर (स्वदेशी)	1121	1133	14.27	22.31
कुल प्राप्त सामग्री (आयातित)	223	362	22.62	35.18
कुल प्राप्त सामग्री	2002	1952	18.60	14.74
ऑनलाइन माँगपत्र	1530	1516	1.13	1.68
स्थानीय खरीद (ऑनलाइन आरसी सहित)	5461	8980	5.79	13.89
भण्डार से जारी की गइ कुल सामग्री	8259	6096	0.61	3.08
वित्तीय वर्ष 2012-13 में समायोजित बकाया शेष			8.97	26.71
वित्तीय वर्ष 2011-12 में सीमा शुल्क से छूट प्राप्त राशि का उपयोग			26.40	24.89
वित्तीय वर्ष 2011-12 में उत्पाद शुल्क से छूट प्राप्त राशि का उपयोग			2.49	6.15

अनुपयुक्त वस्तुओं का निपटान: वर्ष के अन्त में अनुपयुक्त वस्तुओं का निपटान: खाली वस्तुओं, कबाड़, प्लास्टिक की वस्तुएँ, फर्नीचर, एम.एस.स्टील, ई-वेस्ट, प्रायोगिक संयंत्र की निपटान गतिविधियाँ पूरी की गईं और उनसे रु. 52.26 लाख की राशि प्राप्त हुई ।

Stores and Purchase

Numerical indicators of work/activities completed

Item	Numbers		Value (₹ in Crores)	
	2011-12	2012-13	2011-12	2012-13
Total indents received and processed	1595	1519	113.17	64.22
Total orders placed (imported)	223	290	37.00	34.42
Total order placed (indigenous)	1121	1133	14.27	22.31
Total consignments received (Imported)	223	362	22.62	35.18
Total consignments received (Indigenous)	2002	1952	18.60	14.74
On-line indents	1530	1516	1.13	1.68
Local purchases (including on-line RC)	5461	8980	5.79	13.89
Total stores issues	8259	6096	0.61	3.08
Outstanding balance adjusted during the financial year 2012-13			8.97	26.71
Utilization of custom duty exemption during financial year 2011-12.			26.40	24.89
Utilization of excise duty exemption during financial year 2011-12			2.49	6.15

Major Equipments/other items procured/processed

Sr. No	Item Name	Value (₹in Lakhs)
1	Atomic force microscope	50.00
2	GCMS	42.50
3	Instrument for TPD and Physisorption analysis of catalysis	43.00
4	GCMS	32.00
5	High pressure reactor	43.50
6	High resolution X-ray microcomputed tomography imaging system	362.40
7	Flow cytometer	30.80
8	Multipurpose Physisorption system	35.23
9	Chemisorption and Physisorption system	35.12
10	Ekspert MicroLC System	67.16
11	Multichannel Electrochemical workstation	72.00
12	Semiconductor parameter analyser	34.50
13	Isothermal Calorimetry instrument	45.00
14	Microscope for cell imaging	41.75
15	Multichannel potentiostat galvanostat	27.50
16	Spectrophotometer fluorescence	24.60
17	Solar simulator	47.75
18	Field emission scanning electron microscope	283.50
19	Quadrupole mass spectrometer	48.00
20	DSC-TGD	28.00
21	Glove box	26.10
22	JANUS std.Varispan MDT Liquid handling system	28.80
23	Multi mode microplate reader	27.25
24	HPLC	36.00
25	Automated liquid handling system	46.75
26	Waters binary HPLC	26.80
	TOTAL	1586.01

Disposal of Unserviceable items: Disposal activity of empty drums, bottles, scraps, plastic wares, furniture items, M.S. steel, e-waste, pilot plant equipments was completed in the month of March, 2013 and a sum of ₹ 52.26 lakhs was released.

ANNEXURES

Patents Granted: Foreign

Title	Inventor(s)	Country/ Region and Grant No.
Taste Masked Pharmaceutical Compositions Comprising A PH Sensitive Polymer Providing Enhanced Bioavailability Of Polymorphic Bitter Drugs	Mohan Gopalkrishna Kulkarni; Anupa Ramesh Menjoge	CN: ZL200380110831.4
Antifungal Compounds Containing Benzothiazinone, Benzoxazinone or Benzoxazolinone And Process Thereof	Borate Hanumant Bapurao; Maujan Suleman Riyajsaheb; Sawargave Sangmeshwer Prabhakar; Kelkar Ramesh Ganesh; Wakharkar Radhika Dilip; Chandavarkar Mohan Anand; Vaiude Sharangi Ravindra; Joshi Vinay Anant	US: 8129369
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	CN: 101238090B
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	US: 8324227
Thiophene Containing Analogues Of Fluconazole As Antifungal Agents And Process Thereof	Borate Hanumant Bapurao; Sawargave Sangmeshwer Prabhakar; Maujan Suleman Riyajsaheb; Chandavarkar Mohan Anand; Vaiude Sharangi Ravindra; Joshi Vinay Anant	US: 8236840
Process Of Manufacturing Of Fatty Acid Alkyl Esters	Darbha Srinivas; Paul Ratnasamy; Sanjeevani Amrit Pardhy; Thirumalaiswamy Raja; Shilpa Shirish Deshpande; Vijay Vasant Bokade; Kashinath Joti Wagmare; Arshia Altaf Lalljee; Surya Prakash Babu; Karukappadath Kunjimoideen Abdul Rashid; Khaliji Anas; Chennampilly Ummer Aniz	US: 8124801
Method For The Preparation Of Biofuels From Glycerol	Darbha Srinivas; Lakshmi Saikia; Paul Ratnasamy	NZ: 588450 SG: 164736
Transesterification Catalyst, Process For Preparation Thereof And A Process For Transesterification Using The Catalyst	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	NZ: 567600 JP: 5006329 AU: 2006300758
A Novel Dicarbonic 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	Gnanou Yves; Matmour Rachid; More Arvind Sudhakar; Wadgaonkar Prakash Purushottam	JP: 5048687
Process For Producing Hydrocarbon Fuel	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	JP: 5001287
A Novel PH Sensitive Polymer Useful For Taste Masking And Gastric Delivery Of Drugs	Mohan Gopalkrishna Kulkarni; Anupa Ramesh Menjoge	JP: 5000890 EP: 1694724 ES: 1694724 FR: 1694724 GB: 1694724 SE: 1694724 CH: 1694724
Room Temperature Electrochemical Process For Synthesizing Titanium Dioxide Nanoneedles	Rajeshkumar Shankar Hyam; Reshma Kanta Bhosale; Satishchandra Balkrishna Ogale	ZA: 2011/05212
An Apparatus For Disinfection Of Sea Water / Ships Ballast Water And A Method Thereof	Ranade Vinayak Vivek; Pandit Anirudha Bhalachandra; Anil Agra Chandrashekhar; Subhash Shivram Sawant; Ilangovan Dandayudapani; Madhan Rajachandran; Pilarisetty Venkat Krishnamurthy	SG: 143311

Patents Granted: Indian

Title	Inventor(s)	Patent No
An Improved Process For The Preparation Of Lubricants	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	254487
A New Process For The Synthesis Of Micron/Nano Sized Inorganic Materials	Murali Sastry; Debabrata Rautray	254459
A Process For The Preparation Of Novel Macroporous Beaded Crosslinked Copolymers	Varsha Bhikoba Ghadge; Chalnattu Khizhakke Madhath Raman Rajan; Surendra Ponrathnam	254221
An Improved Process For Preparation Of N-Substituted Acrylamides	Bhalchandra Shripad Lele; Mohan Gopalkrishna Kulkarni	254132
Bile Acid Derived Steroidal Dimers Novel Amphiphilic Topology Having Antifungal Activity	Deepak Bhalchandra Salunke; Dr. Braja Gopal Hazra; Dr.Vandana Sudhir Pore; Mukund Vinayak Deshpande; Pallavi Balaram Nahar	253965
Process For Preparation Hydrogen Peroxide	Vasant Ramchandra Choudhary; Chanchal Samanta; Prabhas Jana	253888
An Improved Process For The Preparation Of Diol Functionalized UV Absorbers	Thanki PN; Singh RP	253836
A Process For The Preparation Of Primary Alkyl Glycerol Ethers Useful As Biofuel Additive From Glycerol	Darbha Srinivas; Paul Ratnasamy; Lakshmi Saikia	253826
A Macromonomer Based Copolymer Soluble In Aqueous Medium Above PH6 And A Process For The Preparation Thereof	Suvarna Pathaki Rupali Kedar; Kulkarni Mohan Gopalakrishna	253643
A Novel Device For Production Of Hydrogen From Effluents Of Internal Combustion Engine	Sanmati Annaray Mirji	253553
A Process For The Preparation Of Doped Conducting Polymer Films	Radhakrishnan S; Deshpande SD	253331
Composition Of Polymer Microcapsules Of Biocide For Coating Material	Parshuram Gajanan Shukla; Sivaram Swaminathan; Absar Ahmad	252557
Polyurethane Microcapsules Containing Biocide And Process For Preparation Thereof	Parshuram Gajanan Shukla; Sivaram Swaminathan	252555
A Novel Catalyst Composite Materials Useful For Desulfurization Of Hydrocarbon Feedstocks And Process For The Preparation Thereof	Shilpa Shirish Deshpande; Sanjeevani Amrit Pardhy; Subramanian Sivasankar	252412
Novel 1-Bromo-4-(4Bromophenoxy)-2-Pentadecyl Benzene And Preparation Thereof	More Arvind Sudhakar; Wadgaonkar Prakash Purushottam	252323
A Process For Preparation Of Hydrocarbon Fuel	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	251994
Novel Bisphenol Compounds And Method For Preparation Thereof	More Arvind Sudhakar;Wadgaonkar Prakash Purushottam	251565
A Novel Transesterification Catalyst And A Process For The Preparation Thereof	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	251432
An Improved Process For The Preparation Of Crosslinked Polyallylamine Polymer	Kulkarni Mohan Gopalkrishna; Kanawade Sandeep Thakaji; Benjamin Swapnanjali Babu	250997

Ph.D. Theses

Author	Title	Guide
Tripathi D.	Asymmetric synthesis of biologically active cyclic ethers and polyols employing proline catalyzed reactions and hydrolytic kinetic resolution (HKR)	Kumar P.
Akhtar S.	Biochemical studies of Nitrite Reductase in Mycobacterium sp.	Sarkar D.
Mishra A.	Biochemical studies on Reactive Oxygen species Generation and its Physiological role in Mycobacterium Sp.	Sarkar D.
Gupta R.	Biosynthesis of novel Sophorolipids using Candida bombicola ATCC 22214: Characterization and applications.	Prabhune A.
Kantak J. B.	Biotransformation: In Synthesis of Fatty Acid Alkyl Esters From Jatropha and Pongamia Oil	Prabhune A.
Sreedhar K.	Conformationally restricted PNA analogues synthesis and biophysical studies of cationic pyrrolidyl PNA	Ganesh K. N.
Sane P. S.	Designed Macromolecular Architecture by Controlled Polymerization Methods	Wadgaonkar P. P.
Shedge S. V.	Development and application of non-iterative methods for calculation of electric response properties within density functional theory	Pal S.
Chaudhary P.	Development of Novel Antifungal Agents using Fungal cell wall as a target.	Deshpande M. V.
Sadavarte N.	Difunctional Monomers Starting from Cashew Nut Shell Liquid (CNSL) and High Performance Polymers Therefrom	Wadgaonkar P.
Reddy S. R.	Enantioselective Synthesis of Bioactive Molecules via Hydrolytic Kinetic Resolution of Alkoxy Epoxides, Dihydroxylation of Alkenes and CuCN-Mediated Annulations in C-C, C-O Bond Formation	Sudalai A.
Rawat V.	Enantioselective Synthesis of Bioactive Molecules via Proline Catalyzed α Functionalization, Asymmetric Epoxidation and Synthetic Methodologies Involving Pd-Catalyzed Reductive Cyclization, Selective Hydrosilylation of Carbonyl Compounds	Sudalai A.
Rai G.	Enthalpy effects in Ionic Liquids and mixing schemes in Aqueous Ionic systems.	Kumar A.
Patil R. S.	Functional and biologically active oligosaccharide mimics of carbohydrate processing enzymes and their application for pathogen detection: An exercise with mycobacterium tuberculosis	Ramana C. V.
Inamdar S. R.	Global optimization of chemical processes	Kulkarni B. D.
Shaikh A. W. A	Highly Porous Poly (HIPE) Materials: Synthesis and Characterization	Ponrathnam S.
Kapoor M.	Host-Pathogen Interaction in Metarhizium Anisopliae and its insect Host Helicoverpa Armigera.	Deshpande M. V. & Sen A.

Ph.D. Theses

Author	Title	Guide
Shedge A. S.	Hydrophobically modified Water soluble polymers : Syntheses, Characterization & Rheology.	Badiger M. V.
Mishra M.	Interactions between diverse proteinase inhibitors from Capsicum annuum and insects pest : biochemical & molecular approach	Gupta V.S.
Vishwakarma R. K.	Isolation, Cloning and Characterization of Terpenoids Biosynthesis Pathway gene(s) from Bacopa monniera	Khan B. M.
Taware R. V.	Isolation, Purification and Characterization of Secondary metabolites form endophytic fungi of Phyllanthus Sp.	Ahmad A.
Santoshkumar	Isolation, cloning and characterization of Cinnamate 4 hydroxylase (C4H) Gene from Leucaena Leucocephala and its expression studies	Khan B. M.
Patel P.	Metal mediated Novel Nitro-Alkyne cycloisomerizations: studies toward the total synthesis of isatisine A	Ramana C. V.
Rajwade A. V.	Molecular and biochemical characterization of high and low alpha-linolenic acid containing Indian flax (Linum usitatissimum L.) varieties	Gupta V. S.
Menon V	Molecular and functional aspects of Hydrolyases / Inhibitors with emphasis on Aspartic Protease Inhibitor	Rao M.
Kodgire V. V	Organic Inorganic Hybrids : Preparation, Characterization and Applications in Adhesives and Coatings	Badiger M. V.
Yadav A. P.	Polymer Derived Functional Carbon and Carbon Based Nanocomposites	Jog J. P.
Jagtap R. S.	Preparation of some organozinc compounds and their enantioselective addition to aldehydes	Joshi N. N.
Manjare Y. S.	Preparation of some supramolecular assemblies of an adamantanedicarboxilic acid	Pedireddi V. R.
Bhonsle H. S.	Regulation of glycation in Diabetes: Identification and characterization of glycated proteins	Kulkarni M. J.
Biradar S. C.	Role of polymer functionality and architecture on morphology of gold nanoparticles	Kulkarni M. G.
Singh M.	Selective Carbon-Carbon Coupling Reactions of Phthalides: Synthesis of anti-Helicobacter pylori agents the CJ-molecules and Oxygen Containing Bioactive Natural Products	Argade N. P.
Pandey P. S.	Studies in Asymmetric Catalysis for Hydrformation Reactions	Chaudhari R. V.
Shingote S. K.	Studies in catalytic transfer hydrogenation reactions	Deshpande R. M. & Kelkar A. A.
Raju D.	Studies on Metal Accumulation and Synthesis of Inorganic Nanomaterials in Plants and their Applications.	Ahmad A.
Bhavsar K. P.	Studies on Phytase from Aspergillus Niger NCIM 563 Under Solid state Fermentation and its Correlation with submerged Phytase I and II	Khire J. M.

Ph.D. Theses

Author	Title	Guide
Jamalpure T. M.	Studies on the Alkaline Amylase from an Alkalophilic Streptomyces species NCL 716	Lalitha Kumar
T. Gaydhankar	Studies on the solid acid catalysts containing Group VI Elements: Synthesis, Characterization and Screening for their catalytic activities	Waghmare K. J. & Nikalje M. D.
Nagarajan V.	Study of some Supramolecular Assemblies Mediated by N-H-O, N-H-N and N-H-S Hydrogen Bonds	Pedireddi V. R.
Narute S. B.	Sugar Alkynol Cycloisomerization Approach towards the total synthesis of Aflastatin A, Zooxanthellamide D; and Synthesis of some C-Gycosyl Analogues of B-DPA as novel antitubercular agents	Ramana C. V.
Selukar B. S.	Synthesis and Characterization of Biodegradable Polymers using Organomodified Clay	Garnaik B.
Ghorpade R.	Synthesis and Characterization of High Refractive Index Hydrophobic Polyacrylates	Ponrathnam S.
Bagmare S.	Synthesis and biophysical properties of Nucleic acid analogues bearing 5-atom achiral amide and chiral D/L-amino acid- derived linkages	Kumar V. A.
Sangave D. V.	Synthesis and characterization of two stage crosslinkable Resins	Kulkarni M. G.
Malvi B.	Synthesis of “Clickable” SBA-15 and MCM-41 Mesoporous Materials and Their Applications in Catalysis and Bio-Catalysis	Sengupta S.
Kar M.	Synthesis of "Clikable" Polypeptide by NCA Polymerization and their Application as Biomaterials	Sengupta S.
Patil M. T.	Synthesis of isomeric cyclitols and their derivatives / analogs from myo-inositol and the associated structural studies.	Shashidhar M. S.
Sivaranjani S.	Synthesis, Characterization and Application of Hetero Atom Doped Mesoporous TiO_2	Gopinath C. S.
Gurale B. P.	Synthesis, related mechanistic and strustural studies of Cyclitols and their derivatives	Shashidhar M. S.
Harale K.	Synthetic studies towards Stemoamide, Paroxetine, Femoxetine,3-Hydorxypipecolic Acid and Development of Synthetic Mehodology.	Chavan S.
Khairnar L. B.	Synthetic studies towards pipecolic acid, its 3-hydroxy derivatives and development of synthetic methodology	Chavan S. P.
Chendake Y. J.	Transport of acids through polymeric membranes	Kulkarni B. D.

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. It is aimed to share the excitement of science and technology with school students. Following talks were organized during the year.

Topic	Speaker
The Art and Science of Colour	Dr. Sayam Sen Gupta, CSIR-NCL
Discovery of Elements	Dr. K. Guruswamy, CSIR-NCL
Crystal Growing	Dr. Nandini Devi, CSIR-NCL
Tropical Infectious Diseases: Biology & Global Impact on Human Health And Economy	Dr. Dhanasekaran Shanmugam, CSIR-NCL
How knowing the small is helping in our fight against diseases	Dr. Neetu Singh, CSIR-NCL
The forces that bind molecules: From basic Science to New Technology	Dr. M. Cynthia Goh, Institute for Optical Sciences, University of Toronto, Canada
Reaction Energetics	Prof. M. G. Finn, Georgia Institute of Technology, USA
Chemistry that you can eat: The Science behind food and cooking	Dr. Magesh Nandagopal, CSIR-NCL
Fun with maths	Prof. Anisa Chorwadwala, IISER-Pune
An Introduction to the Nanotechnology of Gold	Dr. Mathias Brust, University of Liverpool, UK
Chemistry with sweet compounds	Dr. Srinivas Hotha, IISER-Pune
Science And our Community	Dr. Murali Sastry, DSM India Innovation Centre, Gurgaon
What we should learn from Nature	Dr. Arvind Anant Natu, IISER-Pune
Molecules Medicine and Life	Dr. Ravi Singh, CSIR-NCL

CSIR-NCL Customers

Indian Customers

- GAIL (India) Limited
- ONGC
- Unichem Laboratories Ltd.
- Odyssey Organics Pvt. Ltd.
- RIL
- Cadbury India Ltd.
- Albert David Ltd.
- Gadre Marine Exports Pvt. Ltd.
- Tridiagonal Solutions Pvt. Ltd.
- Deepak Novochem Technologies Ltd.
- Hindustan Polyamides and Fibres Ltd.
- I S Industries Pvt. Ltd.
- Cipla Ltd., Mumbai
- Torrent Pharmaceuticals Ltd.
- BASF India Ltd.
- Morganite Crucible (India) Ltd.
- Emcure Pharmaceuticals Ltd.
- S. C. Johnson Products Pvt. Ltd.
- Godrej Consumer Products Ltd.
- Tata Chemicals Ltd.
- SRF Ltd.
- Bayer Crop Science Ltd.
- Aquapharm Chemicals Co Pvt. Ltd.

Foreign Customers

- Sherwin-Williams Company
- Solvay SA, Belgium
- GlaxoSmithkline LLC
- Benefuel Incorporation
- Solvay SolexisS.p.A., Italy

Publicly Funded Customers

- DST
- DBT
- Ministry of New & Renewable Energy
- IFCPAR (CEFIPRA)
- Ministry of Food Processing Industries
- Ministry of Environment & Forest

Deputations Abroad: Staff

Name	Place	Purpose	Period
Dr. (Mrs) A. V. Pundle	Netherlands	DBT-CREST Award	March 18 – July 17, 2013
Dr. (Mrs) Moneesha Fernandes	Austria	Conference	Oct 7 – 11, 2012
Dr. (Mrs) V. G. Puranik	France	2nd Bilateral Indo French symposium	July 11 – 16, 2012
Dr. (Ms) S. B. Umbarkar	France	2nd Bilateral Indo French symposium	July 11- 13, 2012
		Invited professor	May 17– June 17, 2012
		'ACHEMA 2012	June18 - 22, 2012
Dr. A. P. Giri	Israel	Scientific Collaboration & Paper Writing	May 7- 20, 2012
Dr. A. R. Joshi	Thailand	Conference ICBEE 2012	Sep 1 – 2, 2012
	Kenya	Project discussion	May 7 – 14, 2012
	Netherlands	Course on Super Pro Designer	Oct 25 – 26, 2012
Dr. A. Sudalai	Israel	Sabbatical leave	Oct 1, 2012 – Feb 28, 2013
Dr. Anil Kumar	China	Keynote speech at the 3rd APCIL Conference	Oct 17 – 19, 2012
	Spain	Bilateral Exchange NARILAR Project	Mar 16 – 24, 2013
Dr. Ashish K. Lele	Portugal	Conference	Aug 5 – 8, 2012
Dr. Avalokiteswar Sen	Thailand	Conference on Wild Silkmoth & Silk	Nov 22 – 24, 2012
Dr. B. L. V. Prasad	USA & UK	Gordan Conference, Kansas State University, USA Liverpool University UK	June 15 – July 6, 2012
	Germany	CSIR-RAMAN Fellowship	Sep 10 - Dec 8, 2012
Dr. C. S. Gopinath	France	Erasmus Mundus Fellowship	May 1 - 31, 2012
	Japan	Conference on Electronic Materials 2012	Sep 23 - 28, 2012
	South Korea	Conference and talk at KAIST	June 24 – 29, 2012
Dr. C. V. Rode	Japan	JST Program	May 27 - 30, 2012
		National Institute of Advanced Industrial Science & technology Sendai, Japan	April 14 – 23, 2012
	Spain	NARILAR Project Work	Feb 15 – Mar 31, 2013
		Invited talk	Nov 2 – 7, 2012
	South Korea	Talk on Renewable feedstock for clean energy	Jan 3 – 11, 2013
Dr. D. Srinivas	Singapore	Conference on Molecular & Functional Catalyst	July 30 – 31, 2012
	UK	Plenary Talk	Mar 24 – 27, 2013
Dr. Ganesh Pandey	Netherlands	Tetrahedron symposium	June 26 – 29, 2012
Dr. K. B. Sonawane	Malaysia	Separation Science Asia 2012	June 27 - 28, 2012
Dr. K. Guruswamy	UK	Research Workshop in Adv. Materials	Sep 16 – 23, 2012
	USA	Symposium on Macro Molecules	June 24 – 29, 2012
Dr. K. Krishnamoorthy	Australia	Collaboration	June 10 - 24, 2012
Dr. K. R. Patil	Spain & Portugal	Project work NARILAR	Oct 1- Nov 21, 2012

Deputations Abroad: Staff

Name	Place	Purpose	Period
Dr. M. V. Badiger	Japan	Gel sympo	Oct 9 - 12, 2012
	France	IFCPAR Project	Sep 3 – 24, 2012
Dr. M. V. Deshpande	USA	Discussion and visit Rutgers University, NJ,	June 22 – July 1, 2012
Dr. Magesh Nandagopal	Belarus	Scientific - Practical Conference TRIIN 2012	Oct 17 - 19, 2012
Dr. P. G. Shukla	USA	Seminar & discussion collaboration	Oct 1 - 5, 2012
Dr. P. P. Barve	Germany	Discussion on process development	Oct 3 – 5, 2012
Dr. Pankaj Poddar	UK	Talk at Meeting : Nano Material Futures	Feb 17 – 20, 2013
		Magnetic Measurement Under Indo-UK Project	Aug 16 - 26, 2012
Dr. Paresh L. Dhepe	France	Bilateral Indo French symposium	July 11 – 13, 2012
Dr. R. Nandini Devi	France	Bilateral Indo French symposium	July 11 – 13, 2012
Dr. Rahul Banerjee	Belgium	To attend The Editors Symposium	Mar 2 - 4, 2013
	UK	Talk at Cambridge University and attend RSC's Cryst Eng Command Editorial Board Meeting	May 13 – 19, 2012
	Canada	Conference : Challenges in Inorganic & Materials Chemistry	July 19 – 22, 2012
	China	2nd China India Singapore Symposium	Nov 19 – 23, 2012
Dr. S. B. Ogale	France	Annual Meeting	May 23 - June 10, 2012
	South Korea	NANO Korea 2012 Symposium	Aug 16 – 17, 2012
	Italy	AIP/ICTP Industrial Physics Forum	April 16 – 20, 2012
	Australia	PV and Solar Thermal Workshop	Oct 14 – 21, 2012
	UK & France	Collaborative Visit, to conduct PhD Exam	July 16 – 25, 2012
Dr. S. S. Tambe	USA	AICHE Meeting & Visiting OPCONSYS	Oct 28 - Nov 4, 2012
Dr. Sanjay Nene	Germany	Meeting & discussion on Bilateral Project	Oct 1 – 5, 2012
Dr. Sourav Pal	Nepal	Workshop on Theoretical Chemistry Atoms	April 30 - May 3, 2012
	USA	Seminar at University of Florida	Oct 3 – 6, 2012
	Germany	Discussions on DST-DAAD project	Mar 21 – 25, 2012
Dr. Sudip Roy	USA	Gordon conference	July 22 – 27, 2012
Dr. V. V. Ranade	Netherlands	Gordan Conference	Sep 2 – 7, 2012
	UK	BHR Consortium Conference	Oct 12 – 16, 2012
Ms. Anuya Nisal	Portugal	Short Course - Colloidal Suspension Rheology & ICR 2012 Conference	Aug 3 – 10, 2012
Shri H. V. Pol	Portugal	Conference	Aug 5 – 8, 2012
Shri K. D. Deshpande	Japan	To visit Fujitsu Technologies various Data Centre	Mar 3 – 9, 2013

Deputation Abroad: Students

Name	Place	Period
Anal Kumar Ganai	Japan	Sep 5 - 9, 2012
Ankit Ajit Jain	USA	Mar 17 - 20, 2013
Anumon C. Divakaran V.D.	Japan	Oct 9 - 12, 2012
Anupam Subhash Samanta	Japan	Sep 5 - 9, 2012
Chandrashekhar RamsnehiPrasad Sharan	Australia	Oct 12 - Dec 14, 2012
D. V. Rami Reddy Narasimha Reddy	Italy	Mar 3 - 7, 2013
Deepti Atulkumar Mishra	Spain	July 2 - 5, 2012
Edwin Soloman Gnanakumar	Italy	Mar 3, 2013 - Mar 2, 2014
Joby P. V. Sebastian	Japan	July 28 - Aug 1, 2012
K. Sivaranjani Kumarsrinivasan	Germany	July 1 - 6, 2012
Kalyani Suresh Chikhalikar	Portugal	Aug 3 - 11, 2012
Khaja Mohaideen Kamal	South korea	July 8 - 13, 2012
Mandakini Mahendra Biswal	Singapore	Jan 15 - Mar 14, 2013
Mangesh B Mahajan	South korea	July 8 - 13, 2012
Manojkumar Surapu Varada	Canada	Aug 5 - 9, 2012
Mrityunjoy Kar	Czech Republic	July 1 - 5, 2012
	France	May 23 - July 17, 2012
Mudit Dixit	France	July 11 - 13, 2012
Neha Sandeep Mahajan	China	Sep 24 - 28, 2012
Neha Shivdatt Tiwari	Italy	Mar 3 - 7, 2013
Nishita Satyendra Lucas	Japan	July 28 - Aug 1, 2012
Onkar Sharad Game	Singapore	Feb 1 - Mar 31, 2013
	UK	Nov 1 - Oct 30, 2012
Pavan Manohar More	France	May 23 - July 17, 2012
Prakash Lohani Chandra	France	July 11 - 13, 2012
Prashant Arvind Patil	Portugal	Aug 3 - 11, 2012
Pravin Narayan Shinde	UK	Sep 16 - Dec 15, 2012

Deputation Abroad: Students

Name	Place	Period
Priyanka Anil KumarSingh	Israel	July 1 - Dec 31, 2012
Rahul Sadashiv Tanpure	Israel	May 5 - Oct 31, 2012
Raja Das	UK	Feb 14 - Mar 16, 2013
	Italy	Sep 9 - 14, 2012
Rajesh Ramkrishna Jadhav	Germany	Sep 1 - Oct 31, 2012
Rajesh T.	Belgium	Aug 29 - 31, 2012
Ramtenki Vilas	U K	Sep 16 - Dec 15, 2012
Rasika Bharat Mane	South Korea	Jan 3 - 11, 2013
	Japan	April 14 - 23, 2012
Sagar Hindurao Patil	Portugal	Sep 15 - Dec 14, 2012
Samruddhi B Kamble	Portugal	Aug 3 - 11, 2012
Sandip Mallikarjun Kale	USA	Jan 16 - Dec 31, 2013
Shashikant Sabhajeet Shukla	UK	Aug 5 - 10, 2012
Shraddha Yashwant Chhatre	Switzerland	Sep 15, 2012 - Feb 15, 2013
	UK	May 1 - July 20, 2012
Shruti Agarkar	U K	July 8 - 20, 2012
Sonali B Rohamare	U K	Sep 19, 2012 - Sep 18, 2013
Subha Sujit Sadhu	UK	Feb 17 - 20, 2013
Sushma Kumari	Italy	Mar 3 - 7, 2013
Tanay Madhusudan Kundu	Canada	July 19 - 22, 2012
Trupti Vyankatesh Kotbagi	France	July 11 - 13, 2012
Venu BabuKotikam Venkatswararao	Canada	Aug 5 - 9, 2012
Vidhya Changdev Ghantani	France	July 11 - 13, 2012

Awards / Recognitions

Dr. A. K. Bhattacharya	- Fellow of Maharashtra Academy of Sciences
Dr. Alok Sen	- Fellow of Maharashtra Academy of Sciences
Dr. Amol Kulkarni	- Humboldt Ambassador Scientist
Dr. Ashish Lele	- Infosys Prize
Dr. (Mrs.) Asmita Prabhune	- Fellow of Maharashtra Academy of Sciences
Dr. A. T. Biju	- OPPI Young Scientist Award
Dr. B. L.V. Prasad	- CRSI Bronze Medal - Young Career Award
Dr. C. G. Suresh	- Fellow of Maharashtra Academy of Sciences
Dr. G. J. Sanjayan	- CRSI Bronze Medal - Shanti Swaroop Bhatnagar (SSB) Prize

Dr. Pradeep Kumar receiving OPPI Young Scientist Award

Dr. Sourav Pal receiving the Best Laboratory Award from Union Defense Minister Shri A. K. Antony

Awards / Recognitions

Dr. M. S. Qureshi	• Consulting Editor of the International Journal- 'Journal of Pharmaceutical Analysis (JPA)'
Dr. M. S. Shashidhar	• Fellow of the National Academy of Sciences (NASI), Allahabad, India
Dr. Mugdha Gadgil	• CSIR Young Scientist Award
Dr. Pradip Kumar	• OPPI Young Scientist Award • Professor A.S.R. Anjaneyulu 60th Birthday Commemoration Award
Dr. R. A. Mashelkar	• Chairperson of the Academy of Scientific & Innovative Research (AcSIR)
Dr. Srinivasa Reddy	• CDRI Award
Dr. Sourav Pal	• A. V. Rama Rao Foundation Lecture in Chemistry • Chairman of Royal Society of Chemistry (West India Section) • Member of the Advisory Board of CSIR • Member of the Governing Council of Central Water and Power Research Station (CWPRS)
Dr. V. V. Bokade	• Member of the Editorial Board of New Journal on Conference Papers in Energy to be published by Hindawi Publishing Corporation, Cairo, Egypt.
Dr. V. V. Ranade	• Outstanding Achievement Award R&D– Individual Excellence

NCL Research Foundation

The National Chemical Laboratory Research Foundation (NCL RF), a not-for-profit organization, was established in 1991 with a mission to promote excellence in science and technology and create an environment in which creative and innovative endeavours in scientific, technical and R&D support areas are recognised and rewarded. It aims to bring creative research, novel technologies and organisational innovations into clear focus and encourages those core values which NCL considers important for the well being of the organisation.

Awards and Lectures

NCL RF gives various awards on NCL Foundation Day and National Science Day. Besides organizing invited lectures on the occasion of NCL Foundation Day, National Science Day and National Technology Day, NCL RF organizes several special lectures in memory/ honour of former NCL Directors:

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

Network Projects

Following CSIR network projects continued during the year:

Title of the project	Project leader
A multi-scale Simulation and Modeling Approach to Designing Smart Functional Materials for use in Energy, Electrochemistry and Bio-mimetics	Dr. Sourav Pal
Advanced Drug Delivery System	Dr. Sayam Sen Gupta
Affordable Cancer Therapeutics	Dr. S. P. Chavan
Biocatalysts for Industrial Applications & Greener Organic Synthesis	Dr. H. V. Thulasiram
Bioprospection of plant resources and other natural products	Dr.(Mrs.) Vidya Gupta
Catalysts for Specialty Chemicals	Dr. Pal Singh Anand
Catalysts for Sustainable Energy	Dr. D. Srinivas
Centre for BIOtherapeutic Molecule Discovery	Dr. G. J. Sanjayan, Dr. A. P. Giri
Centre for Surface and Interface Science Research	Dr. C. S. Gopinath, Dr. C. P. Vinod
Clean Coal Technology	Dr. D. Srinivas
Clean Coal Technology	Dr. Vivek Vinayak Ranade, Dr. Rajnish Kumar
Creating Intellectual Property and capabilities for the development of improved security features and subtrates for the Indian currency note	Dr. V. Premnath
CSIR-NCL-IGIB Joint Research Initiative: Interfacing Chemistry and Biology	Dr. H. V. Thulasiram
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. V. M. Bhandari Dr. Sanjay P. Kamble
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

Network Projects

Title of the project	Project leader
Genomics of medicinal plants and agronomically important traits	Dr. A. P. 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
Innovate, develop and up-scale modular, agile, intensified and continuous (Indus MAGIC) processes and plants	Dr. Vivek Vinayak Ranade
Innovative solutions for Solar Energy storage	Dr. C. S. Gopinath, Dr. (Mrs.) 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. Venkateswarlu 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. P. R. Rajamohanan
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

Network Projects

Title of the project	Project leader
Plant-Microbe and Soil Interactions	Dr. N. Y. Kadoo
Research Initiative for Low Emissions	Dr.(Mrs.) S. B. Umbarkar
Screening molecules in lead exploration	Dr. Mahesh J. Kulkarni
Technologies and Products for Solar Energy Utilization through Networks	Dr. K. 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 Centre	Dr. Jayant Malhar Khire
Zero Emission Research Initiative for Solid Wastes from Leather	Shri Deenadayalan

CSIR-800

CSIR-800 was launched in June 2011 and a partnership to promote Cluster Innovation Centers was announced by CSIR and the National Innovation Council (NInC).

It is an initiative to reach to 800 million Indians at the base of the economic pyramid through various CSIR technologies. The objective is to achieve the inclusive growth and improved quality of life and bring smiles to the faces of 800 million citizens of India through socially and economically relevant science and technology interventions.

CSIR-800 program is being executed through Micro, Small and Medium Enterprises (MSMEs) to benefit from CSIR Technologies through 'Cluster Innovation Centres' and by the establishment of Gram Vigyan Kutir (GVK, Techvil).

The Gram Vigyan Kutirs are being established by the laboratories to disseminate appropriate technology solutions and typical technological assistance. CSIR-NCL is setting-up Gram Vigyan Kutir in Wada/Vikramgad block in tribal belt of Thane District of Maharashtra. This Gram Vigyan Kutir is expected to benefit to 15-20 villages and around 40,000 population of tribal area of Thane District.

Dateline CSIR-NCL

02/04/2012	Symposium on Materials Science Research- Details required
12/04/2012	CSIR-NCL Research Scholars Meet - Life in Science - A perspective by Padma Shree Dr. G. C. Mishra, Former Director, NCCS, Pune
13/04/2012	Prof. K. Venkataraman Memorial Lecture on Synthetic Studies on Organoselenium Compounds as Antioxidants by Prof. S. Chandrasekaran, IISc, Bangalore
25/04/2012	Prof. B. D. Tilak Memorial Lecture on The Odyssey of Community Service: A Personal Reflection by Dr. Prakash Amte
11/05/2012	National Technology Day Lecture by Dr. R. R. Sonde, Executive Vice President, Thermax Ltd. Pune on science – engineering – technology – market: Non – linear pathways with special reference to clean energy technologies
17/05/2012	75th Birth Day Felicitation Function of Prof. M.M. Sharma FRS by Dr. A.V. Rama Rao
06/06/2012	Visit of Dr. Ashwani Kumar, Hon ble Minister of State for Planning, Science & Technology and Earth Sciences, Govt. of India- Photo
11/06/2012	Seminar on Current Trends in Industrial Catalysts
15/06/2012	Workshop on Industrial Waste Water Treatment: Recycle & Reuse
22/08/2012	Public Lecture on Stories of Emerging Paradigms in Translational Cancer Research by Prof. Shiladitya Sengupta, MIT, Cambridge, USA
25/09/2012	CSIR Foundation Day Lecture by Dr. S. R. Shetye, Vice Chancellor, Goa University on Physical processes in monsoonal estuaries of India : Need for a new research approach
10/10/2012	ACS on campus event @ NCL - An initiative from the American Chemical Society
19/11/2012	Public Lecture on Science of Compassion by Prof. Pradeep Deshpande
22/11/2012	Symposium on Proteomics beyond IDs
27/12/2012	INSA Anniversary General meeting
07/01/2013	NCL Foundation Day Lecture by Prof. Ei-ichi Negishi, Nobel Laureate on Magical Power of Transition Metals: Past, Present, and Future
19/01/2013	Symposium on 100 Years of X-Ray Diffraction
07/02/2013	Distinguished Public Lecture on The Greek Key super secondary structural motif in the crystalline appears essential to maintain the transparency of the human eye lens: A case where structure determines the function by Professor D. Balasubramanian, L.V Prasad Eye Institute , Hyderabad
11/02/2013	RSC India one-day Roadshow Symposium at CSIR-NCL Pune
28/02/2013	National Science Day Lecture on Changing Paradigm of Indian Science by Prof. W. N. Gade , Vice Chancellor , University of Pune
07/03/2013	National Safety Day lecture by Mr. M. Rama Krishna, VP, Alexandria Equities Management (India) Pvt. Limited, Hyderabad
22/03/2013	CSIR- NCL, HRD programme of Faculty Training and Motivation for Teachers

राजभाषा रिपोर्ट

राजभाषा कार्यान्वयन रिपोर्ट

भारत सरकार की राजभाषा नीति का अनुपालन करने की दृष्टि से सीएसआईआर - राष्ट्रीय रासायनिक प्रयोगशाला में प्रत्येक स्तर पर प्रयास किए जाते हैं। यह एक वैज्ञानिक प्रयोगशाला है, जहां अधिकांश कार्य वैज्ञानिक तथा तकनीकी स्वरूप का होता है तथा शेष प्रशासनिक कार्य हिन्दी भाषा में किया जाता है। इस प्रयोगशाला में किए जा रहे राजभाषा कार्यान्वयन संबंधी उल्लेखनीय प्रयास निम्नानुसार है।

राजभाषा अधिनियम की धारा 3(3) के अंतर्गत जारी होने वाले सभी दस्तावेज अनिवार्य रूप से द्विभाषी जारी किए जाते है।

इस प्रयोगशाला में राजभाषा विभाग द्वारा जारी वार्षिक कार्यक्रम में निर्धारित किए गए लक्ष्यों की प्राप्ति की ओर विशेष ध्यान दिया जाता है।

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% से अधिक कर्मचारी वृंद ने हिन्दी का कार्यसाधक ज्ञान प्राप्त कर लिया है, राजपत्र में अधिसूचित किया गया है।

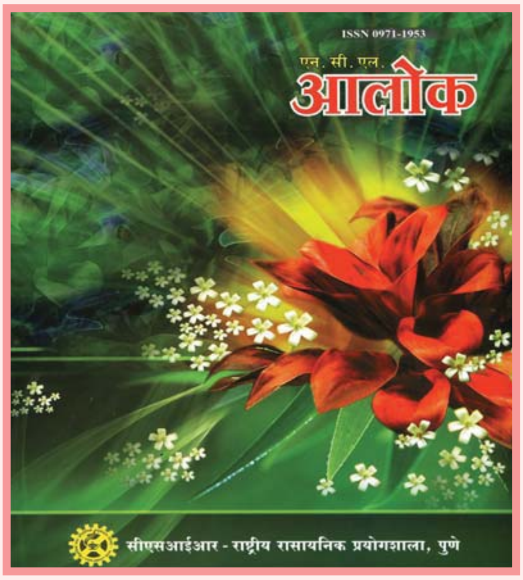
प्रयोगशाला के 98% कर्मचारियों को हिन्दी, हिन्दी टंकण एवं आशुलिपि का प्रशिक्षण दिया जा चुका है।

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।

प्रत्येक तिमाही में प्रयोगशाला की राजभाषा कार्यान्वयन समिति की 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 है।

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 कार्याशालाओं 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।

प्रयोगशाला में प्रतिवर्ष हिन्दी गृहपत्रिका ''एनसीएल - आलोक'' का प्रकाशन नियमित रूप से किया जाता है। गृहपत्रिका प्रकाशन का मूल उद्देश हिन्दी भाषा में लिखे गए वैज्ञानिक लेखों का प्रचार-प्रसार तथा कर्मचारियों की हिन्दी में लेखन और अभिव्यक्ति क्षमता को प्रोत्साहित करना है।



प्रयोगशाला के हिन्दी कक्ष व्दारा प्रतिदिन हिन्दी सुविचार तथा अँग्रेजी शब्द के अर्थ का प्रेषण मेल व्दारा सभी कर्मचारियों को किया जाता है, ताकि कर्मचारियों में हिन्दी भाषा के प्रति रूचि उत्पन्न हो सकें।

इसके अलावा राजभाषा हिन्दी के प्रचार - प्रसार तथा राजभाषा हिन्दी के प्रगामी प्रयोग को बढावा देने के उद्देश से विभिन्न राजभाषा सम्मेलनों तथा राजभाषा संगोष्ठियों का आयोजन भी किया जाता है। इसी क्रम में गुरूवार, दिनांक 24 जनवरी, 2013 को राजभाषा हिन्दी : एक उद्योग नामक विषय पर एकदिवसीय स्थानीय संगोष्ठी का आयोजन किया गया।

वैज्ञानिक कार्यों में राजभाषा के प्रयोग को बढावा 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 7 मई, 2013 को कार्बनिक रूपान्तरण में उत्प्रेरक का प्रयोग नामक विषय पर एकदिवसीय विज्ञान संगोष्ठी का आयोजन किया गया।

प्रयोगशाला में सभी मानक प्रपत्र, फार्म तथा आवेदन पत्र इत्यादि द्विभाषी रूप में तैयार किए गए हैं।

प्रयोगशाला की वैबसाइट को द्विभाषी रूप में प्रदर्शित किया गया है।

प्रयोगशाला के सभी कम्प्यूटरों में द्विभाषी रूप से कार्य करने की सुविधा उपलब्ध है।

प्रयोगशाला के सभी साइनबोर्ड, नाम - पट्टों तथा रबर की मोहरों को द्विभाषी बनाया गया है।

प्रशिक्षण कार्यक्रमों में मिली - जुली भाषा का उपयोग किया जाता है।

प्रयोगशाला के निदेशक एवं वरिष्ठ हिन्दी अधिकारी नगर राजभाषा कार्यान्वयन समिति की बैठकों में नियमित रूप से भाग लेते है।

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।

प्रयोगशाला के पुस्तकालय हेतु प्रतिवर्ष हिन्दी पुस्तकें खरीदी जाती हैं।

प्रयोगशाला में प्रतिवर्ष हिन्दी सप्ताह का भव्य आयोजन किया जाता है। इस अवसर पर स्टाफ के लिए विभिन्न हिन्दी प्रतियोगिताओं तथा सांस्कृतिक कार्यक्रमों का आयोजन किया जाता हैं। हिन्दी सप्ताह के आरंभ में हिन्दी दिवस के अवसर पर प्रतिवर्ष प्रयोगशाला की वार्षिक गृहपत्रिका का विमोचन किया जाता है।

प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानों एवं संगोष्ठियों की रिपोर्ट हिन्दी एवं अँग्रेजी दोनों भाषाओं में सीएसआईआर - समाचार में प्रकाशनार्थ राष्ट्रीय विज्ञान संचार एवं सूचना स्त्रोत संस्थान (निसकेयर), नई दिल्ली को नियमित रूप से भेजी जाती है।

सीएसआईआर मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यो 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।

इसके अतिरिक्त प्रयोगशाला में आयोजित होने वाले विभिन्न वैज्ञानिक कार्यक्रमों तथा अन्य समारोंहों का संचालन भी हिन्दी माध्यम से किया जाता है।

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 प्रस्तुत करते हैं।

भारतीय राजभाषा विकास संस्थान, देहरादून व्दारा वर्ष 2012 में शिमला में आयोजित राजभाषा सम्मेलन में प्रयोगशाला के वरिष्ठ वैज्ञानिक डॉ. डी. सी. अग्रवाल ने भाग लेकर अपना शोध पत्र प्रस्तुत किया। इस अवसर पर उन्हें स्मृति चिन्ह एवं प्रमाणपत्र देकर सम्मानित किया गया।

प्रयोगशाला से जारी होने वाली सभी निविदा सूचनाएँ तथा विज्ञापन इत्यादी द्विभाषी रूप में प्रकाशित किए जाते हैं।

विज्ञान शिक्षा के प्रति रूचि 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 है।

प्रयोगशाला के स्टाफ को हिन्दी में कार्य करने हेतु प्रोत्साहित करने की दृष्टी से यहाँ विभिन्न राजभाषा प्रोत्साहन योजनाएँ लागू 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।

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।

राजभाषा रिपोर्ट

हिन्दी सप्ताह समारोह का आयोजन

भारत सरकार की राजभाषा नीति का राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में कड़ाई से कार्यान्वयन/अनुपालन किया जाता है। इसी संवैधानिक प्रावधान के अधीन प्रयोगशाला में प्रतिवर्ष सितम्बर मास में हिन्दी सप्ताह समारोह का आयोजन किया जाता है। इस उपलक्ष्य में स्टाफ हेतु विभिन्न हिन्दी प्रतियोगिताएँ आयोजित की जाती हैं और प्रयोगशाला की वार्षिक राजभाषा पत्रिका एनसीएल आलोक का लोकार्पण भी किया जाता है। इस वर्ष सीएसआईआर - एनसीएल में 14 से 21 सितम्बर, 2012 की अवधि में हिन्दी सप्ताह समारोह का आयोजन किया गया। इस अवधि में प्रयोगशाला स्टाफ के लिए विभिन्न प्रतियोगिताएँ आयोजित की गईं जिनमें बड़ी संख्या में वैज्ञानिकों/अधिकारियों/कर्मचारियों ने भाग लिया।

14 सितम्बर, 2012 को हिन्दी दिवस के अवसर पर प्रयोगशाला की वार्षिक राजभाषा पत्रिका एन.सी.एल. आलोक का लोकार्पण किया गया। इस अवसर पर मुख्य अतिथि के रूप में समारोह में उपस्थित उच्च ऊर्जा पदार्थ अनुसंधान प्रयोगशाला, पुणे के वरिष्ठ वैज्ञानिक एवं उप निदेशक, डॉ. राजकिशोर पाण्डेय ने सीएसआईआर-एनसीएल जैसी वैज्ञानिक अनुसंधान प्रयोगशाला व्दारा राजभाषा पत्रिका के प्रकाशन पर प्रसन्नता व्यक्त की और कहा कि हिन्दी के माध्यम से हम वैज्ञानिक अनुसंधानों को देश की जनता तक पहुँचा सकते हैं। डॉ. पाण्डेय ने कहा कि इस पत्रिका में सामान्य लेखों के साथ - साथ कुछ ऐसे महत्वपूर्ण तकनीकी लेखों को भी प्रकाशित किया गया है जिनकी सामाजिक उपयोगिता बहुत अधिक है। उन्होंने सरकारी कामकाज में राजभाषा हिन्दी के प्रयोग को अति आवश्यक बताया।

इस समारोह में अध्यक्ष के रूप में उपस्थित प्रयोगशाला के वरिष्ठ प्रधान वैज्ञानिक, डॉ. दिनेशचन्द्र अग्रवाल ने अपने सम्बोधन में हिन्दी की अपरिहार्यता को स्पष्ट किया और कहा कि हिन्दी अब तो केवल भारत की ही नहीं, बल्कि एक विश्व भाषा बन गई है। उन्होंने कई उदाहरणों व्दारा हिन्दी की राष्ट्रीय एवं अन्तर्राष्ट्रीय महत्ता को स्पष्ट किया। डॉ. अग्रवाल ने कहा कि आज समूचा विश्व एक वैश्विक गाँव (ग्लोबल विलेज) बन गया है जिससे विश्व के सभी देशों के बीच व्यापार एवं संस्कृति का आदान - प्रदान होने लगा है। इस कारण हिन्दी अपनी राष्ट्रीय सीमाएं लाँघकर अन्तर्राष्ट्रीय स्तर पर जा पहुँची है। इससे हिन्दी के प्रयोग के क्षेत्र की विशालता और व्यापकता सिध्द होती है।

हिन्दी सप्ताह के दौरान दि. 17 सितम्बर को प्रयोगशाला के स्टाफ हेतु हिन्दी निबन्ध प्रतियोगिता का आयोजन किया गया। इस प्रतियोगिता में कई कर्मचारियों ने भाग लिया। दि. 18 सितम्बर को पूर्वाह में हिन्दी सामान्य ज्ञान प्रतियोगिता तथा उसी दिन अपराह में हिन्दी शुध्दलेखन प्रतियोगिता का आयोजन किया गया। इन प्रतियोगिताओं में भी स्टाफ के सदस्यों ने बढ़चढ़ कर भाग लिया।

हिन्दी सप्ताह का समापन समारोह दि. 21 सितम्बर, 2012 को अपराह 3 बजे प्रयोगशाला में सम्पन्न हुआ जिसकी अध्यक्षता प्रयोगशाला के वरिष्ठ वैज्ञानिक डॉ. ए. जे. वर्मा ने की। इस समापन समारोह में पुणे स्थित राष्ट्रीय विषाणुविज्ञान संस्थान के उप निदेशक डॉ. देवेन्द्र मौर्य मुख्य अतिथि के रूप में उपस्थित थे। डॉ. मौर्य ने इस अवसर पर प्रयोगशाला के लगभग 25 कर्मचारियों को विभिन्न प्रतियोगिताओं में प्रथम, द्वितीय और तृतीय स्थान प्राप्त करने के लिए पुरस्कार प्रदान किए। इसके अलावा में अपना समस्त सरकारी कामकाज हिन्दी में करने वाले कर्मचारियों को भी नकद प्रोत्साहन पुरस्कार प्रदान किए गए।

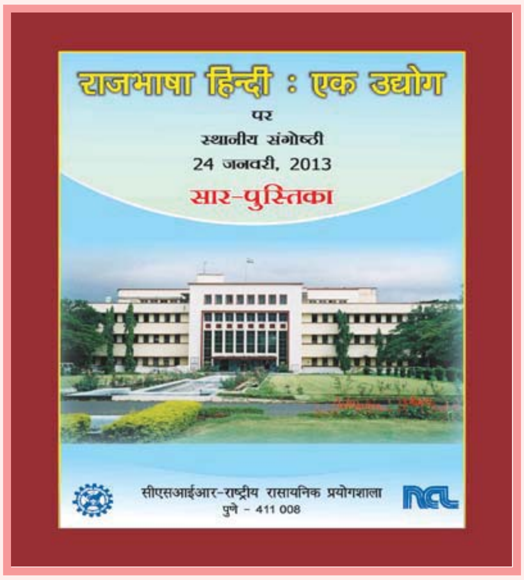
डॉ. मौर्य ने इस अवसर पर कहा कि हम अधिकाँशत: अँग्रेजी में ही बात करना पसंद करते हैं। ऐसा केवल मानसिकता के कारण ही है। हमें अपनी मानसिकता में बदलाव लाना होगा तभी हम अपने राष्ट्र और राजभाषा के प्रति सकारात्मक सोच और प्रेम पैदा कर सकते हैं। डॉ. मौर्य ने कहा कि हमारी राजभाषा ही हमारे विकास का प्रतीक है। विदेशी भाषा को अपनाकर हम आगे नहीं बढ़ सकते। चीन, जापान, फ्रान्स, जर्मनी जैसे देशों ने अपनी ही भाषा को अपनाकर अपना विकास किया और विश्व में अपना एक अलग स्थान बनाया है। उन्होंने कर्मचारियों को आह्वान किया की वे राजभाषा के माध्यम से राष्ट्र के उन्नयन में अपना बहुमूल्य योगदान दें।

समारोह के अध्यक्ष डॉ. ए. जे. वर्मा ने इस अवसर पर अपने अध्यक्षीय भाषण में कहा कि हिन्दी हमारे देश की पहचान है। विश्व में भारत की पहचान हिन्दी के द्वारा ही होती है। हिन्दी का एक अति सुदृढ सांस्कृतिक एवं समाजिक आधार है। इस कारण ही इसे भारतीय संविधान में राजभाषा के रूप में प्रतिष्ठित किया गया है।

राजभाषा रिपोर्ट

एकदिवसीय हिन्दी संगोष्ठी का आयोजन

सीएसआईआर - एन.सी.एल., पुणे में राजभाषा के सुचारू रूप से कार्यान्वयन हेतु अनेक स्तरों पर प्रयास किए जा रहे हैं। इसके अन्तर्गत समय - समय पर हिन्दी संगोष्ठीयों एवं कार्यशालाओं का भी आयोजन किया जाता है। इसी क्रम में गुरूवार, दिनांक 24 जनवरी, 2013 को राजभाषा हिन्दी : एक उद्योग नामक विषय पर **एकदिवसीय स्थानीय संगोष्ठी** का आयोजन किया गया।



राजभाषा हिन्दी : एक उद्योग

पर

स्थानीय संगोष्ठी

24 जनवरी, 2013

सार-पुस्तिका

सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला

पुणे - 411 008

इस अवसर पर हिन्दी विद्वान एवं सुप्रसिध्द लेखक, डॉ. दामोदर खडसे मुख्य अतिथि के रूप में उपस्थित थे। उन्होंने उक्त संगोष्ठी के आयोजन पर प्रसन्नता व्यक्त करते हुए प्रयोगशाला में राजभाषा के उन्नयन एवं विकास हेतु किए जा रहे प्रयासों की सराहना की। अपने विचार व्यक्त करते हुए डॉ. खड़से ने कहा कि आज हिन्दी केवल सरकारी कार्यालयों में राजभाषा के रूप में ही प्रयोग में नहीं लायी जा रही है, बल्कि हिन्दी को उद्योग जगत में व्यवसाय को बढ़ावा देने हेतु भी विशाल स्तर पर प्रयोग में लाया जा रहा है। अपनी विदेश यात्रा का संस्मरण सुनाते हुए डॉ. खड़से ने बताया कि जब भी वे विदेश यात्रा पर गए, वहाँ उन्हें हिन्दी ने ही अन्य भारतीयों से जोड़ने का महत्वपूर्ण कार्य किया है। इस प्रकार हिन्दी ने अन्तर्राष्ट्रीय स्तर पर भी अपनी पहचान बनाई है। प्रयोगशाला के वरिष्ठ वैज्ञानिक एवं भौतिक रसायन प्रभाग के प्रमुख, डॉ. अनिल कुमार ने अपने अध्यक्षीय सम्बोधन में कहा कि यह हमारे लिए गौरव की बात है कि हमारी राजभाषा राष्ट्रीय और अन्तर्राष्ट्रीय स्तर पर उद्योग जगत में प्रयोग में लायी जा रही है। हिन्दी आम आदमी की भाषा है और बड़े - बड़े उद्योग अपने उत्पादों को सामान्य जनता तक पहुँचाने के लिए इसी जनभाषा का प्रयोग करते हैं। इसीलिए देश के कोने - कोने में हिन्दी को व्यवसाय के हर क्षेत्र में प्रयोग में लाया जा रहा है और हिन्दी के कारण कई लोगों को रोजगार भी मिले हैं। उन्होंने आगे कहा कि आज भाषा केवल बोलचाल की वस्तु न होकर अर्थार्जन का बहुत बड़ा साधन बन चुकी है।

इस संगोष्ठी में विशेष अतिथि के रूप में उपस्थित पूर्व उप. निदेशक/निदेशक (भाषाएँ), भारत सरकार, शिक्षा विभाग एवं भाषा विशेषज्ञ, डॉ. किशोर वासवानी ने उपस्थित श्रोताओं को सम्बोधित करते हुए कहा कि आज हिन्दी शिक्षा, उद्योग, मीडिया, सिनेजगत सहित कई क्षेत्रों में सफलता के साथ प्रयोग में लायी जा रही है। इसमें शिक्षित एवं अशिक्षित सभी प्रकार के लोग शामिल हैं। अर्थात हर प्रकार के लोगों की आवश्यकताओं के अनुरूप राजभाषा हिन्दी को प्रयोग में लाया जा रहा है। उन्होंने आगे कहा कि साहित्य एवं सिनेमा के माध्यम से हमें अन्य भाषी समाज एवं उसके साहित्य का परिचय हिन्दी ने ही कराया है। हिन्दी एक सशक्त भाषा है। सदियों से, भारत जैसे बहुभाषी देश की सबसे बड़ी सम्पर्क - भाषा होने के साथ - साथ आज यह विश्व की तीन सबसे बड़ी भाषाओं (चीनी (मंदारीन), हिन्दी और अँग्रेजी) में से एक है। 14 वीं सदी से ही हिन्दी सामाजिक, सांस्कृतिक, धार्मिक और व्यापार विनिमय के क्षेत्रों में, बिना सरकारी आश्रय के एक असरकारी भूमिका निभाती आयी है। डॉ. वासवानी ने आगे कहा कि आज हिन्दी ताकतवर उद्योग का रूप ले चुकी है और अरबों रूपयों का राजस्व कमाकर सरकार को देकर एक कमाऊ सुपुत्री की भुमिका निभा रही है।

इस एकदिवसीय संगोष्ठी में सीएसआईआर एनसीएल एवं पुणे स्थित केन्द्रीय सरकारी कार्यालयों के अधिकारियों ने भाग लिया और राजभाषा हिन्दी : एक उद्योग के सन्दर्भ में अपने - अपने विचार व्यक्त किए। सभी ने मानवजीवन के विभिन्न पहलुओं से हिन्दी को जोड़ते हुए हिन्दी के प्रयोग, उसकी उपयोगिता एवं उसकी मौलिकता पर प्रकाश डाला।

CSIR-National Chemical Laboratory

Council of Scientific and Industrial Research
National Chemical Laboratory

1990- 1999 : Set- up of Catalyst pilot plant.

About CSIR- NCL

CSIR-National Chemical Laboratory, Pune is a research, development and consulting organisation with a focus on chemistry and chemical engineering. **Dr. Sourav Pal**, is the current Director of NCL, Pune.

The purpose of this laboratory is to advance knowledge and to apply chemical science to the good of the people.

Research

Nurturing Chemical Science and Technology

Academic Programme

A journey to the Advancement of Science and Technology

News and Events

13/01/14 Felicitation of Prof C. N. R. ...
13/01/14 Dr. Sourav Pal and Dr. C.V. Ra...
06/01/14 NCL honours scientists on foun...

Partnership with Industry

Your Partner from Concept to Market

Join Us

Open to the Innovative and New Minds

Featured R&D

Hydrogel as enhancer for Zinc Oxide

Quick Links

- RTI
- Library
- Jobs Vacancies
- Tenders
- NCIM
- Guest House

External Links

- Academic Website
- PhD. Admission
- AcSIR
- CSIR Website
- NCL Innovations
- One CSIR

Announcements

- new announcement
- Symposium on "Wonderla...
- International Symposiu...
- CSIR Diamond Jubilee R...
- PhD. Admission Open

Read More >>

Contact

CSIR- National Chemical Laboratory (NCL)
Dr. Homi Bhabha Road, Pune- 411008,
India. Tel. :+91-20-2590 2000, 25893400;
Fax :+91-20-2590 2660.

© Copyright **National Chemical Laboratory (NCL)** . Pune, Maharashtra - 411008, INDIA.

Disclaimers | **Privacy Policy**

www.ncl-india.org

CSIR-National Chemical Laboratory

(Council of Scientific & Industrial Research)

Dr. Homi Bhabha Road, Pune 411 008 (INDIA).
Tel. : +91-20-2590 2600

| www.ncl-india.org |