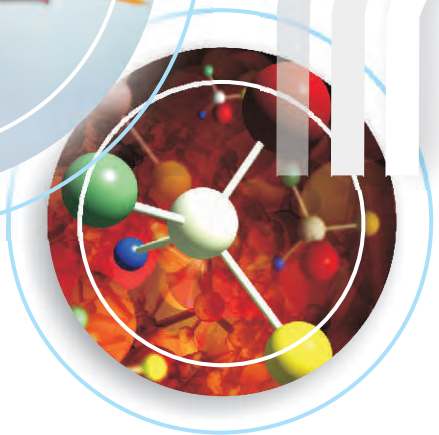




**राष्ट्रीय रासायनिक प्रयोगशाला**  
**National Chemical Laboratory**  
वार्षिक प्रतिवेदन 2008-09



ANNUAL REPORT 2008-09

# NCL

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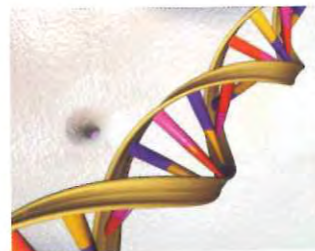
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राष्ट्रीय रासायनिक प्रयोगशाला  
National Chemical Laboratory  
वार्षिक प्रतिवेदन 2008-09



PERFORMANCE



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मुझे राष्ट्रीय रासायनिक प्रयोगशाला, पुणे का वर्ष 2008-09 का वार्षिक प्रतिवेदन प्रस्तुत करते हुए अतीव प्रसन्नता हो रही है ।

नई सहस्राब्दि के प्रथम दशक के अन्तिम समय में प्रवेश करते हुए एनसीएल ने नए उत्साह के साथ आगे की यात्रा जारी रखी है । एनसीएल का विज्ञान का आधार लगातार विस्तृत हो रहा है जिसमें भविष्य की विशाल संभावनाएँ समाहित हैं। इनके अन्तर्गत आन्तर्विधा विज्ञान से समाज में धनार्जन का मार्ग प्रशस्त होगा। इस दिशा में हमने अनेक नए कार्यक्रमों की शुरुआत की है जिससे भविष्य में हमारे विज्ञान, प्रौद्योगिकी और नवोन्मेष का आधार सुदृढ़ होगा । बौद्धिक सम्पदा के कार्यक्षेत्र को व्यापक बनाया गया है जिससे कि प्रारंभिक चरण की वैज्ञानिक खोजों से बौद्धिक सम्पदा अर्जित की जा सके । पेटेण्ट कराने की दृष्टि से अनवरत संवर्धित नवोन्मेषों को कम महत्त्व दिया जा रहा है । प्रारंभिक चरण की खोजों पर आधारित नए केन्द्रों को स्थापित करने की संभावनाओं पर ध्यान केन्द्रित किया जा रहा है ताकि लोगों को जागरूक और शिक्षित बना कर पारिस्थितिकी को अनुकूल बनाया जा सके और इस प्रकार मानसिकता में बदलाव लाया जा सके । अन्ततः वैज्ञानिकों को ही धनार्जन के अवसर सृजित करने होंगे, फिर चाहे उसके लिए उनका व्यावसायिक दृष्टिकोण हो या फिर परोपकारी दृष्टिकोण ।

एनसीएल में वैज्ञानिक अनुसंधान सम्बन्धी कार्यकलापों के निष्पादन की प्रगति का क्रम जारी है । एनसीएल ने वर्ष के दौरान उत्कृष्ट श्रेणी के 421 शोधपत्र प्रकाशित किए जिनका औसत इम्पैक्ट फैक्टर 2.42 था । एनसीएल में शोधकार्य में संलग्न 80 से अधिक छात्रों को पीएच.डी. डिग्री प्रदान की गई । एनसीएल में उत्प्रेरण, पदार्थ विज्ञान, बहुलक विज्ञान, कम्प्युटेशनल रसायन विज्ञान तथा पृष्ठ विज्ञान जैसे विविध कार्यक्षेत्रों में चार नए वैज्ञानिकों ने कार्यभार ग्रहण किया ।

वर्ष के अन्त तक एनसीएल ने रु. 21.05 करोड़ की बाहरी आय का अर्जन किया जिसमें उद्योग जगत् का योगदान रु. 13.1 करोड़ का था । इसमें भारतीय उद्योग से रु. 9.70 करोड़ और वैश्विक उद्योग से 3.40 करोड़ की धनराशि शामिल है । वैश्विक उद्योग से हुई आय की कमी के दो कारण हैं। पहला यह कि विश्व अर्थव्यवस्था में मंदी के कारण अनेक बहुराष्ट्रीय कम्पनियों के अनुसंधान एवं विकास सम्बन्धी बजट में कटौती हो गई जिसके फलस्वरूप उनका निवेश एनसीएल में नहीं हो सका ।

दूसरा और अधिक महत्त्वपूर्ण कारण यह है कि एनसीएल ने वैश्विक कम्पनियों के साथ संविदा अनुसंधान के अन्तर्गत दी जाने वाली सेवाओं से प्राप्त शुल्क के स्थान पर अब सार्वजनिक-निजी भागीदारी मॉडल के अन्तर्गत अनुसंधान लाइसेंस शुल्क और रॉयल्टी के द्वारा धनार्जन करने का निर्णय लिया है । इस नीतिगत परिवर्तन के कारण अल्पावधि में धनार्जन में कमी होना स्वाभाविक है । तथापि मुझे विश्वास है कि भविष्य में इस नए उपाय से शुद्ध संविदा अनुसंधान से प्राप्त आय में हुई कमी की पूर्ति भली प्रकार की जा सकेगी । यह तथ्य सन्तोषजनक है कि वर्ष 2008-09 में रॉयल्टी और प्रीमियम से प्राप्त आय रु. 2.25 करोड़ थी जब कि वर्ष 2007-08 में यह रु.1.6 करोड़ थी । यह बढ़ोतरी जो कि हमारी बाहरी आय का लगभग दस प्रतिशत है, विज्ञान और प्रौद्योगिकी के माध्यम से धनार्जन करने की दिशा में एनसीएल के नए प्रयासों को सिद्ध करती है ।

हमारी अनेक प्रक्रियाओं ने व्यावसायिक क्षेत्र में अच्छी प्रगति की है । रयोंग, थाईलैण्ड में स्थापित 3000 टन प्रति वर्ष की क्षमता का एपिक्लोरोहाइड्रिन संयंत्र वर्ष के दौरान बढ़ी हुई अवधि में भी लगातार संचालित रहा । इससे संयंत्र के संचालन के बारे में गहरी समझ उत्पन्न हुई और उत्प्रेरक की जीवनावधि के बारे में भी कुछ मुद्दे सामने आए । इनके स्वीकार्य समाधान हेतु एनसीएल तथा आदित्य बिड़ला ग्रुप ने संयुक्त रूप से इन मुद्दों का निपटारा किया । एनसीएल ने गोदावरी शुगर मिल्स लिमिटेड, समीरवाडी, कर्नाटक में खोई हेतु बनाए गए वाष्प विस्फोट प्रदर्शन संयंत्र को सफल संचालन के बाद सम्बन्धित प्रौद्योगिकी सहित गोदावरी शुगर मिल्स लिमिटेड को हस्तान्तरित किया । जैवभार से धनार्जन करने के लिए लिग्नो-सेलुलोलिसिक जैवभार पर पूर्व अभिक्रिया मुख्य चरण है । सीएसआईआर के नमिटीली कार्यक्रम के अन्तर्गत प्रौद्योगिकी का हस्तान्तरण एक महत्त्वपूर्ण सफलता थी क्योंकि इससे इस परियोजना में सीएसआईआर द्वारा निवेश किया गया पूरा धन प्रौद्योगिकी हस्तान्तरण के द्वारा वसूल हो गया और साथ ही इस उत्पाद के व्यावसायिक विक्रय से एनसीएल को दीर्घावधि तक रॉयल्टी का भुगतान भी प्राप्त होगा ।

एनसीएल द्वारा 300 टन प्रति वर्ष की क्षमता का प्रदर्शन संयंत्र स्थापित करने के लिए निर्जलीय L(+)- लैक्टिक अम्ल के अनवरत उत्पादन की प्रौद्योगिकी गोदावरी शुगर मिल्स लिमिटेड को हस्तान्तरित की गई । इस सम्बन्ध में विस्तृत अभियांत्रिकी गतिविधियाँ शुरु की गईं और अधिक आन्तर्विधा कार्यकलापों को गति प्रदान करने के लिए एनसीएल ने दो श्रेष्ठता केन्द्र स्थापित किए । पहला केन्द्र वैज्ञानिक अभिकलन से सम्बन्धित था जिसके अन्तर्गत अधिक समन्वयन और सहयोग हेतु विभिन्न सिद्धान्त और कम्प्युटेशनल विज्ञान की क्षमताओं को समाहित किया गया । दूसरा केन्द्र सूक्ष्मरिएक्टर प्रौद्योगिकी से सम्बन्धित था । इसके अन्तर्गत रासायनिक अभियांत्रिकी और कार्बनिक प्रक्रिया रसायन विज्ञान के वैज्ञानिकों को सूक्ष्म रासायनिक प्रक्रियाओं और यूनिट संचालन में सूक्ष्मरिएक्टरों की शक्ति और क्षमता का पता लगाने हेतु एक साथ मिल कर कार्य करने के उद्देश्य से एक मंच पर लाया गया । एनसीएल में हो रहे सूक्ष्मरिएक्टर अनुसंधान कार्य ने रासायनिक उद्योग का भी ध्यान आकर्षित किया है । उनकी सहभागिता को सुविधाजनक बनाने के लिए शुल्क के आधार पर पाँच भागीदारों का एक औद्योगिक संघ बनाया गया



है जो समय-समय पर बैठक करके प्रौद्योगिकी के कार्यान्वयन हेतु परिणामों पर विचार-विमर्श करता है और संभावित अवसरों की सूचना का परस्पर आदान-प्रदान करता है।

हमारे अनेक सहयोगियों ने अपनी-अपनी उपलब्धियों से एनसीएल को गौरवान्वित किया है। डॉ. अनिल कुमार को भारतीय राष्ट्रीय विज्ञान अकादमी, नई दिल्ली का सदस्य बनाया गया। डॉ. बर्वे को नवोन्मेषी रासायनिक प्रक्रिया प्रौद्योगिकी के विकास की दिशा में महत्वपूर्ण योगदान के लिए रसायन विज्ञान एवं प्रौद्योगिकी के क्षेत्र में वासविक पुरस्कार प्रदान किया गया। भारतीय रासायनिक अनुसंधान सोसायटी ने डॉ. सौरव पाल को रजत पदक और डॉ. गोपीनाथ को कांस्य पदक प्रदान किए। डॉ. पंकज पोद्दार को सीएसआईआर का युवा वैज्ञानिक पुरस्कार प्राप्त हुआ तथा डॉ. राजेश गोत्राडे और डॉ. अमोल कुलकर्णी को भारतीय राष्ट्रीय विज्ञान अकादमी के प्रतिष्ठित युवा वैज्ञानिक पुरस्कार प्राप्त हुए।

एनसीएल ने अपनी भौतिक संरचना के निर्माण पर कार्य जारी रखा है। एक अत्याधुनिक बहुलक एवं प्रगत पदार्थ भवन के निर्माण का कार्य पूरा होने के करीब है। इससे एनसीएल में आधुनिक प्रयोगशाला की जगह 80 हजार वर्ग फीट के लगभग बढ़ जाएगी। इसके अलावा सभी विधाओं के वैज्ञानिकों के प्रयोग हेतु 2200 वर्ग फीट क्षेत्रफल की एक आणविक जीवविज्ञान प्रयोगशाला का निर्माण किया गया है। एनसीएल प्रवर्तन पार्क में वर्तमान इमारतों में ही एक 4500 वर्ग फीट की मॉडुलर प्रयोगशाला का निर्माण किया गया है। इस प्रयोगशाला में वेन्चर सेण्टर नामक प्रौद्योगिकी व्यवसाय इनक्यूबेटर स्थित है जिसे एनसीएल ने धारा 25 के अन्तर्गत कम्पनी के रूप में स्थापित किया है।

एनसीएल ने अपने रासायनिक और घरेलू कूड़े-कचरे का जिम्मेदार ढंग से निपटान करने हेतु अनेक कदम उठाए हैं। एनसीएल ने अपने परिसर में ही सूखे और गीले कूड़े-कचरे को व्यवस्थित करने की एक योजना बनाई है। इसके अन्तर्गत कॉलोनी के प्रत्येक क्वार्टर से सूखा और गीला कूड़ा अलग-अलग एकत्रित करके एक केन्द्रीय स्थान पर ले जाया जाता है जहाँ पर गीले कूड़े से कम्पोस्ट खाद बनाई जाती है जिसका उपयोग एनसीएल उद्यान और कॉलोनी के घरों में किया जाता है। सूखे कूड़े का पुनर्चक्रण किया जाता है। इस प्रकार एनसीएल परिसर घरेलू कूड़े के निपटान में आत्मनिर्भर हो गया है। एनसीएल शीघ्र ही एक कार्य योजना लागू करेगी जिसके अन्तर्गत सभी प्रकार के रासायनिक कचरे को एकत्रित करके पुणे शहर के बाहर स्थित केन्द्रीय प्रदूषण नियंत्रण बोर्ड द्वारा स्थापित एवं अनुमोदित खतरनाक कचरा निपटान संयंत्र को भेजा जाएगा। मलजल एवं प्रयोगशाला जल के शुद्धीकरण हेतु एक संयंत्र स्थापित करने की योजना है। इसके द्वारा गन्दे जल को एनसीएल के अन्दर ही शुद्ध किया जाएगा। इन कार्यक्रमों के साथ एनसीएल, पुणे शहर की एक जिम्मेदार संस्था और पड़ोसी बनने के पथ पर अग्रसर है।

एनसीएल जनवरी, 2009 से शुरू हो रहे अपनी हीरक जयन्ती वर्ष में प्रवेश कर रही है। भारत के प्रथम प्रधानमंत्री पण्डित जवाहरलाल नेहरू ने राष्ट्रीय रासायनिक प्रयोगशाला को 3 जनवरी, 1950 के दिन

औपचारिक रूप से राष्ट्र को समर्पित किया था। एनसीएल के इतिहास में इस महत्वपूर्ण अवसर की स्मृति में वर्ष 2009-10 के दौरान अनेक कार्यक्रमों की योजना बनाई गई है। भूतकाल यदि हमारी विरासत है तो भविष्य हमारा भाग्य है। एनसीएल का भावी लक्ष्य एक ऐसा संगठन बनना है जो सर्वोत्तम वैश्विक मानकों का प्रयोग करते हुए बौद्धिक अवरोधों को पार कर सके, राष्ट्र की आवश्यकताओं को पूरा कर सके, औद्योगिक प्रतिस्पर्धा के लिए कुछ नवोन्मेष कर सके, वैश्विक ज्ञानजन्य अर्थव्यवस्था में पूरी तरह भागीदार बन सके तथा राष्ट्र की कमियों का निराकरण कर सके। अपनी स्थापना के बाद से प्रत्येक दशक की समाप्ति पर एनसीएल को नई दिशा तलाशने और एक पृथक् भविष्य का लक्ष्य रखने के लिए चुनौती मिलती रही है। साठ वर्ष की आयु प्राप्त कर लेने तथा नई सहस्राब्दि का प्रथम दशक पूरा कर लेने पर एनसीएल को पूरी आशा और विश्वास है कि वह ज्ञानार्जन, ज्ञान के हस्तान्तरण और उसको प्रयोग में लाकर भविष्य में एक सर्वोत्तम और श्रेष्ठ संस्था के रूप में भारत के लिए प्रासंगिक एवं उपयोगी बनी रहेगी।

मैं अपने वैज्ञानिकों तथा अन्य सभी सहयोगी स्टाफ के प्रत्येक सदस्य द्वारा दिए गए योगदानों के प्रति अपना आभार प्रकट करता हूँ। इन सभी ने मिल कर इस प्रयोगशाला को एक ऐसे सुखद और उत्पादक स्थान के रूप में विकसित किया है जहाँ हम सभी प्रसन्नतापूर्वक कार्य कर सकते हैं। मुझे अपनी जिम्मेदारियों के निर्वहन में प्रयोगशाला की अनुसंधान परिषद और प्रबन्ध परिषद से भी बहुत अच्छा सहयोग मिला है जिसके लिए मैं उनको धन्यवाद देता हूँ। मैं वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद (सीएसआईआर) मुख्यालय के स्टाफ और महानिदेशक महोदय को भी उनके द्वारा एनसीएल को दिए गए सम्पूर्ण और अबाधित सहयोग के लिए धन्यवाद देता हूँ।

एस. शिवराम

एस. शिवराम

### From the Director's Desk



It gives me great pleasure to present the Annual Report for the National Chemical Laboratory, Pune for the year 2008-09.

NCL continues to march ahead with new zeal as we enter the end of the first decade of the new millennium. NCL's science base continues to expand with a grand vision of the future, wherein, interdisciplinary science will create wealth in society. To this end we have set in motion several new initiatives which will strengthen our science, technology and innovation base for the future. The intellectual property function has been strengthened with a focus on creating IP from early stage science discoveries. Incremental innovations are being given less importance from the point of view of patenting. New venture creation possibilities based on early stage discoveries is being brought into center focus with a view to sensitize, educate, create enabling eco systems and lead to transformation of mind sets. In the end it is the scientist who will create new opportunities for wealth creation, driven either by commercial or altruistic motives.

Science performance indicators continue to be healthy. NCL published 421 peer reviewed papers during the year with an average impact factor of 2.42. More than eighty PhD degrees were awarded to students working in NCL. Four new scientists were inducted into NCL in diverse areas such as catalysis, materials, polymer science, computational chemistry and surface science.

NCL closed the year with an External Cash Flow (ECF) of Rs 21.05 Crore (Rs 210 million) with an industry contribution of Rs 13.1 Crore (Rs 131 million). Indian industry contributed Rs 9.70 crore (Rs 97 million) whereas global industry pitched in with 3.40 Crore (Rs 34 million). The drop in revenues from global industry was on account of two reasons. One, the depression in world economy resulted in a cut in R&D budgets of many global multinationals and their consequent investment

in NCL. Second, and more importantly, NCL has progressively shifted its core revenue generation philosophy from pure "fee for service" contract research with global companies to a more desirable and sustainable public-private partnership model with balanced receipts from research, licensing fee and royalty. As we switch tracks there is likely to be an impact on revenue generation in the short term. However, I am confident that in the years to come, new revenue streams will more than make up for the loss of income from pure contract research. It was gratifying to note that the income accruing from royalty and premium was 2.25 Crore in 2008-09 (Rs 22.5 million) compared to 1.6 Crore (Rs 16 million) in 2007-08. This increase, which is about ten percent of our ECF, signifies NCL renewed focus on creating value through science and technology.

Many of our processes continue to make good progress towards eventual commercialization. The 3000 TPA Epichlorohydrin plant at Ryong, Thailand operated continuously for extended periods of time during the year. This led to a deeper understanding of the operability of the plant and brought to fore certain issues regarding catalyst life times. NCL and Aditya Birla group jointly tackled these issues with a view to find acceptable solutions. The Steam Explosion Demonstration Plant for Bagasse at Godavari Sugar Mills Limited (GSML), Sameerwadi, Karnataka, designed by NCL after satisfactory runs was transferred along with the relevant technology to GSML. Pretreatment of lingo-cellulosic biomass is a key step in creating value out of biomass. The transfer of technology was a significant milestone in the NMITLI programme of CSIR in the sense that the entire direct investment made by CSIR in the project was recovered by the transfer of technology with a long term royalty payment to NCL upon commercial sale of the product. The technology for the continuous downstream recovery process for anhydrous L (+) - Lactic Acid was (1 kg/h) was transferred to GSML for setting up a 300 ton per annum demonstration plant. Detailed engineering activities were initiated.

To foster more interdisciplinary interactions, NCL created two Centers of Excellence (CoE). One was for Scientific Computing which brought together under one umbrella the diverse competencies of Theory and Computational Science, for greater synergy and collaboration. The other was for the area of Microreactor Technology which brought together scientists in Chemical Engineering and Organic Process Chemistry to work together to exploit the power of microreactors in fine chemical processes and unit operations. The microreactor research area at NCL also attracted chemical



industry. To facilitate their participation a subscription based industrial consortium consisting of five partners was created which met periodically to discuss results and share potential opportunities for technology deployment.

Several of our colleagues continue to do NCL proud. Dr Anil Kumar was elected to the Fellowship of the Indian National Academy of Science, New Delhi. Dr Barve won the Vasvik Award in Chemical Sciences and Technology for his significant contributions to the development of innovative chemical process technologies. Dr Sourav Pal was conferred the Silver Medal and Dr Gopinath the Bronze Medal by the Chemical Research Society of India. Dr Pankaj Poddar won the CSIR Young Scientist Award, whereas, Dr Rajesh Gonnade and Dr Amol Kulkarni won the coveted INSA Young scientist awards.

NCL continues to pay attention to the creation of physical infrastructure. A state-of-the-art Polymers and Advanced Materials Building is nearing completion. This will add close to 80,000 sq feet of modern lab space to NCL. In addition a 2200 sq feet Molecular Biology Laboratory was created for the use of scientists cutting across disciplines. A 4500 sq ft modular lab was created out of existing buildings in the NCL Innovation Park to house the technology Business Incubator, namely, Venture Center, a Section 25 Company promoted by NCL.

NCL has taken several initiatives to ensure that it handles its chemical as well as domestic wastes in a responsible manner. NCL commissioned a wet and dry garbage handling facility in its campus. A system was implemented, wherein, segregated dry and wet garbage was collected from the door steps of the colony residents and taken to a central location, where, the wet garbage was composted and recycled to the NCL gardens and households. The dry garbage was sent to a recycling plant. Thus, NCL campus became self sufficient in terms of household waste handling. NCL will shortly implement a system, wherein, all chemical waste will be collected and sent to a hazardous waste handling facility, set up and approved by the Central Pollution Control Board, located in the outskirts of Pune. Plans are afoot to build an effluent treatment plant to handle the sewage and laboratory water and fully recycle the water within NCL. With these initiatives, NCL is well on the way to become a responsible institution and neighbour in the city of Pune

NCL enters its Golden Jubilee year beginning January 2009. NCL was formally dedicated to the Nation by the first Prime Minister of India, Pandit Jawaharlal Nehru on January 3, 1950. Several events have been planned throughout 2009-10 to commemorate this significant milestone in the history of an

institution. While the past is our heritage, the future is our destiny. NCL's future vision is to be an organization that will cross intellectual barriers using the best global benchmarks, serve the national agenda, innovate for industrial competitiveness and participate fully in the global knowledge economy and address the national shortfalls. At the turn of every decade since its inception, NCL has been challenged to charter new course and envision a different future. As we turn sixty and complete the first decade of the new millennium, NCL looks to the future with renewed optimism and commitment, confident that it will continue to stay relevant to India in the years to come by sustaining an institution with enduring values of excellence devoted to acquisition, transmission and application of knowledge.

I wish to gratefully acknowledge the contributions of every one of my staff, scientific as well as supporting, who make this laboratory a pleasant and productive place for all of us to work. I also wish to place on record the wonderful support I have been receiving from the Research and the Management Council of this Laboratory in the discharge of my responsibilities. I also thank DG CSIR and the staff at CSIR Headquarters for their unstinted support to NCL.

**S. Sivaram**





### Vision

# Vision

- ✦ To be a globally recognized and respected R&D organization in the area of chemical sciences and engineering
- ✦ To become an organization that will contribute significantly towards assisting the Indian chemical and related industries in transforming 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



### Mission

# Mission

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

### Guiding Principles & Values

# Guiding Principles & Values

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

Management Council

**DIRECTOR**

Research Council

Secretariat

Scientific Divisions

Heterogeneous Catalysis

Chemical Engg & Process Dev.

Polymer Science & Engineering

Biochemical Sciences

Organic Chemistry

Physical and Materials Chemistry

Plant Tissue Culture

Resource Centres

Catalyst Pilot Plant

Center for Materials Characterization

Central NMR Facility

Digital Information and Knowledge Resource Center

National Collection of Industrial Microorganisms

NCL Innovations

National Repository of Molecules

Intellectual Property Management

Strategic Planning

Research Planning and Audit

Publication and Science Communication

Human Resource Management

Safety Management

Engineering Services

Glass Blowing

Administration

Finance and Accounts

Stores and Purchase

Business Development

Business Development

Contract & Legal Support

Public Relations and Events Management

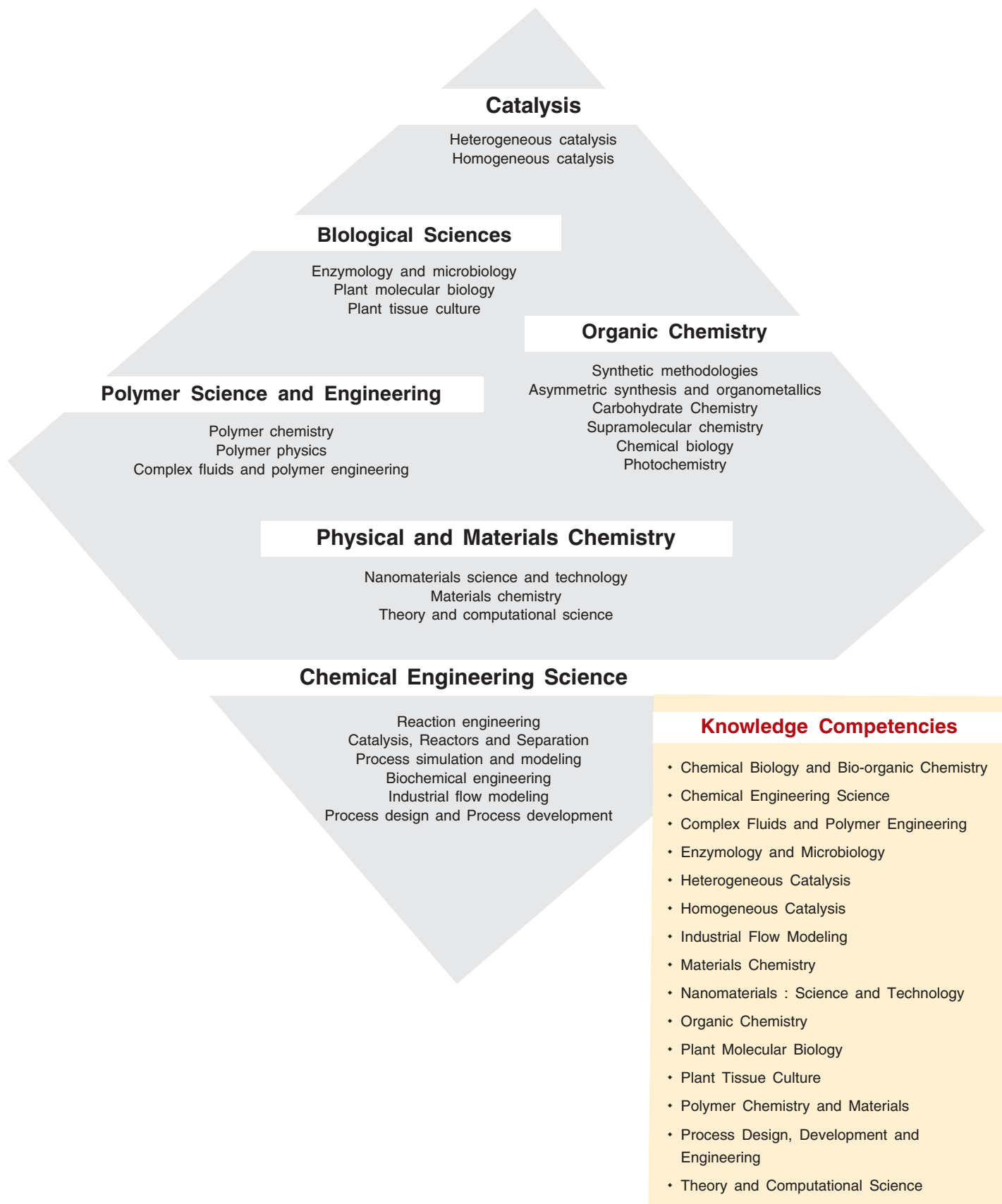
Management Information System

Organization Chart



ORGANIZATION CHART

## Research Areas



## Research Council

**Chairman****Prof. D. Balasubramanian**

Research Director  
L.V. Prasad Eye Institute  
Road No. 2, Banjara Hills  
Hyderabad 500 034.

**Members****Dr. Amit Biswas**

Senior Vice President (R&T)  
Reliance Industries Limited  
Swastik Mill Compound  
V. N. Purav Marg, Chembur  
Mumbai 400 071.

**Prof. S. Chandrasekaran**

Department of Organic Chemistry  
Indian Institute of Science  
Bangalore 560 012.

**Prof. Dipankar Chatterji**

Molecular Biophysics Unit  
Indian Institute of Science,  
Bangalore 560 012.

**Dr. K. C. Gupta**

Acting Director  
Institute of Genomics and  
Integrative Biology  
University Campus Mall Road  
Delhi 110 007.

**Prof. A. K. Shukla** (till Feb. 2009)

Director  
Central Electrochemical Research  
Institute, Karaikudi 630 006.

**Dr. Pradip K. Bhatnagar** (till July 2008)

Senior Vice President  
New Drug Discovery Research  
Ranbaxy Laboratories Limited  
Plot No.20, Sector 18  
Udyog Vihar Industrial Area  
Gurgaon 122 015.

**Prof. S. K. Sopory**

Group Leader  
Plant Molecular Biology  
International Centre for Genetic  
Engineering & Biotechnology  
Aruna Asaf Ali Marg  
New Delhi 110 067.

**Dr. Javed Iqbal** (from July 2008)

Director  
Institute of Life Sciences  
University of Hyderabad  
Gachibowli  
Hyderabad 500 046.

**Dr. Naresh Kumar**

Head  
R&D Planning Division (CSIR)  
Anusandhan Bhavan  
Rafi Marg  
New Delhi 110 001.

**Mr. R. Saha**

(till Feb. 2009)  
Adviser & Head  
Science & Society Division  
Department of Science &  
Technology,  
Technology Bhawan, New  
Mehrauli Road  
New Delhi 110 016.

**Dr. S. Sivaram**

Director, NCL

**Member Secretary****Dr. G. S. Grover**

Head, Research Planning &  
Audit Unit  
NCL

Management Council

**Chairman**

**Dr. S. Sivaram**  
Director, NCL

**Members**

**Dr. B. D. Kulkarni**  
Deputy Director, NCL

**Dr. S. Ponrathnam**  
Scientist, NCL

**Dr. B. M. Khan**  
Scientist, NCL

**Dr. B. L. V. Prasad**  
Scientist, NCL

**Dr. (Mrs.) V. A. Kumar**  
Scientist, NCL

**Mr. R. P. Purandare**  
Technical Officer, NCL

**Mr. G. Prabhakaran**  
Scientist, NCL

**Ms. Mariamma John**  
F&AO, NCL

**Member Secretary**

**Mr. B. B. Kasture**  
Administrative Officer, NCL



## PERFORMANCE INDICATORS

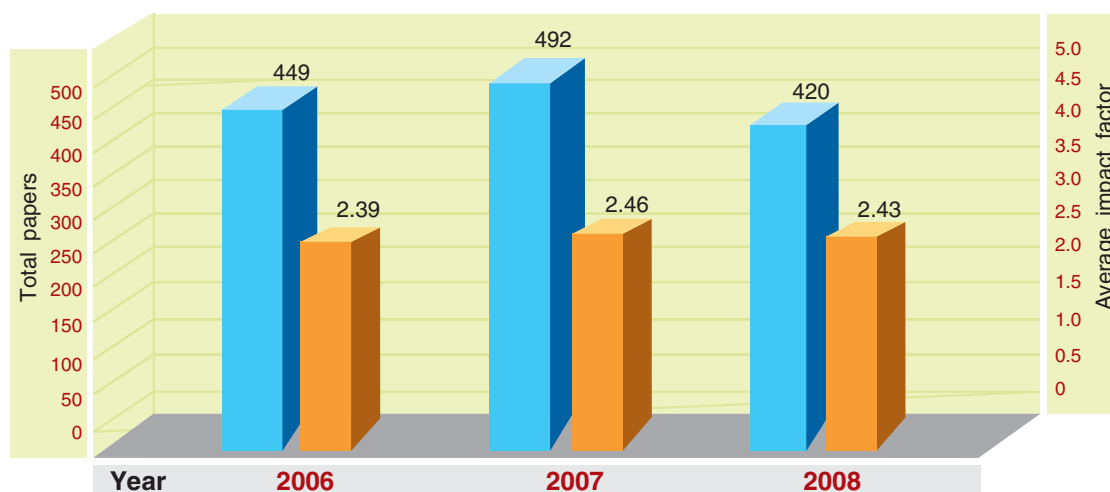
Science Performance Indicators	014
Technology Performance Indicators	015
Human Resource Indicators	016
Financial Performance Indicators	018
Outputs and Outcomes	023



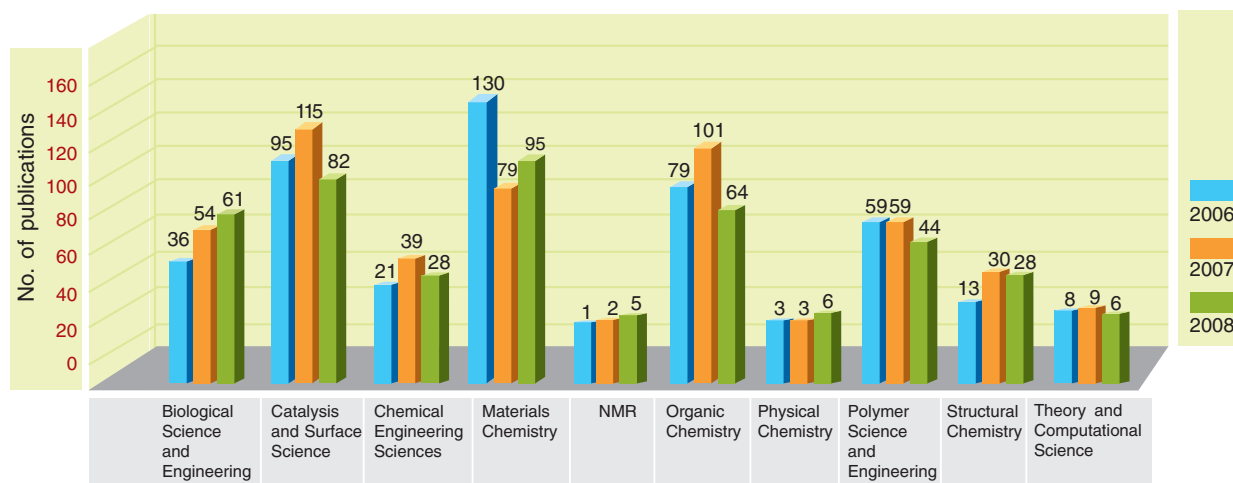
## Science Performance Indicators



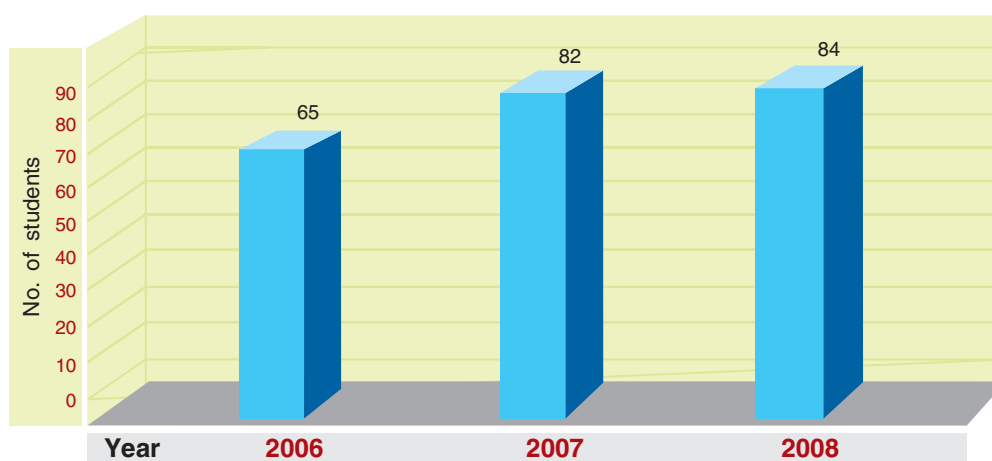
### Research Output : Publications



### Areawise Publications



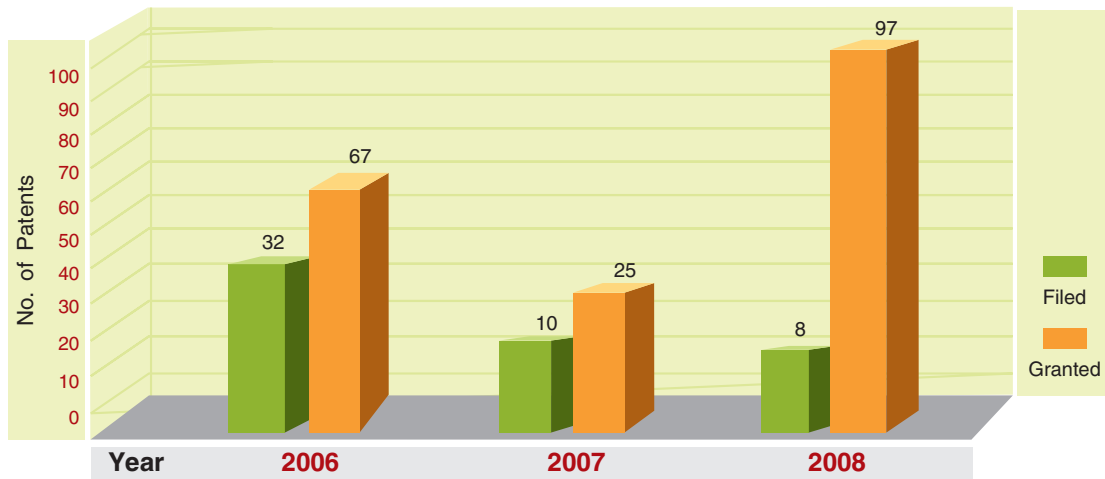
### PhDs Awarded



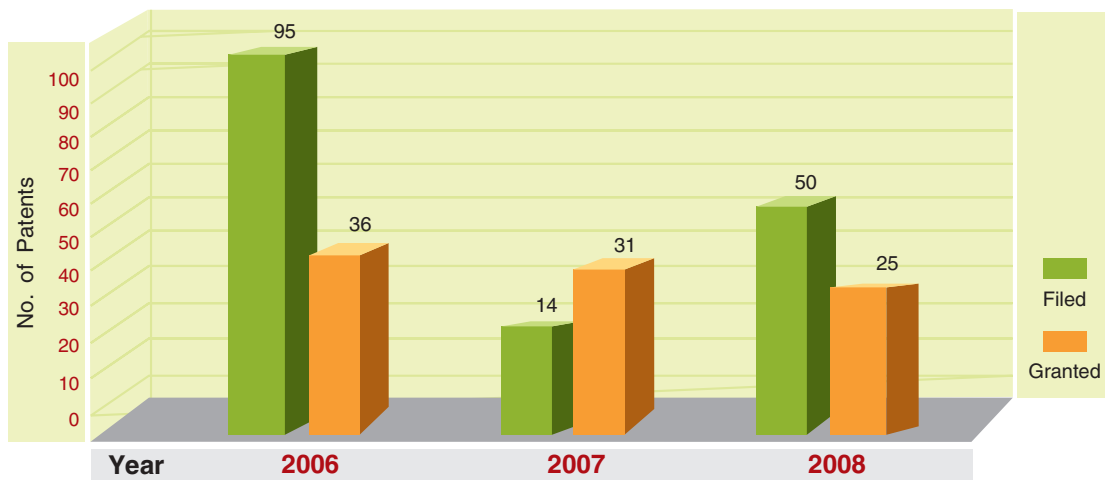
Technology Performance Indicators



Indian Patents : Filed and Granted



Foreign Patents : Filed and Granted



Premia / Royalty Earnings



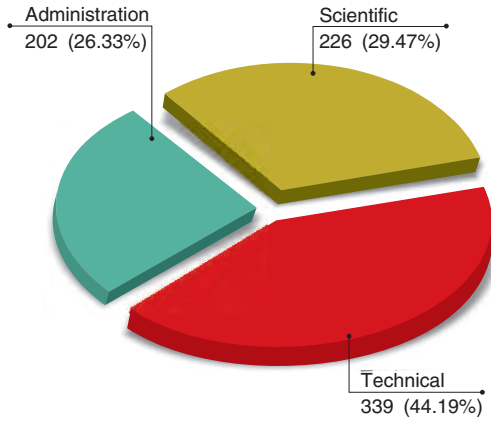


Human Resource Indicators

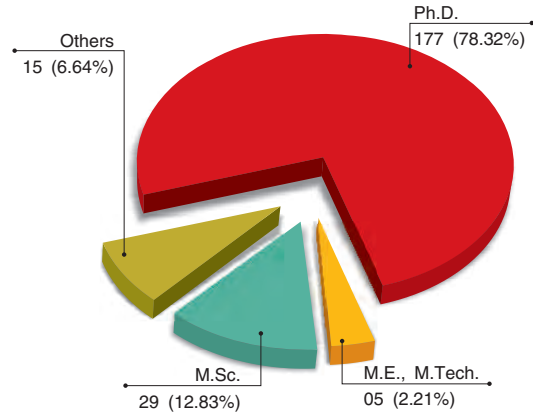
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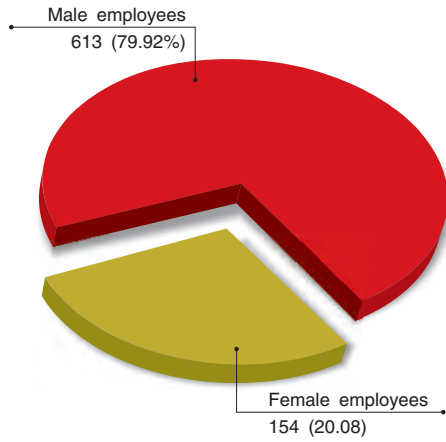
Total Staff : 767



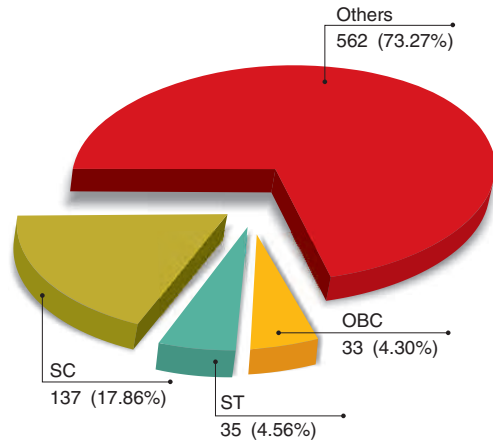
Scientific Staff : 239



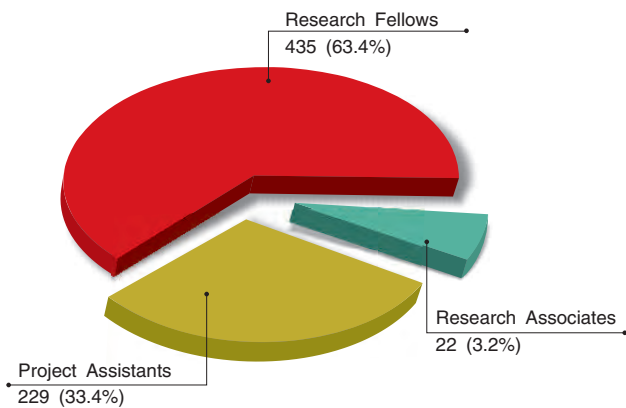
Male : Female Ratio



SC, ST and OBC Employees



No. of Students and Project Staff: 686



Scientist : Agewise Distribution

Grade	Number	Average age (in Year)
Sci. B	18	35.57
Sci. C	36	38.74
Sci. EI	45	50.59
Sci. EII	74	52.83
Sci. F	39	54.53
Sci. G	13	57.13
Sci. H / Director	01	62.45
Total	226	

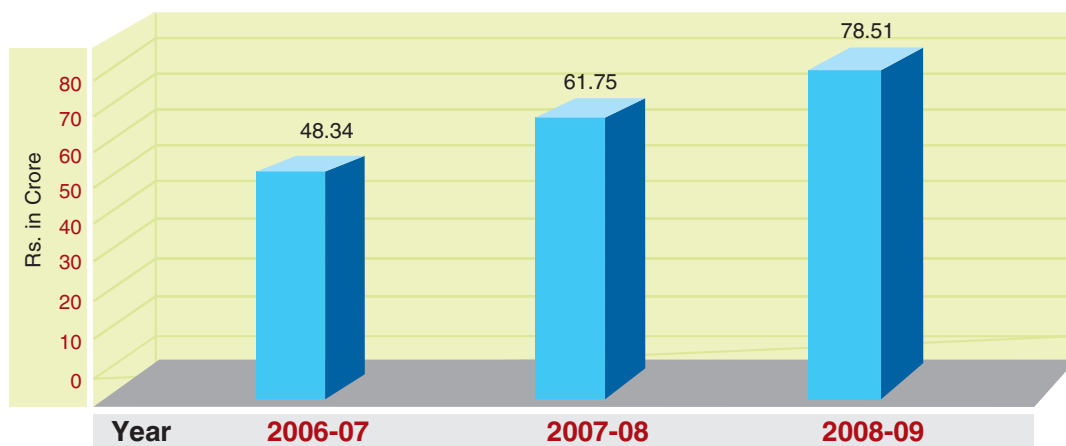


Name and date of joining	Area and Qualifications
 <p>Dr. Sanjay Pandurang Kamble (2 June 2008)</p>	<p><b>Chemical Engineering Science</b></p> <ul style="list-style-type: none"> <li>✦ Scientist, National Environmental Engineering Research Institute, Nagpur (2005-2008)</li> <li>✦ PhD, Institute of Chemical Technology (Formerly UDCT), University of Mumbai (2007)</li> <li>✦ Mariwala Associate (Lecturer grade), Institute of Chemical Technology, University of Mumbai (2004 - 2005)</li> <li>✦ Lecturer, Institute of Chemical Technology, University of Mumbai (2003-2004)</li> </ul>
 <p>Dr. Neelanjana Sengupta (4 Aug. 2008)</p>	<p><b>Computational Biophysics and Chemistry</b></p> <ul style="list-style-type: none"> <li>✦ PhD, University of California, Irvine, USA (2008)</li> <li>✦ Teaching and Research Assistantships, Dept. of Chemistry, University of California, Irvine, USA (2003-2008)</li> </ul>
 <p>Dr. Rahul Banerjee (8 Sept. 2008)</p>	<p><b>Crystal Engineering and Structural Chemistry</b></p> <ul style="list-style-type: none"> <li>✦ Post Doctoral Research Fellow, University of California Los Angeles, Los Angeles, USA (2006-2008)</li> <li>✦ PhD, University of Hyderabad (2001-2006)</li> </ul>
 <p>Dr. Rajesh Kumar Singh (3 Oct. 2008)</p>	<p><b>Molecular and Structural Biology</b></p> <ul style="list-style-type: none"> <li>✦ Post Doctoral Research Fellow, University of Greifswald, Germany (2006-2008)</li> <li>✦ PhD, Protein Crystallography, EMBL-University of Heidelberg, Germany (2002-2006)</li> </ul>
 <p>Dr. Sudip Roy (1 Jan. 2009)</p>	<p><b>Theoretical Chemistry</b></p> <ul style="list-style-type: none"> <li>✦ Post Doctoral Research Fellow, Technical University Darmstadt, Germany (2005-2008)</li> <li>✦ PhD, University of Saarland, Germany (2000-2005)</li> </ul>
 <p>Dr. Magesh Nandagopal (30 March 2009)</p>	<p><b>Technology Management and Commercialization</b></p> <ul style="list-style-type: none"> <li>✦ MBA, Finance and Operations Management, University of Connecticut, Storrs, USA (2008)</li> <li>✦ PhD, Polymer Science, University of Connecticut, Storrs, USA (2005)</li> </ul>

## Financial Performance Indicators

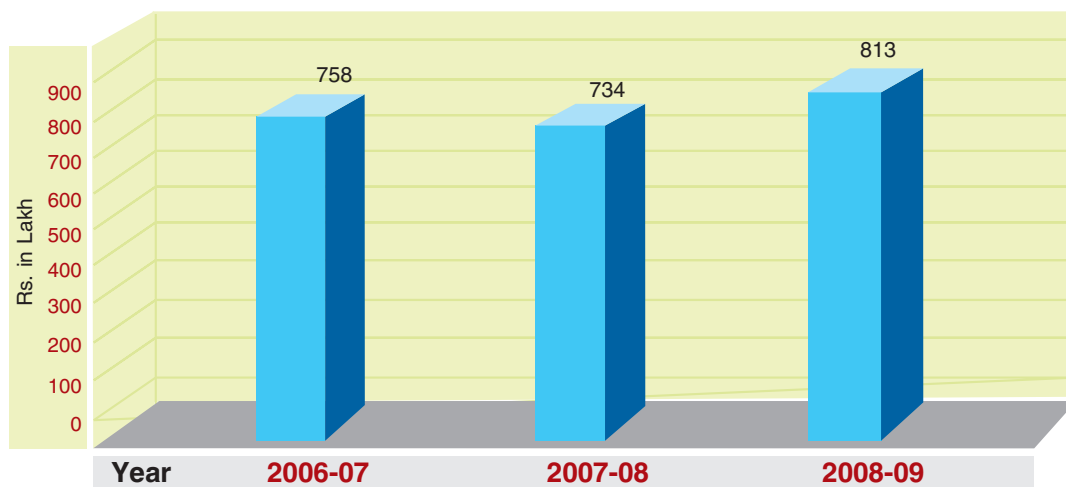


### CSIR Budget



2006-07 (CSIR Budget : 43.38 + Network Project : 04.18 + NMITLI Projects : 00.78)  
 2007-08 (CSIR Budget : 52.26 + Network Project : 06.06 + NMITLI Projects : 03.43)  
 2008-09 (CSIR Budget : 54.63 + Network Project : 19.00 + NMITLI Projects : 04.88)

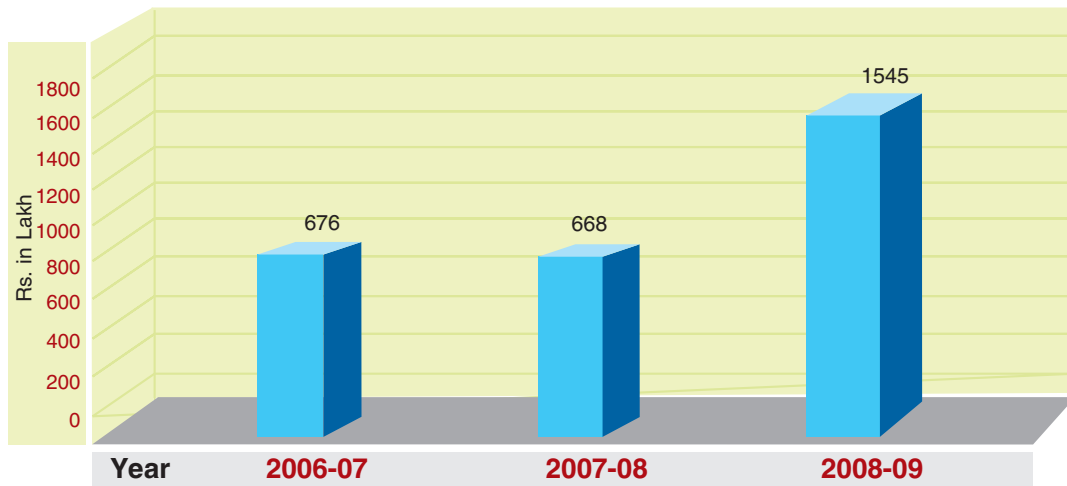
### Laboratory reserve: Receipts



Financial Performance Indicators

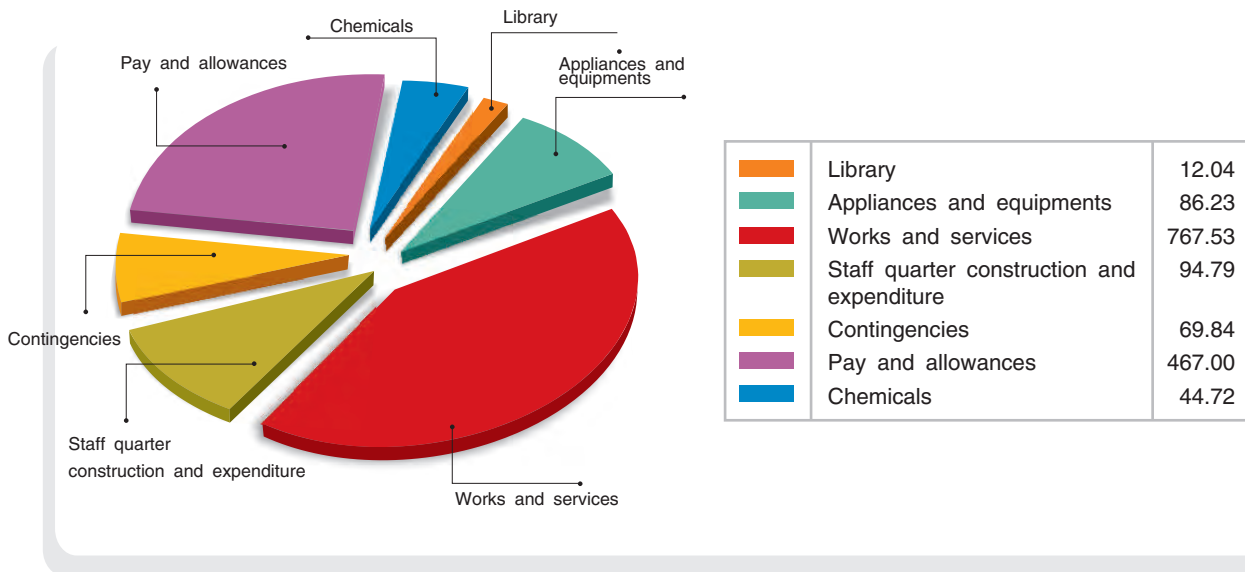


Laboratory reserve: Expenditure



10 lakh=1 million / 1 crore=10 million

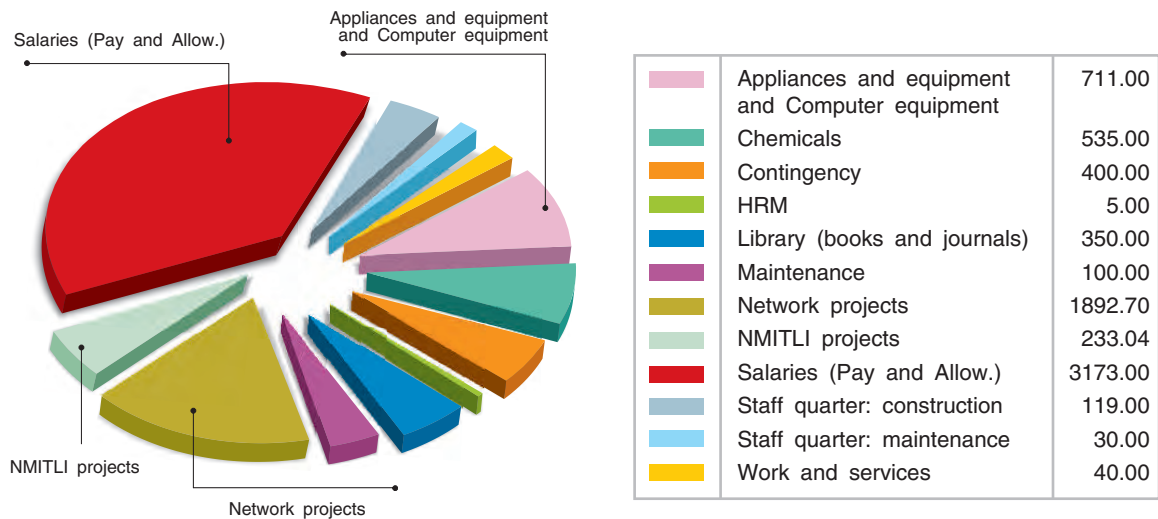
Expenditure: Laboratory reserve 2008-09 (Rs. in Lakhs)



## Financial Performance Indicators



### Expenditure:CSIR and Network Projects 2008-09 (Rs. in Lakhs)



### External Income



10 lakh=1 million

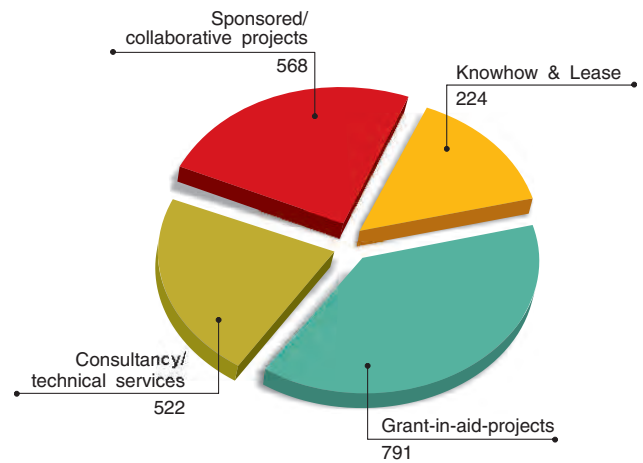
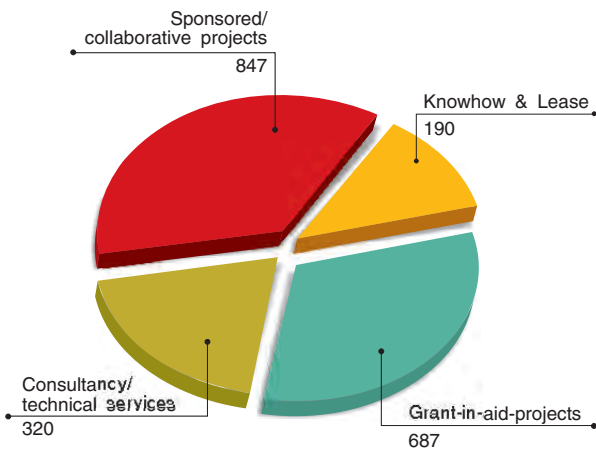
Financial Performance Indicators



ECF : Project wise break-up

2007 - 08 : Rs. 2044 lakhs

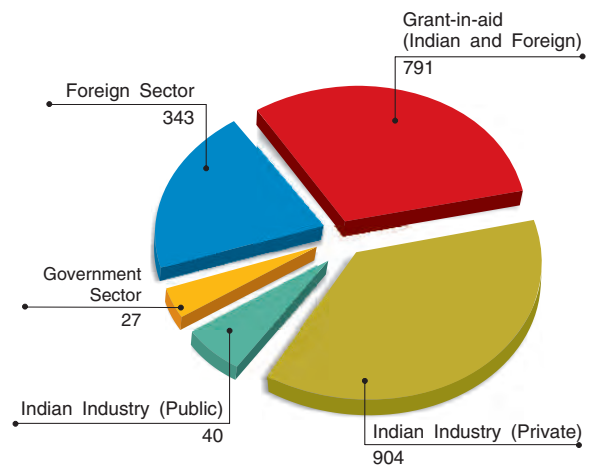
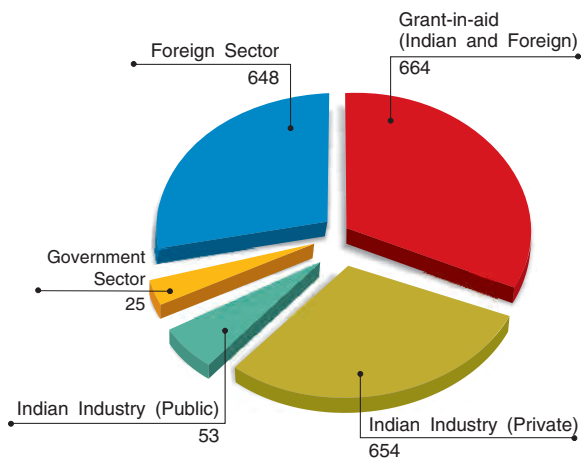
2008 - 09 : Rs. 2105 lakhs



ECF : by source

2007 - 08 : Rs. 2044 lakhs

2008 - 09 : Rs. 2105 lakhs



10 lakh=1 million

Financial Performance Indicators



**Capital and Recurring Expenditure on R&D (2007-2009)**

Rs. in lakh

Source	Capital		Recurring	
	2007-08	2008-09	2007-08	2008-09
CSIR	1177	711	590	535
Lab Reserve	250	86	56	45
Projects	455	335	1289	1199
Network Projects	360	1173	108	720
NMITLI Projects	95	88	194	145
<b>Total</b>	<b>2337</b>	<b>2393</b>	<b>2237</b>	<b>2644</b>
Percentage %	<b>51%</b>	<b>48%</b>	<b>49%</b>	<b>52%</b>

**Ongoing Publicly Funded Mission Mode and Internal Projects (2008-09)**

Sr. No.	Description	Rs. in Lakh
1	CSIR NMITLI	488
2	Major publicly funded projects (DST, DBT, NPSM, SDC, McNIGHT etc.)	791
3	Network projects	1900
4	Internal projects *	213
	<b>Grand Total</b>	<b>3392</b>

\* - Funded from Lab Reserve of NCL

**Scientific Budget (2008-09)**

Funding Source	Rs. in lakh		
	Recurring	Capital	Total
CSIR	4243	1220	5463
LR	582	963	1545
<b>Total</b>	<b>4825</b>	<b>2183</b>	<b>7008</b>

10 lakh=1 million

Outputs and Outcomes



Select Outputs and Outcomes of NCL

Category of benefits	Benefit	Indicators	2006-07	2007-08	2008-09
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in foreign journals/ publications (Calendar year)	426	468	394
		Number of papers published in Indian journals(Calendar year)	24	22	26
		Average Impact Factor	2.39	2.46	2.43
		Number of invention disclosure (Calendar year)	10	31	47
		Number of patents filed in India (Calendar year)	32	10	8
		Number of patents filed outside India (Calendar year)	95	14	50
		Number of patents licensed / assigned	5	6	1*
		Number of major national/ regional collections, compilations, databases	3	3	3
	Highly trained man-power	Number of PhDs produced (Calendar year)	65	82	84
		Number of NET/GATE qualified students joined (including DBT JRF)	34	39	43
	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	11	10	9
	Pride and standing among nations; National image	Number of international awards won	1	-	-
		Memberships of major international academies and learned societies (Cumulative membership years)	7	7	7
		Memberships of editorial boards of international peer-reviewed journals (number of editorships for International Journals)	31	33	54
		Number of papers in foreign journals	426	468	394
		Number of IF research papers	432	451	384
		Number of foreign patents granted (Calendar year)	36	31	25
	Representation in global affairs	Official(s) in global/ trans-national organizations like the UN, WHO etc - IUPAC (Cumulative years of office held) (Data given in no. of years)	6	6	6

1 Crore = 10 Million

\* Licensed through NMITLI Project.



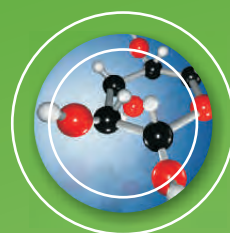
## Outputs and Outcomes



Category of benefits	Benefit	Indicators	2006-07	2007-08	2008-09
Private goods	Research, consulting, teaching and analytical services	Total earnings from projects done for Indian & Foreign businesses/ industry (Rs. in Crore) (Industrial ECF, excluding Grant-in-Aid)	13.17	13.56	13.14
	Continuing education	Total earnings from continuing education / training programs (Rs. in Crore)	NA	-	-
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (Rs. in Crore)	0.91	1.599	2.24
Strategic goods and options	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (Rs. in Crore)	0.78	3.43	4.88
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (Rs. in Crore)	8.97	6.87	7.91
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	Number of papers in foreign peer-reviewed journals	426	468	394
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	17	17	19
		Number of PhDs granted where lab scientists were research guides	65	82	84
		Number of staff who are members of National academies (Cumulative)	27	29	30
		Number of Bhatnagar awardees (Cumulative)	14	14	14
	Number of Padma awardees (Cumulative)	5	5	5	
	Lab's standing with industry	Total worth of projects with industry (only industry: both Indian & foreign) (excluding Grant-in-Aid) (Rs. in Crore)	13.17	13.56	13.14

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

1 crore = 10 million



## RESEARCH & DEVELOPMENT REPORTS



Advanced Materials	026
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Centers of Excellence	162



## Hybrid materials



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Application of solid-state NMR for the study of advanced functional materials

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- ✦ K. V. Ramanathan, IISc, Bangalore

Solid-state NMR is a very powerful experimental technique from which information about the structure and dynamics of a range of materials can be extracted. Our research is focused on the study of important materials using solid-state NMR techniques. Some of the ongoing research activity is described below:

### Polymers

The mechanical properties of polymers are dependent on the presence/absence of segmental motions of the main-chain and the molecular motions of side-groups. Solid-state NMR is a powerful technique which can probe molecular motions in the range of a few MHz (relaxation techniques) to ~100 kHz (separated local field spectroscopy) and to a few Hz using CODEX experiments. We have developed some of the above techniques and use them for probing the molecular motions in polycarbonate copolymers, and polylactic acid. The degree of crystallinity is an important parameter that influences the mechanical property of crystalline polymer.

### Strontium aluminate

Strontium hexaluminate ( $\text{SrAl}_{12}\text{O}_{19}$ ) has a hexagonal magnetoplumbite structure similar to that of  $\text{SrFe}_{12}\text{O}_{19}$ , the well known hard ferrite material with many technological applications. Strontium aluminate is used for a wide variety of applications in the field of ceramic composites, catalytic substrates, photo luminescent, and thermoluminescent materials. When activated with a suitable dopant (e.g. europium), it acts as photoluminescent phosphor with long persistence of phosphorescence. It is known from earlier X-ray crystallographic studies that  $\text{SrAl}_{12}\text{O}_{19}$  has five distinct Al sites, one tetrahedral  $\text{AlO}_4$ , one trigonal bipyramidal  $\text{AlO}_5$ , and three octahedral  $\text{AlO}_6$  sites. The octahedral sites are of different symmetry.

Later crystallographic studies on single crystals reported that the known 'central atom model' with bipyramidal geometry for the five-coordinated Al atoms gives a slightly larger residual (R) factor (0.0340) when compared to a 'split atom model' with distorted tetrahedral sites with lower R factor (0.0331) for the same space group of  $P6_3/mmc$ . The  $\text{Al}^{3+}$  ion in the mirror plane (2b site in the central atom model) is shared between two sites (4e site with half occupancy in the split atom model) instead of being in theoretical five-fold coordination, providing a distorted tetrahedral environment for Al. Although the coordination behavior of different Al centers in strontium aluminate is known from X-ray crystallographic studies, solid-state nuclear magnetic resonance

(NMR) is a powerful tool to extract information regarding the local structure and coordination environment of the material. Especially, this tool becomes very handy to locate the substitutional sites when Al in  $\text{SrAl}_{12}\text{O}_{19}$  is substituted by other elements by which the properties of the material can be altered.

Strontium hexaluminate is an interesting system that can be studied in detail by solid-state NMR techniques because of the existence of the different coordination environment for aluminium. Using  $^{27}\text{Al}$  5-quantum magic angle spinning (5QMAS) studies at 7.05 T, Jansen et al. have shown that there is an  $\text{AlO}_5$  site with high shielding ( $\delta_{\text{iso}} = 18$  ppm) and a quadrupolar coupling constant ( $C_q$ ) of 2.1 MHz, where the high shielding observed is ascribed to the distorted nature of the penta-coordinated Al as expected in the 'central atom model'. In all the earlier studies using magic angle spinning (MAS) NMR, an unambiguous proof for the existence of this site was not available since this site overlapped with the  $\text{AlO}_6$  sites in the MAS spectrum. Recently, from high-field NMR studies at 14.1 and 18.8 T, Du and Stebbins have observed a site with a large quadrupolar coupling constant of 21 MHz in this system.

They have assigned this to a distorted tetrahedral aluminium site and have argued that the 'split atom model' is the correct description and have ruled out the possibility of a penta-coordinated aluminium being present in this system. Thus, there is no

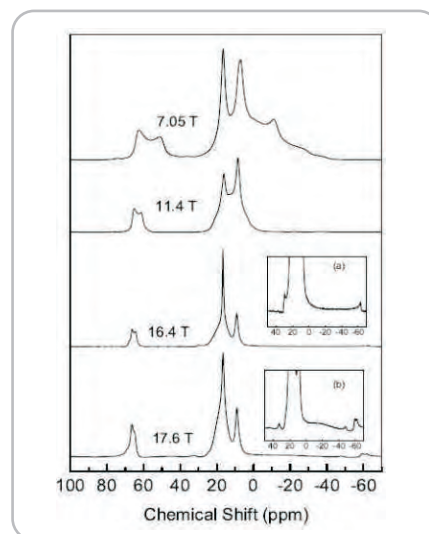


Figure 1: The  $^{27}\text{Al}$  magic angle spinning (MAS) Solid-state NMR spectrum of  $\text{SrAl}_{12}\text{O}_{19}$  recorded at 7.05 T, 11.4 T, 16.4 T and 17.6 T. Insets (a) and (b) are the zoomed spectra at 16.4 T and 17.4 T which clearly show the presence of a site with a quadrupolar coupling constant of ~20 MHz



consensus on the nature of coordination of Al sites from solid-state NMR studies, as the two opposing results are based on studies at either low or high magnetic fields. We have carried out studies on a single phase material to obtain fresh insights into the coordination behavior of the fifth Al site with solid-state NMR experiments in both low and high magnetic fields.  $^{27}\text{Al}$  MAS experiments have been carried out both in low and high magnetic fields and multiple-quantum magic angle spinning (MQMAS) at low magnetic field to get the  $^{27}\text{Al}$  resonances of various crystallographic sites present. Our studies give evidence for simultaneous presence of both the five coordinated and the distorted four coordinated sites in  $\text{SrAl}_{12}\text{O}_{19}$ .

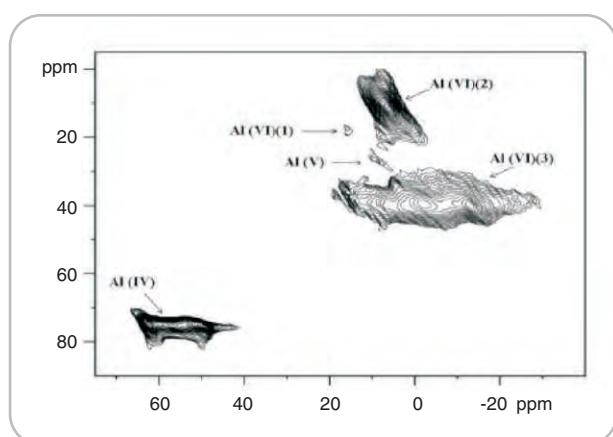


Figure 2: The  $^{27}\text{Al}$  MQMAS spectrum of  $\text{SrAl}_{12}\text{O}_{19}$  at 7.05 T which clearly shows the presence of a five-coordinated  $\text{Al(V)}$  aluminium, apart from a three octahedral  $\text{Al(VI)}$  and a tetrahedral aluminium  $\text{Al(IV)}$

## Inorganic-organic hybrid materials

Heterogenization of homogenous catalytic materials has been an effective strategy to overcome the difficulties involved in the separation, purification and reusability of homogenous catalysts. One of strategies that have been adopted for the same is the encapsulation of the homogenous catalytic molecules into porous materials. Heteropolyacids (HPA) like phosphotungstic acid (PTA) are promising catalysts for many acid catalyzed reactions like benzoylation of phenol. PTA can be heterogenized by impregnation or encapsulation on porous supports like silica. But due to its weak bonding interaction with the silanol group, leaching will occur. We have immobilized PTA on the surface of fumed silica by means of chemical bonding with certain organic groups like amines, imidazole and methyl imidazole. This chemical bonding was done by an alkoxy silyl group. We expect that this will result in the strong anchoring of PTA in the support and will prevent leaching. Solid-state NMR is the most important characterisation technique that can confirm the organic modification of silica or the mesoporous materials. We have carried out a NMR investigation with  $^{29}\text{Si}$ ,  $^{13}\text{C}$ ,  $^1\text{H}$  and  $^{31}\text{P}$  solid-state NMR. Comparison of  $^{31}\text{P}$  CPMAS spectra of anchored PTA and neat PTA showed the confirmation of anchoring.

Hybrid materials



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Dipti Dhakras, PAII  
Raunak Naphade, PA-II

Collaborator:

✦ Safish Ogale, NCL

Functional polymer nanocomposites

Background / objectives

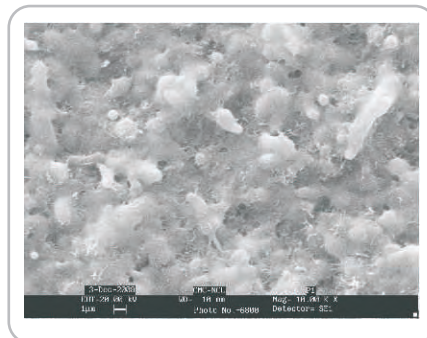
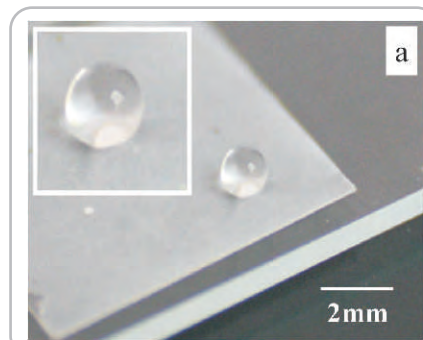
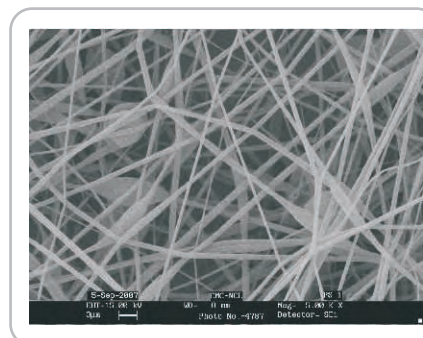
Recently, the possibility of using polymer nanocomposite materials for application in the electronics devices, including light emitting diodes, solar cell, and transistors has led wide scientific and technological interest for several decades. Use of polymer nanocomposites based on organic materials in FET devices offers many advantages such as light weight, flexibility, easy processing and improved durability. However, in order to realize these applications it is highly desirable that one need to process these polymer nanocomposites in thin film phase while retaining its bulk characteristics. Additionally these nanocomposites should also possess high dielectric permittivity in order to improve the charge storage density.

Work done and discussion

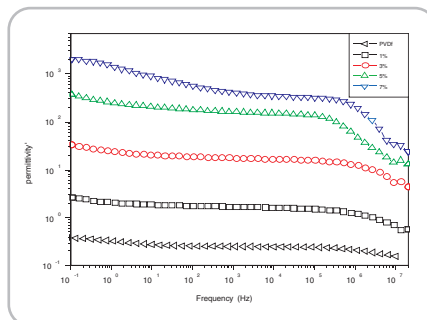
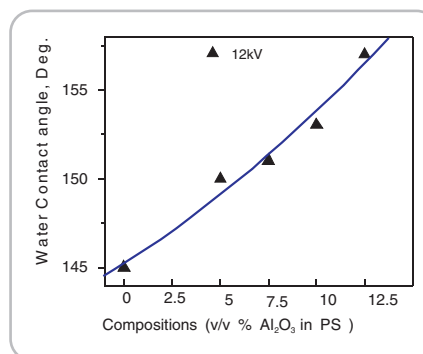
High quality thin films of ferroelectric Poly (vinylidene fluoride) (PVDF) embedded with multiwalled carbon nanotubes (MWNT) were prepared using pulsed laser deposition (PLD) technique. FTIR and XRD measurements indicate effective transfer of the polymer into thin film phase. The dielectric property dependence of MWNT composites on both volume fraction of filler and frequency is investigated. A remarkable enhancement in the permittivity is found with increasing MWNT loading.

Superhydrophobic polymer nanocomposites

Super hydrophobic surfaces are generally made by controlling the surface chemistry and surface topography of various expensive materials. A simple method of electrospinning was used to generate superhydrophobic membrane which showed fiber and beads morphology in Polystyrene /Nano-active alumina fibers



SEM morphology PVDF/MWNT thin films



Dielectric permittivity of PVDF and PVDF/MWNT

Selected Publications:

- ✦ *J Polymer Science: B: Polymer Physics*, 2008, 46, 2539
- ✦ *E-Polymers*, 2009, art. no. 112

## Hybrid materials



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Polypeptide grafted silica nanoparticles: Synthesis and applications

### Members:

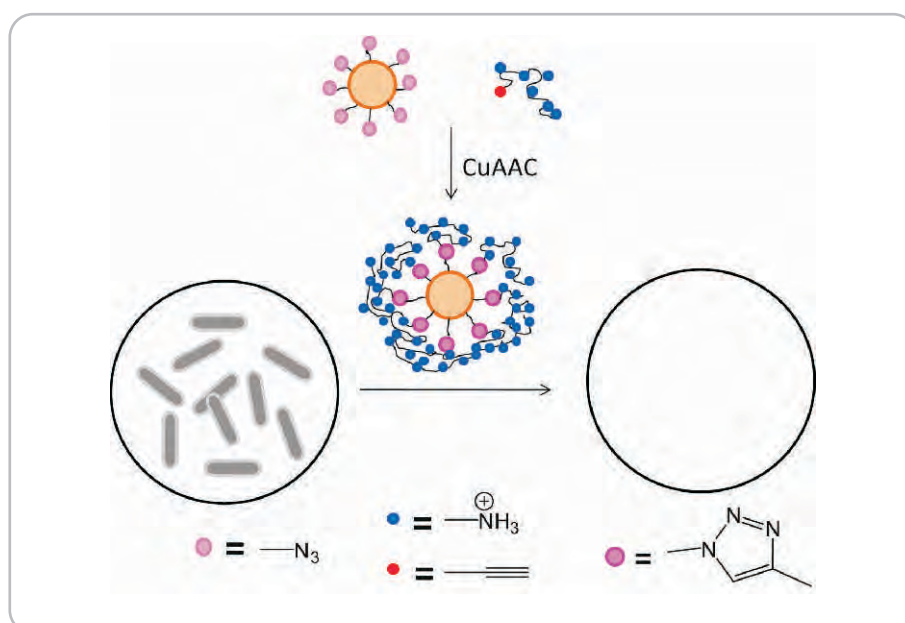
Mrityunjoy Kar, SRF  
P. S. Vijayakumar, PDF

Polypeptide polymer grafted silica nanoparticles are of considerable interest because the ordered secondary structure of the polypeptide grafts imparts novel functional properties onto the nanoparticle composite. Synthesis of polypeptide grafted silica nanoparticles such as poly-L-lysine grafted silica nanoparticles, would be of particular interest since the high density of cationic charges on the surface could lead to many applications such as gene delivery and antimicrobial agents. We have developed a 'grafting to' approach using a combination of

NCA polymerization and "click chemistry" to synthesize polypeptide grafted silica nanoparticle with a high graft density of 1 chain/nm<sup>2</sup>. Poly-L-lysine grafted silica nanoparticle, synthesized by this methodology, was tested as an antimicrobial agent on both Gram-negative *E. coli* and Gram-positive *bacillus subtilis*. It was found that 50 µg/mL of PLL-silica was sufficient for a considerable (>90%) reduction of bacterial count, thus showing its potential usage as antimicrobials.

### Collaborator:

✦ BLV Prasad, NCL



Poly-L-lysine grafted silica nanoparticles synthesized using NCA polymerization and "click chemistry" is shown to have antibacterial properties

### Selected publication:

✦ *J. Materials Chemistry*, 2009, 22, 1409

## Magnetic materials



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S. D. Bhamre, SRF  
S. Deka, SRF

### Collaborator:

- T. G. Ajithkumar, NCL

### Magnetism and magnetic materials

#### Objectives

- Development of magnetostrictive smart materials with high magnetostriction at low magnetic fields based on sintered ceramic oxide magnetic materials
- Studies on the structural and magnetic characteristics of different types of magnetic nanoparticles as a function of particle size
- Studies on the magnetic interactions in magnetic nanoparticles to understand the role of interparticle magnetic interactions in magnetic nanoparticles, as this information is very crucial for various applications
- Synthesis and studies on superparamagnetic iron oxide nanoparticles capped with various biocompatible molecules for biomedical and environmental applications

#### Work done and discussion

Magnetic nanoparticles are useful for biomedical and environmental applications. For these applications, the magnetic nanoparticles need to be biocompatible and less toxic. Important factors which determine the biocompatibility and toxicity of these materials are the nature of the magnetically responsive component. Superparamagnetic iron oxide nanoparticles (SPIONs) of  $\gamma\text{-Fe}_2\text{O}_3$  (maghemite) or  $\text{Fe}_3\text{O}_4$  (magnetite) are the most suitable candidates for biomedical and environmental applications. Understanding the magnetic characteristics of the nanoparticles, especially after coating with suitable surfactants, is very important for various applications. We have studied the magnetic characteristics of  $\text{Fe}_3\text{O}_4$  nanoparticles before and after coating with highly bio-compatible molecules such as citric acid, chitosan, dextran, ascorbic acid, etc. The emphasis is to study the changes in the magnetic properties after surface modification because such knowledge is very essential for the applications of the magnetic nanoparticles. Considerable changes in the

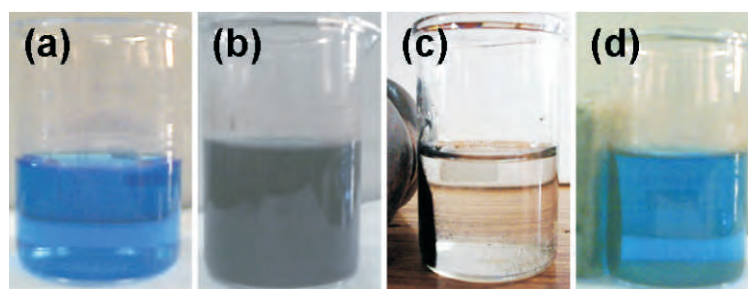
properties have been observed, after coating, because of the changes in the magnetic interactions between the particles. This information is very useful for the various applications of magnetic nanoparticles.

For magnetic nanoparticles, the exchange interactions at the surface of a particle will be different from those inside, due to changes in the coordination behaviour at the surface. Therefore, studying and understanding the coordination and distribution behaviour of the different metal ions in the nanoparticles of spinel-type oxides is very important to understand the changes in the magnetic properties. Solid state NMR study which is a useful and important technique to obtain information on local structural variations, has been made on nanoparticles of non-magnetic spinel oxides of crystal structure similar to that of magnetite and maghemite. Apart from the usual tetrahedral and octahedral coordinations present in the bulk material, the presence of 2- and three-coordination environments have been observed in nanoparticles.

Disposal of wastewater from dyeing industries poses one of the major environmental problems. Activated carbon (AC) is extremely useful as an adsorbent for the removal of toxic wastes from water such as dyes, heavy metals, arsenic, oil, etc. Adsorption by AC is an effective and widely employed method for waste water treatment. AC is known to be an excellent adsorbant for varieties of dyes and the used carbon can be easily regenerated with various techniques. Nanocomposite containing activated carbon attached to superparamagnetic  $\text{Fe}_3\text{O}_4$  is found to be very efficient and highly suitable for removing dissolved dyes and other contaminants from waste water by a simple magnetic separation process after adsorption on AC.

### Selected publications:

- J. Phys. Chem.*, 2008, C, 112, 14737
- Int. J. Nanoscience*, 2008, 7, 43
- J. Amer. Ceram. Soc.*, 2008, 91, 1976
- J. Nanosci. Nanotech.*, 2008, 8, 3955



Photographs showing (a) methylene blue (MB) solution, (b)  $\text{Fe}_3\text{O}_4\text{-AC}$  nanocomposite dispersed in the MB solution, (c) separating the nanocomposite particles by a small laboratory magnet after 5 minutes, and (d) separating the  $\text{Fe}_3\text{O}_4$  nanoparticles after dispersing for 5 minutes in the MB solution.

## Nanostructured materials



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Epoxy-dispersible carbon nanotubes

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### Background / objectives

Carbon nanotubes (CNTs) are unique nanostructured materials with remarkable physical and mechanical properties such as high tensile strength and Young's modulus, high thermal conductivity as well as high current density. Due to their excellent properties, CNTs can be used as fillers in polymer composite systems in order to enhance the electrical conduction, thermal transport, and mechanical properties of the original polymer materials. Among various polymers, high strength epoxy systems are very important materials for aircraft, space shuttle, electronics products and many other industrial applications.

CNT-reinforced epoxy systems hold the promise of delivering superior composite materials with high strength, light weight, and multi-functional features. The realization of this CNT-reinforced composite application, however, poses some problems: the lack of interfacial adhesion, which is critical for load transfer in composites and the poor dispersion of nanotubes in the matrix, which is also significant for the fabrication of reinforced composites. The dispersion of CNTs within the matrix is important to achieve efficient and effective load transfer to the nanotubes.

Chemical functionalization of CNTs is always recommended to obtain good dispersion and achieve strong interface. The covalent functionalization of nanotubes with carboxylic (-COOH), carboxylate (-COO) and hydroxyl (-OH) groups has been reported to improve the nanotube dispersion in solvents and polymers. The amino-functionalized CNTs show improved compatibility with epoxy resin and thus, more homogeneous dispersion in the matrix. The project is therefore aimed to evolve suitable functionalization strategies facilitating the preparation of CNT-reinforced epoxy composites with enhanced mechanical properties.

### Work done and discussion

CNTs were purified by chemical and thermal treatments. The purified CNTs were refluxed in acid solutions at different concentrations for carboxylic functionalization. The CNT samples, purified as well as COOH-functionalized, were characterized by SEM, EDX, TEM, TGA/DTA, Raman, FTIR and XPS. The dispersibility of COOH-functionalized CNTs in different solvents was studied by UV-VIS spectroscopy.

The electron microscopic images (SEM and

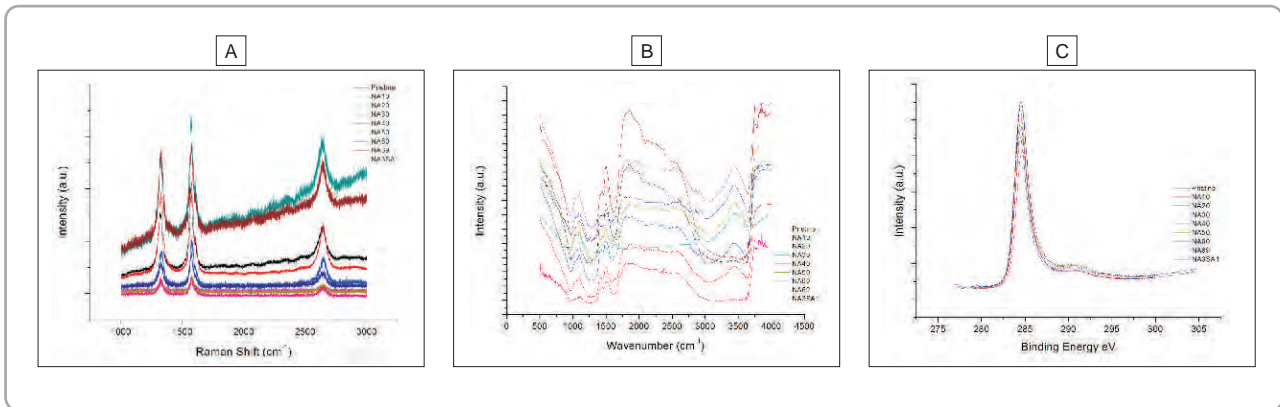
TEM) of purified CNTs confirmed that the residual catalyst and amorphous carbon impurities were successfully removed from the material. The nanotubes having uniform diameter in the range of 15 - 20 nm appeared to be entangled with each other. The EDX measurements revealed that the sample of purified CNTs consisted predominantly of carbon. In the purified CNT sample, the carbon content was found to be 98.5 wt% and the impurities consisting of Fe, Co, Ni, Mo, Mn and O elements altogether to be 1.5 wt%. The % content of impurities present in the samples and thermal stability of the nanotubes were estimated from thermogravimetric analysis. After purification, the amorphous carbon reduced to 1 - 1.5% and the metal impurity was around 1%. The estimated purity of the CNTs was ~ 98%. The CNTs started decomposing near 600 °C and burnt off completely at 775 °C showing high thermal stability of the nanotubes.

In the Raman spectra of pristine and COOH-functionalized CNTs, the strong peaks around 1575 cm<sup>-1</sup> correspond to the graphite-related G-band and the peaks around 1323 cm<sup>-1</sup> correspond to the disorder-induced D-band for graphitic carbon. The peaks around 2647 cm<sup>-1</sup> can be assigned to the first overtone of D-band. The intensity ratio of D-band to G-band (ID/IG) indicates the extent of distortion of CNTs or damages on the nanotube surface. The smaller the value of ID/IG is, the lesser the distortion or damages would be. The FTIR spectra of the CNT samples show the broad bands around 3600 cm<sup>-1</sup>, which are attributed to the presence of O-H groups on the surface of the COOH-functionalized CNTs.

The peaks around 1650 cm<sup>-1</sup> can be attributed to the C=O stretching from COOH group. The XPS analysis of all CNT samples provides the binding energies data. Along with the main intense C-C peak at 284.4 eV, the peak at higher binding energy 290.9 eV represents the -C=O contribution from COOH-functionalized CNTs.

For dispersibility measurements by UV-VIS spectroscopy, the CNT samples were dispersed in different solvents such as water, toluene, THF, methanol and acetone. The UV-VIS spectra measured the absorbance of all dispersed CNT samples in relation to the dispersibility of COOH-functionalized CNTs in different solvents. The COOH-functionalization also enabled a good dispersion of CNTs in epoxy resin.





Raman, FTIR and XPS spectra of pristine and COOH-functionalized carbon nanotubes



Photographs of carbon nanotube dispersion in various solvents – visual examination (1 - Water, 2 - Toluene, 3 - THF, 4 - Methanol, 5 - Acetone)

## Nanostructured materials



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Materials science, nanomaterials

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- ✦ Pravin Narvankar, Applied Materials Inc, USA
- ✦ Prof. Dilip Joag, University of Pune
- ✦ M. A. More, University of Pune
- ✦ S. S. Suryawanshi, Solapur University

### Objectives

- Synthesis of nanostructured and mesoporous material; DST funded project
- Deposition of thin and thick oxide films suitable for gas sensing applications
- Synthesis of metal oxides nanowires suitable as field emitter
- Synthesis and characterization of nanostructured ferrite as gas sensors
- In collaboration with Applied Materials Inc, USA, a sophisticated low temperature chemical vapour deposition set-up has been installed. Now ultra thin films can be deposited in this unit

### Work done and discussion

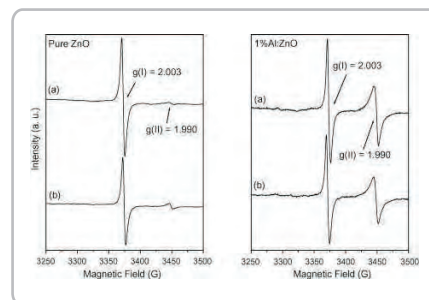
We have developed strength in synthesis of nanostructured materials in various forms such as wires, tetrapods, spheres, flowers, pyramids, triangle etc. We have used techniques such as dip-coating, ultrasonic atomization, spin coating and conventional spray deposition with and without surfactants, Thermal deposition, Microwave hydrothermal and molten solid salt solution route. Nanostructured ZnO, SnO<sub>2</sub>, α-Fe<sub>2</sub>O<sub>3</sub> and different ferrites, in the pure and doped form were synthesized in bulk and film form and characterized by HRTEM, SEM and XRD, EPR, XPS etc. We have found selectivity of these materials towards NO<sub>2</sub>, H<sub>2</sub>S, CO, and liquid petroleum gas, we also observed some of the material as a good humidity sensor. The field emission and photoluminescence properties of some of the material was carried out in collaboration with University of Pune.

### EPR and DRS evidence for NO<sub>2</sub> sensing in Al-doped ZnO

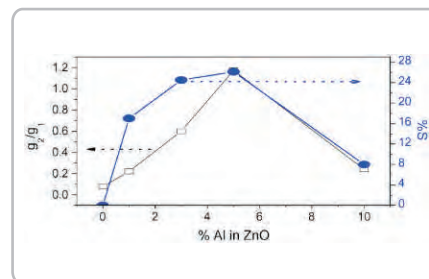
Doping of ZnO with group III elements has found to enhance its gas sensing properties. We have investigated the selective gas response in Al-doped ZnO towards 20ppm of NO<sub>2</sub> gas at the lower operating temperature of 100°C. Gas sensors based on ZnO make use of chemical sensitivity of its surface to the different adsorbed gases that cause change in its resistance. The EPR analysis confirmed the NO<sub>2</sub> response of these samples at lower operating temperatures.

The EPR spectra of pure and Al-doped ZnO show two signals, these signals have been assigned to O- and Zn interstitial defects. The intensity of the signals corresponds to the concentration of defect sites produced. The Al-doped samples show higher intensity of signal II (1.990) than that for pure ZnO. The ratio of intensities of these two signals (II/I) are different for Al:ZnO as compared with pure ZnO. On exposure to NO<sub>2</sub> the intensity ratio of signal-II/signal-I in Al-doped ZnO decreases, indicating electron transfer

from sample to NO<sub>2</sub>. Such a trend in spectral behaviour is not found in pure ZnO. The intensity of signal II in fact increased marginally for NO<sub>2</sub> exposed pure ZnO. The gain in intensity of signal II in pure ZnO might have come from a decrease in intensity of signal I. This is a key evidence to confirm that pure ZnO does not adsorb NO<sub>2</sub> at low temperatures indicating the role of Al in responding towards NO<sub>2</sub> gas.



The NO<sub>2</sub> sensing behaviour of the Al-doped samples correlated with the variation in intensity ratio of signals II/I, indicates that these defect sites (1.990) are the active sites in Al:ZnO for NO<sub>2</sub> sensing. The maximum response was found for 5 wt.% Al:ZnO at 100°C as the defects for this concentration are the highest as evinced by the EPR results.



### H<sub>2</sub>S gas sensitive In-doped ZnO thin films: Preparation and characterization

High quality indium-doped ZnO (IZO) thin films (~100 nm) have been deposited onto the glass substrates by using a spray pyrolysis technique. Precursors such as zinc acetate, indium chloride with a non-ionic surfactant were used. The films variations in (1 0 0), (0 0 2) and (1 0 1) intensities with indium doping. The SEM images showed 50–70nm sized grains, while the TEM confirms formation of grains by ~10nm sized particles. The 3 at% In-doped ZnO showed response as high as 13,000 for 1000ppm H<sub>2</sub>S at 250°C. It exhibits fast response (~2 s) and recovery time (~4 min). The gas response strongly depends on the morphology and indium concentration. The high gas response of IZO is explained on the basis of thickness dependent trap state density.

### Selected publications:

- ✦ *J. American Ceramic Society*, 2008, 91, 2724
- ✦ *Thin Solid Films*, 2008, 516, 6388
- ✦ *Talanta*, 2008, 75, 1315
- ✦ *Sensors and Actuators, B : Chemical*, 2008, 130, 668

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- ✦ K. Vijayamohan, NCL
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- ✦ S. N. Kale, Fergusson College, Pune
- ✦ A. A. Athawale, University of Pune

## Selected publications:

- ✦ *Adv. Mater.*, 2009, 21, 2282
- ✦ *Electrochemistry Commun.*, 2009, 11, 103
- ✦ *Appl. Phys. Lett.*, 2008, 93, 243108; 92, 012512
- ✦ *Phys. Rev. E*, 2008, 77, 066111

## Nanostructured materials

Functional nanomaterials and coatings for solar cells, photocatalysts and biomedical applications



Our research focuses on the development, studies and applications of various metal oxide based as well as semiconductor functional nanomaterials and thin films/coatings. Some of our major activities are:

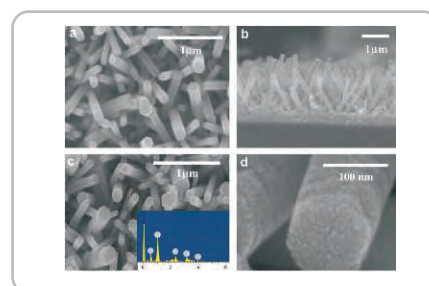
- Shape controlled synthesis of different functional and bifunctional metal oxide nanostructures and exploration of their photocatalysis and energy conversion properties.
- Synthesis and functionalization of metal oxide and semiconductor based hybrid materials and investigation of their optical and magnetic properties.
- Synthesis of magnetic nanomaterials for biomedical applications (hyperthermia).

### Manipulation of magnetic nanostructures through low temperature metal-oxygen chemistry

Dense nanodot and nanotip type morphologies are shown to self-evolve in ultrathin cobalt films during growth under vacuum, depending on the level of oxygen incorporation and temperature. Nanodot morphology is formed at room temperature and the corresponding magnetic hysteresis shows exchange bias (~35 Oe shift along the field axis), which is attributed to the presence of CoO and its exchange coupling with cobalt. The morphology evolves into nanotip features with increase of growth temperature, with concurrent elimination of the oxide component and exchange bias. This work was done in collaboration with CSR, Indore.

Chemical bath deposition of CdS quantum dots on vertically aligned ZnO nanorods for quantum dots-sensitized solar cells  
In this work, done in collaboration with Hanyang University, Korea, formation of CdS

quantum dots (QDs) was achieved on the vertically aligned ZnO nanorods electrode by chemical bath deposition. The diameter and thickness of ZnO nanorods were ~100–150 nm and ~1.6 μm, respectively, and CdS QDs on ZnO nanorods had a diameter smaller than 15 nm. In application of the QD-sensitized solar cells the composite film exhibited a power conversion efficiency of 0.54% under air mass 1.5 condition (80mW/cm<sup>2</sup>), and incident-photon-to-current conversion efficiency showed 18.6%.

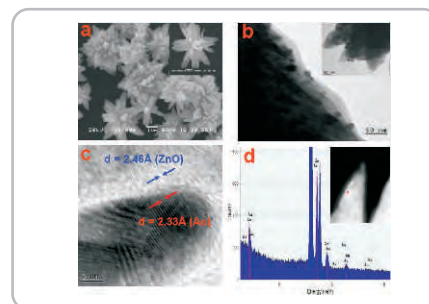


### Enhanced conversion efficiency in dye-sensitized solar cells based on ZnO bifunctional nanoflowers

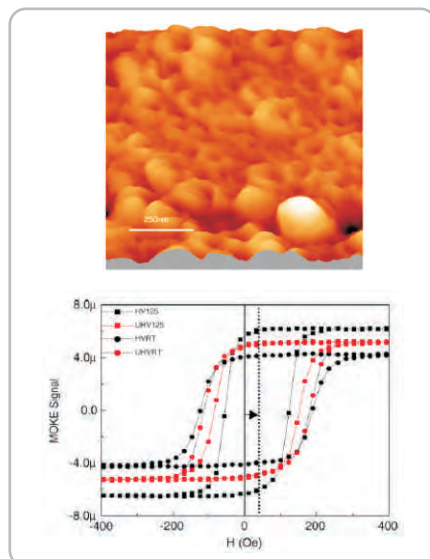
ZnO nanoflowers loaded with gold (Au) nanoparticles (NPs) were synthesized by hydrothermal route using mixed precursors and controlled conditions. The I-V characteristics for N3 dye-sensitized ZnO nanoflower film and Au NP loaded ZnO-nanoflower film were examined. The ZnO nanoflowers with Au NPs showed power conversion efficiency of 2.5%, which is considerably higher than that of ZnO nanoflowers without Au Nps.

### N-Doped TiO<sub>2</sub> nanoparticle-based visible light photocatalyst by modified peroxide Sol-Gel method

In this work good-quality N-doped titania nanoparticles exhibiting visible light



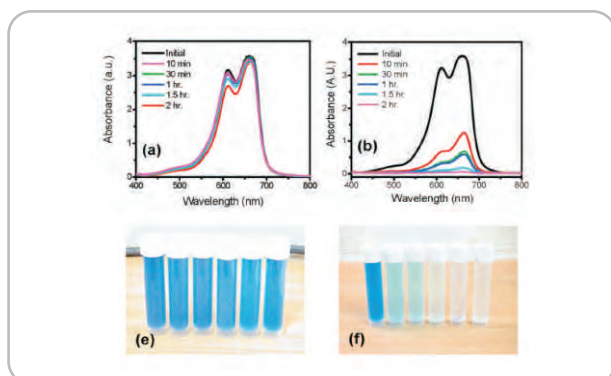
photocatalysis were synthesized at low temperature by the peroxide gel route by incorporating a nitrogen precursor in the sol itself. Nitrogen incorporation in the O-Ti-O matrix and its evolution upon thermal annealing treatment were brought out by various techniques. Specifically, the optical



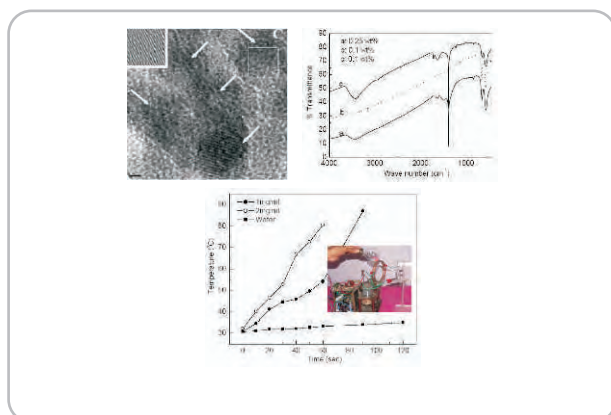


absorption of the nitrogen-incorporated TiO<sub>2</sub> NPs shifts to the visible region in the form of an extended band tailing. It was found that above 400°C, nitrogen escapes the O-Ti-O matrix.

## Nearly monodispersed multifunctional NiCo<sub>2</sub>O<sub>4</sub> spinel nanocrystals: Magnetism, infrared transparency and RF absorption



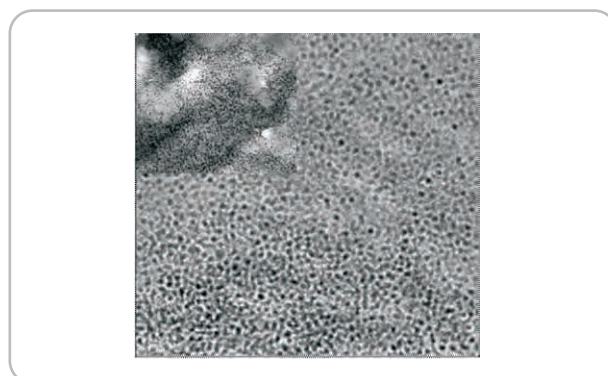
In this study low temperature combustion synthesis of nearly monodispersed NiCo<sub>2</sub>O<sub>4</sub> nanoparticles was achieved. Importantly, these nanoparticles show a high (~83%) infrared transparency and significant radiofrequency (RF) absorption causing substantial heating of their aqueous dispersion that should have potential applications for magnetic hyperthermia.



## Silicate nanoparticles by bioleaching of glass and modification of the glass surface

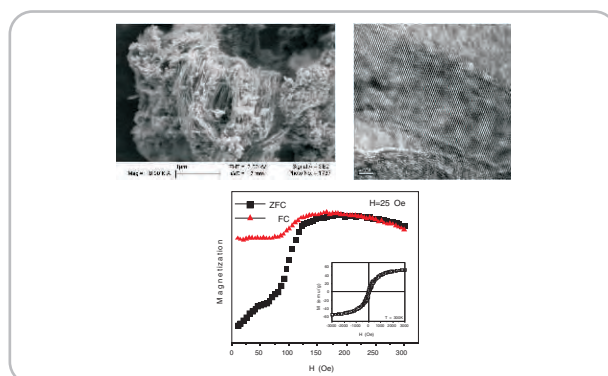
Bioleaching was examined as a low temperature (50°C) soft chemical approach to nanosynthesis and surface processing. We demonstrated that fungus based bioleaching of borosilicate glass enables synthesis of nearly monodispersed ultrafine (~5 ± 0.5 nm) silicate nanoparticles. Using various techniques such as X-ray diffraction, X-ray photoelectron spectroscopy and FTIR, we compared the constitution and composition of nanoparticles with that of the parent glass, and established the basic similarities between the two. The bioleaching process was shown to enhance the non-bridging oxygen component and correspondingly influence the Si-O-Si network. The root mean square roughness of glass surface was seen to increase from 1.27 nm for bare glass to 2.52 nm for 15 h fungal processed case, this increase being equivalent to that for glass annealed at 500°C.

## Non-templated hydrothermal growth of anisotropic magnetite nanostructures using hexamine as the directing agent



Anisotropic growth of magnetite (Fe<sub>3</sub>O<sub>4</sub>) nanoparticles was achieved in hydrothermal synthesis using hexamine to play a dual role of oxide forming and directing agent. Anisotropic structures such as nanorods and nanotubules are revealed and these are shown to exhibit good sensing properties for carbon monoxide and methanol.

## Low temperature synthesis of magnetite and maghemite nanoparticles

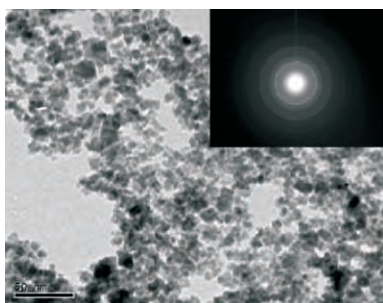


Magnetically controlled resistive switching in CFO/LSMO system

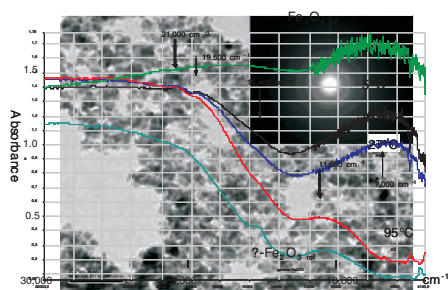
In this work we synthesised iron oxide nanoparticles below 100°C by a simple chemical protocol. The uniqueness of the method lies in the use of Ferrous ammonium sulphate (in conjugation with FeCl<sub>3</sub>) which helps maintain the stability of Fe<sup>2+</sup> state in the reaction sequence thereby controlling the phase formation. Hexamine was added as a stabilizer. The nanoparticles were synthesized at three different temperatures viz, 5°C, 27°C, and 95°C. The nanoparticles synthesized at the lowest temperature exhibit magnetite phase while increase in growth temperature to 95°C leads to the maghemite phase.

## Anomalous microwave heating effects in Ce-doped La<sub>0.7-x</sub>Ce<sub>x</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>: Possible role of grain boundary capacitative effects across cerium solubility limit

In this work microwave heating effects were examined for the case of Ce-doped manganese bulk nanocompacts La<sub>0.7-x</sub>Ce<sub>x</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>. The heating effect was found to be a non-monotonic function of cerium concentration with anomalously high heating (burning) observed for a small concentration



TEM of sample made at 27°C

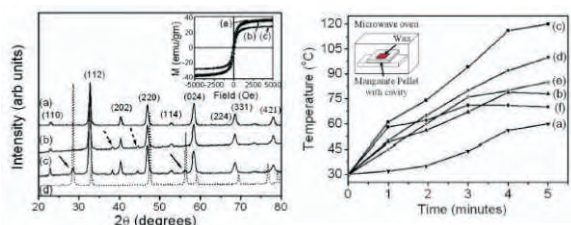


Optical data of various samples

window near  $x=0.03$ . X-ray diffraction studies showed signatures of  $\text{CeO}_2$  phase just emerging in the  $x=0.03$  sample. Various concentration dependent characterizations collectively pointed to the key role of a developing grain boundary  $\text{CeO}_2$  layer that leads to highest capacitive intergrain-coupling and related charging-discharging effects when it is thinnest near the Ce solubility limit.

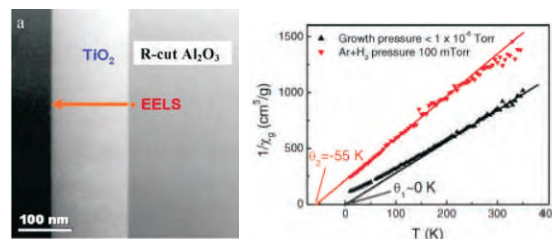
### Mixed state scenario of ferromagnetism in diluted magnetic semiconductor $\text{Co}:\text{TiO}_2$

In this work, we provided a combined window of high resolution scanning transmission electron microscopy and electron energy-loss spectrometry, X-ray absorption (XAS)/X-ray



X-ray diffraction data from (a-c) with increasing Ce concentration in LSMO. The pattern in (d) is for  $\text{CeO}_2$ . Notice appearance of  $\text{CeO}_2$  peaks at intermediate concentration. Right panel shows RF heating data. The data of (c) corresponds to  $x=0.03$ , i.e. 3% Ce in LSMO

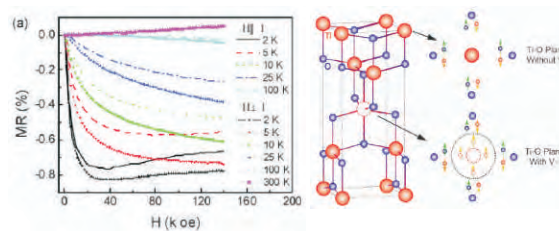
magnetic circular dichroism (XMCD), and magnetization measurements on epitaxial rutile  $\text{Co}_x\text{Ti}_{1-x}\text{O}_2$  ( $x = 0-0.06$ ) system (the first discovered oxide-DMS, which continues to be controversial) grown at low temperature ( $400^\circ\text{C}$ ) under different ambient atmospheres. The study brought out a mixed-state scenario of ferromagnetism involving intrinsic DMS (uniform dopant distribution at low dopant concentration) and coupled cluster magnetism, involving cobalt associations within the matrix at higher concentrations.



Highly uniform dilutely cobalt doped  $\text{TiO}_2$  film without cobalt metal clusters (EELS data showed uniformity of cobalt concentration across film). The right panel shows mixed state ferromagnetism for films grown under different conditions

### Magnetic effect in a non-magnetic transparent oxide semiconductor with non-magnetic ion doping: anatase $\text{Nb}:\text{TiO}_2$

Magnetic effect was observed in a transparent non-magnetic oxide doped with a non-magnetic dopant ( $\text{Ti}_{1-x}\text{Nb}_x\text{O}_2$ ). Temperature-dependent measurement of resistivity, the Hall effect, and MR collectively demonstrate the introduction of magnetic moments in the lattice. The origin of such magnetic moments is attributed to cation vacancies, as shown by X-ray photoelectron spectroscopy and X-ray absorption spectroscopy measurements, and is further supported by first-principles calculations. This suggests that defect ferromagnetism has a potential promise for spintronics.



Temperature and field direction/magnitude dependent magnetoresistance. Model of defect responsible for magnetic moment

## Nanostructured materials



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Biophysics

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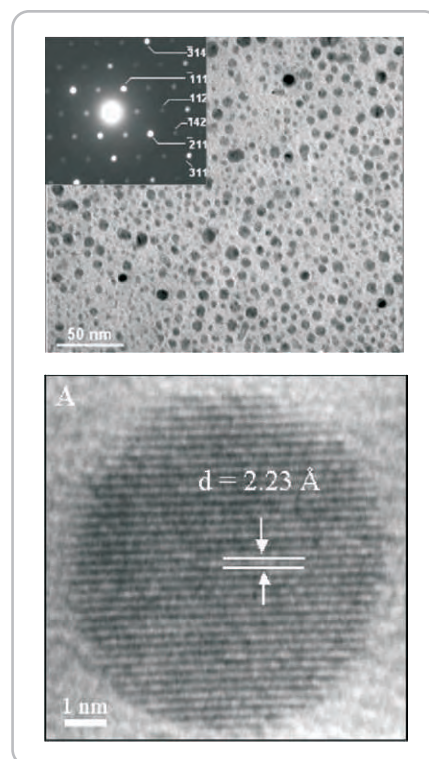
### Collaborators:

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- ✦ K. Selvaraj, NCL

After the advent of novel chemical and microbial techniques, providing control over grain size and shape of the nanomaterials, several binary-oxide materials have been explored in size less than 10 nm for their tunable physical properties.  $\text{Bi}_2\text{O}_3$  nanoparticles have also redrawn attention due to their excellent properties, mostly as optoelectronic material. Here, our key objectives were:

- The room-temperature biosynthesis of  $\text{Bi}_2\text{O}_3$  nanoparticles in a size range of 5–8 nm by extra-cellularly challenging the plant pathogenic fungus—*Fusarium oxysporum* with the bismuth nitrate as precursor
- To synthesis these particles with good stability at room temperature
- To study the structure-property relation in  $\text{Bi}_2\text{O}_3$  nanoparticles

The as-synthesized particle-surfaces are inherently functionalized by a robust layer of proteins which provides them very good stability in the aqueous medium. Structural investigation using selected area electron diffraction, high resolution transmission electron microscopy and powder XRD shows that particles are almost perfectly single crystalline and primarily crystallize in  $\alpha$ -phase with monoclinic structure.



### Selected publications:

- ✦ *J. Nanoscience Nanotech.*, 2008, 8, 3909
- ✦ *J. Appl. Physics*, 2008, 104, 063901
- ✦ *J. Electron Microscopy*, 2008, 57, 113
- ✦ *Applied Biochem. Biotech.*, 2008, 157, 463

Nanostructured materials



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- ✦ A. A. Prabhune, NCL
- ✦ Varsha Pokharkar, Poona College of Pharmacy, Pune
- ✦ Anjali Shiras, NCCS, Pune

Nanoparticle dispersions in different media and diverse applications

The key objectives of work are:

- Finding suitable conditions to make both aqueous dispersions of monolayer ligand protected nanoparticles
- To select the above mentioned ligands such that they effect the dual action – reducing and capping – of the nanoparticles
- Performing appropriate surface functionalization on these nanoparticles for specific applications (drug delivery, cell uptake, decreasing the toxic effects etc.)
- Investigating the application potential of these surface functionalized nanoparticles

Identification of suitable agents for the making of aqueous dispersions of nanoparticles

Through the screening of several reagents, based on the previous work carried out by us and by judicious selection from the screened reagents we could identify sophorolipids, Bovine serum albumin and natural gums (gellan gum, xanthan gum etc) as possible candidates to act as reducing and capping agents to make silver and gold nanoparticles (Fig. 1). We could also show that such particles are stable against aggregation under strong conditions like pH changes and electrolyte additions. Thus these could be potential candidates for drug, fluorescent label loading for drug delivery and cell update experiments.

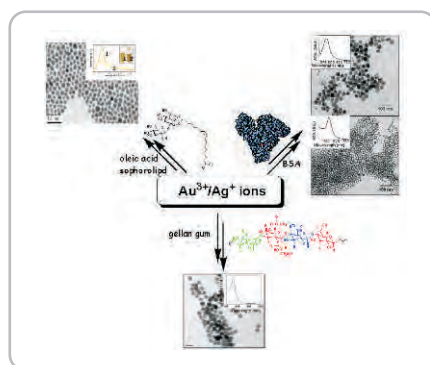


Figure 1: One step aqueous medium based metal nanoparticle synthesis (Au or Ag) using different molecules

Drug delivery applications of gellan gum reduced Doxorubicin loaded gold nanoparticles

In this study, "Gellan Gum" widely used in food and confectionary industry as thickening and gelling agent has been employed as a reducing and stabilizing agent for the synthesis of gold nanoparticles. These nanoparticles displayed great stability

to electrolyte additions and pH changes as compared to the traditional citrate and borohydride reduced ones. Subsequently these have been used to load one of the anthracycline ring antibiotic Doxorubicin hydrochloride. The drug loaded on nanoparticles showed enhanced cytotoxic effect on human glioma cell lines LN-18 and LN-229.

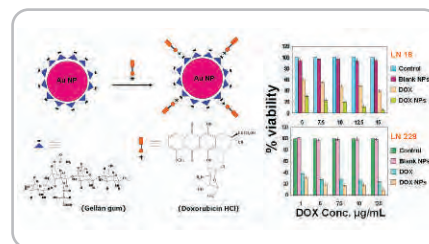


Figure 2: Synthetic scheme of the synthesis of gold nanoparticles reduced/capped by gellan gum and the subsequent drug loading

Cell uptake studies of BSA reduced/capped gold nanoparticles

The uptake behaviour of BSA capped gold nanoparticles (~15 nm) against cancer and normal cell lines have been investigated in detail. We could show that the presence of BSA capping, specifically enhances uptake of these nanoparticles into cancerous cells as compared to normal fibroblast cells. The results show that, extent of their uptake by human glioma cells is critically dependent on the surface chemistry of these nanoparticles.

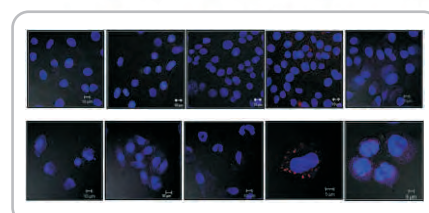


Figure 3: Cell up-take studies with NIH 3T3 (upper panel) and Human Glioma -LN229 (lower panel) cell lines. Notice the enhanced uptake of BSA capped nanoparticles into LN229 cell lines



Concept  
Recent Synthetic Applications of Nanoparticles in Organic Synthesis  
J. M. Corchado et al.

WILEY-VCH

0302-1839(201105)23:05<DOI:10.1002/anie.201100183>1.0.TX:2-#

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## Nanostructured materials



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Ultracapacitor for electric and hybrid vehicle applications

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### Objectives

- Failure mode analysis of Commercial Supercapacitor
- Preparation and characterizations of functionalized carbon nanotubes-Nafion composites as hybrid solid polymer electrolytes for ultracapacitors
- Preparation and characterizations of MWCNT / PEDOT electrodes for super capacitor applications
- Fabrication and analysis of prototype supercapacitors

### Work done and discussion

A commercial supercapacitor was cut opened and analysis of various components of supercapacitor was carried out to understand the materials and basic structure supercapacitor fabrication. The supercapacitor components were analyzed by using SEM, XRD, FT-IR spectroscopy, EDAX, NMR, cyclic voltammetry and electrochemical impedance spectroscopy.

Introduction of solid polymer electrolytes enables thin film fabrication dramatically flexible and convenient with high power density and cycle life. We synthesized sulfonic acid functionalized carbon nanotubes based Nafion composite membrane (NasM) as the electrolyte for all solid-state supercapacitor. The improved capacitance of (NasM) over commercial Nafion electrolyte membranes was confirmed by cyclic voltammetry and galvanostatic charge-discharge measurements. Enhancement in capacitance to the presence of electrostatically linked network structures due to sulfonic acid on the sidewalls of carbon nanotubes which increases the interfacial charge density of the device as confirmed by small angle X-ray scattering studies.

PEDOT-MWCNT composites prepared by ex-situ and in-situ polymerization of EDOT on MWCNT. This study mainly points out the advantage of ex-situ polymerization of EDOT on MWCNT compared to that of in-situ polymerization. The materials were characterized by using SEM, FT-IR spectroscopy, XRD and Cyclic voltammetry. The FT-IR and XRD study confirms the presence of PEDOT on MWCNT. The cyclic

voltammetry studies showed the enhanced performance of PEDOT-MWCNT composites prepared by ex-situ polymerization compared to that of composites prepared by in-situ polymerization.

Prototype supercapacitors were fabricated using the electrode prepared by coating PEDOT-MWCNT and MWCNT on SS 316 mesh. Polypropylene membrane was used as separator for the separation of electrodes in membrane electrode assembly. Non aqueous electrolytes such as 1M LiClO<sub>4</sub> in CH<sub>3</sub>CN and 1 M Tetrabutylammonium-hexafluorophosphate in propylene carbonate were used as electrolyte. Operating voltage of supercapacitor with 1 M LiClO<sub>4</sub>/CH<sub>3</sub>CN electrolyte was 2.5 V and that of 1 M tetrabutylammonium hexafluorophosphate in propylene carbonate was 3.2 V.

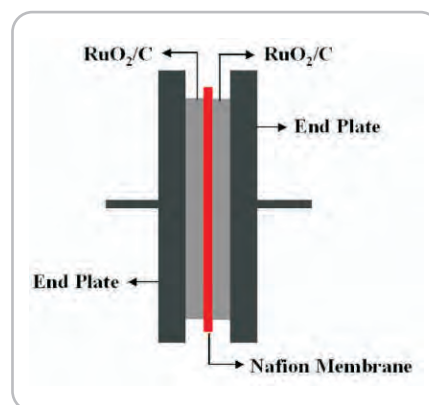


Fig.1 Schematic representation of all solid-state supercapacitor fabricated for analysis

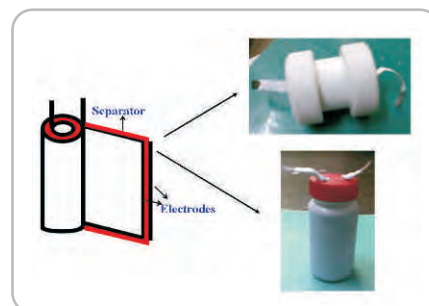


Fig. 2 Prototype supercapacitor fabricated in our lab

### Selected publication:

- ✦ *J. Appl. Electrochem.*, 2009, 39, 1097



Complex fluids and polymer engineering



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Soft condensed matter / synthesis, light scattering and rheology of thermo-sensitive microgels near glassy region

**Objectives**

- To synthesize thermo-sensitive Poly(N-isopropyl acrylamide) microgels of varying cross-linking density using emulsion polymerization
- To investigate the structure and dynamics of these microgels at high concentration especially in the glassy region using light scattering, rheology and confocal microscopy
- To study the effect of softness and the role of interparticle interactions in determining the structure

**Work done and discussion**

Poly(N-isopropyl acrylamide) gels of varying cross linking density were prepared using emulsion polymerization technique. These particles undergo a volume phase transition (VPT) at a temperature about 32°C by expelling water. Dynamic light scattering was used to measure the hydrodynamic diameter of these particles. The particles are found to be highly monodisperse with a polydispersity index less than 1%. We prepared particles in the size range 100-300 nm by changing the cross linker density. With higher cross-linking density, the particles become more compact as can be seen from smaller hydrodynamic diameter in Figure 1.

From static light scattering we measured the 2<sup>nd</sup> virial coefficients which give an idea about the interaction between the microgel particles (Figure 2). We found that the interaction potential is a function of temperature. The interaction potential is repulsive for temperatures below volume phase transition temperature (VPT)(~ 32°C) and become s attractive for temperatures above VPT. We have also prepared ionic microgels by incorporating Acrylic acid group (AAc) during PNIPAM polymerization which gives excellent pH control apart from being temperature sensitive. Figure 3 and 4 respectively shows the changes in zeta potential as well as hydrodynamic radius as a function of solution pH.

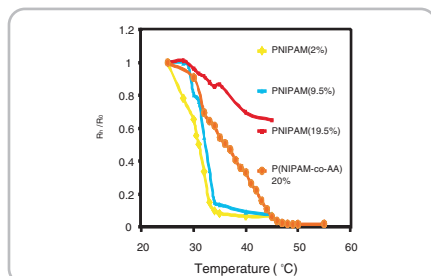


Figure 1: Hydrodynamic radius  $R_h$  for Poly(N-Isopropyl acrylamide) particles for different crosslinker densities as a function of temperature

The rheological measurements done for neutral PNIPAM at a sufficiently high volume fraction shows a glassy like behaviour at temperature below VPT, but it relaxes to liquid like for temperatures above VPT

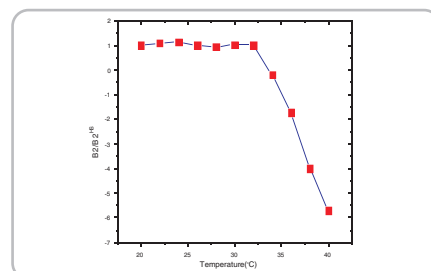


Figure 2: Virial coefficient for PNIPAM particles as a function of temperature. The particles become attractive at higher temperatures

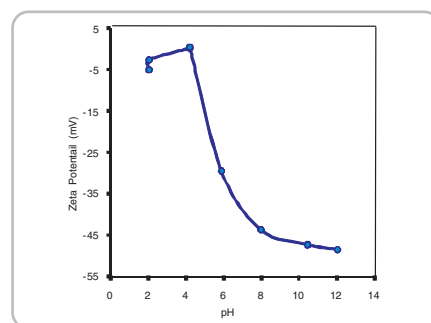


Figure 3: Zeta potential for ionic microgels as a function of solution pH

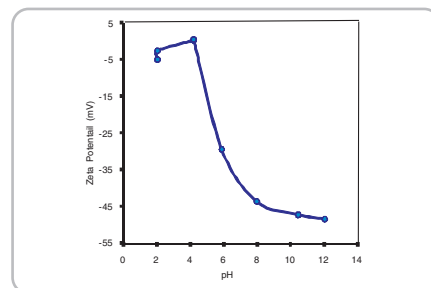


Figure 4: Hydrodynamic radius of ionic microgels as a function of pH

because of the volume phase transition. However at a critical temperature (~32°C) the viscosity is seen to dramatically increase probably because the particles are forming a macroscopic gel due to the attractive nature of their interactions for temperatures above VPT. The behaviour of ionic microgels at higher concentration is very different from neutral microgels. A detailed investigation to study this interesting behaviour is underway.

The interaction potential between the microgels is a function of temperature. The potential changes from repulsive to attractive for temperatures above the volume phase transition. At sufficiently high volume fractions, the microgel suspension show a glassy like behaviour for temperature below VPT, but a dramatic rise in viscosity is seen for temperatures near and above VPT due to the formation of macroscopic gels. The behaviour of ionic microgels in the similar concentration range yielded different results.

## Complex fluids and polymer engineering



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Complex fluids and polymer engineering

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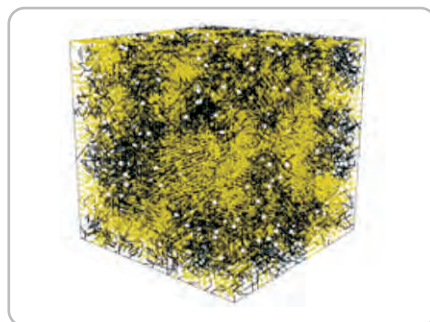
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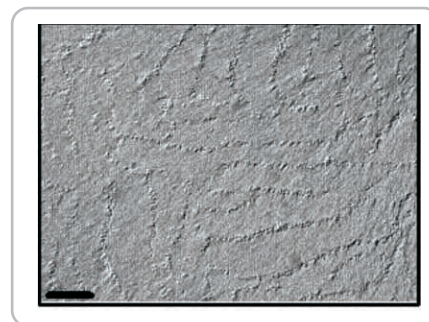
**Influences of additives on polymer melt crystallization**

We used dynamic Monte Carlo simulations to explore the crystallization of polymers doped with a "sticky" antiplasticizer. The effects observed are non-intuitive. Crystallization decreases with increasing stickiness and content of the additive - however, the pathway to the phase transition is altered at intermediate levels of stickiness.

**Particle organization in surfactant hexagonal mesophase**

We have investigated the organization of silica nanoparticles in an organized mesophase of nonionic surfactant. We report a systematic transition in behaviour when the particle size is increased relative to the characteristic mesophase spacing. Our work indicates that the characteristic  $H_1$  length scale delineates different regimes of particle organization in a natural way.

Particles smaller than the characteristic size behave like solvents and swell the space between surfactant cylinders while probably changing the cylinder curvature. Particles comparable to the characteristic size are partitioned - they are partly accommodated in the  $H_1$  phase and partly expelled to form aggregated strands. Even larger particles phase separate from the hexagonal phase to form particulate strands that organize to form



a nanoparticulate mesh. Unusually, the isotropization temperature is increased in the composites as the particles nucleate the formation of the hexagonal phase.

**Selected publications:**

- ✦ *J. Chemical Physics*, 2009, 131, 74905
- ✦ *J. Phys. Chem., B* 2009, 113, 3423



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Complex fluids

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Objectives

- Large amplitude oscillatory shear rheology of soft glassy solids
- Investigating role of chain architecture on the neck-in behaviour of cast films

Work done and discussion

The overarching research theme in the CFPE group is to understand how microstructure develops in complex fluids by the interplay between molecular structure, state variables and imposed deformation parameters. We also attempt to quantitatively understand how the molecular architecture of polymer influences its extrusion behaviour. In pursuit of this theme, we have looked at several types of complex fluids over the past one year. Two examples are described below.

We have investigated the non-linear rheology of soft glasses (for example, PNIPAm microgels, xanthan gum) by using the so called LAOS experiment in the Strain Rate Frequency Sweep (SRFS) mode. In this test, a large amplitude shear strain of sinusoidal frequency is imposed on the sample, and the stress response is deconvoluted into a Fourier series of odd harmonics. Various moduli are computed from this data, and they represent the non-linear response of the material. Interestingly

we found that when this test is done under conditions of SRFS all harmonic moduli can be horizontally shifted to create mastercurves with identical shift factors as shown in Figure 1. This implies that the non-linear response of a complex non-equilibrium material such as soft glass is in fact dictated by only one dominant shear rate dependent relaxation time. This finding has implications in the processibility of soft glassy materials.

Film casting is an industrially relevant process for making packaging films from thermoplastics. When a web of molten viscoelastic polymer is extruded from a slit die and wound on a cooled roll, it undergoes stretch induced necking and edge thickening (Figure 2). Both phenomena are undesirable as they reduce the usable width of the film and cause non-uniform thickness distribution. The extent of necking can be controlled by chain architecture of the polymer, provided a deeper understanding of links between the chain structure, rheology and casting process can be obtained. We are investigating these links using a combination of experiments and simulations. Figure 2 also shows rheology of a LDPE resin in shear and extension, fit of the data to the pom-pom model and comparison of CFD simulations of slit flow with experiments using the pom-pom model.

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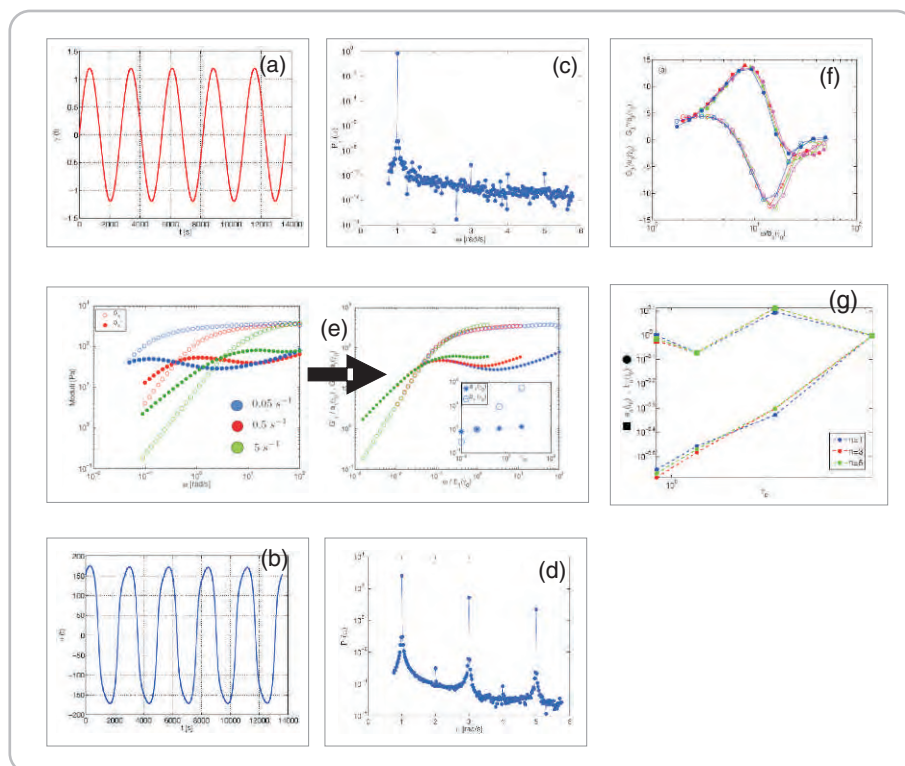


Figure 1: LAOS of soft glassy PNIPAm gels. (a) & (b) show imposed strain and measured stress signals; (c) & (d) show power spectrums of the strain and stress signals; (e) shows SRFS of the first harmonic; (f) shows SRFS of third harmonic and (g) shows shift factors for harmonics 1,3 & 5.

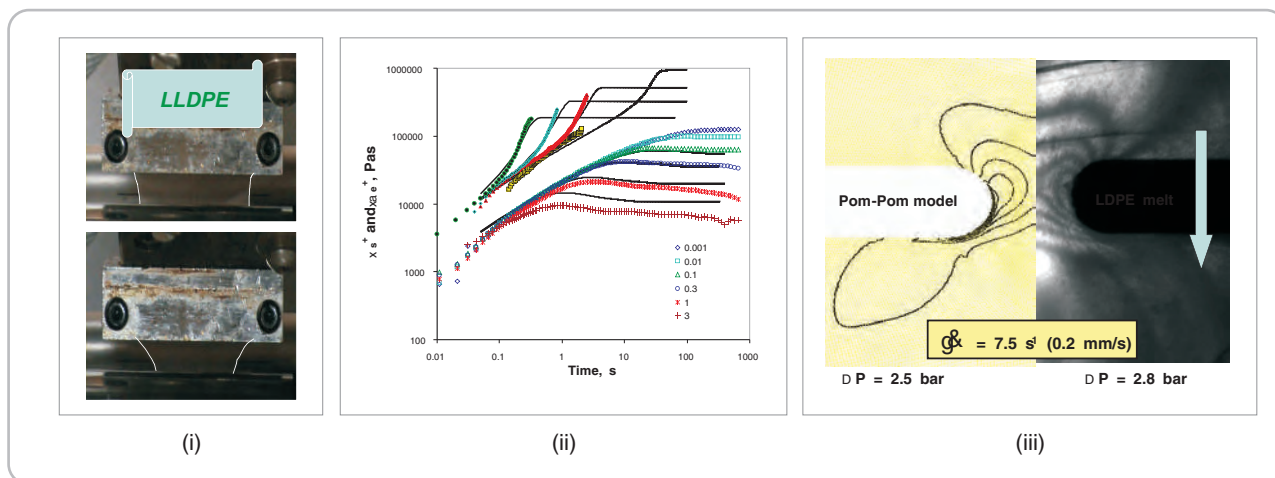


Figure 2: (i) Necking of LLDPE films at low (top) and high (bottom) speeds; (ii) experimental shear and extensional rheology of LDPE (points) and fits to pom-pom model (lines); (iii) comparison of CFD and experimental data on flow through slit in a MPR.

The LAOS experiments showed an interesting flow property of soft solids, namely, that the relaxation spectrum in non-linear deformation is dictated by the imposed rate of deformation, which was not known before. Studies on the industrially relevant film casting process are under way. Specifically, the

links between chain architecture, rheology and complex flows are being studied using rheology, flow birefringence, casting experiments and matching CFD simulations.

## Functional polymers



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## Investigation into the self-organization in urethane methacrylate comb polymers

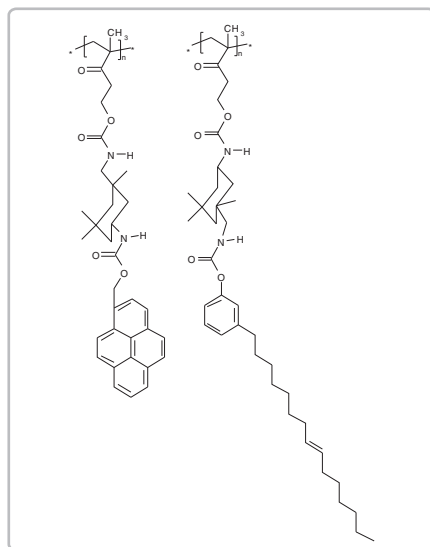
## Background / objectives

Side chain urethane methacrylate polymers with pendant pyrene or cardanol units were synthesized and investigated for their self-organizing process in solution by UV-VIS, and fluorescence spectra and in film by scanning electron microscope (SEM), transmission electron microscope (TEM) and fluorescence microscope.

## Work done and discussion

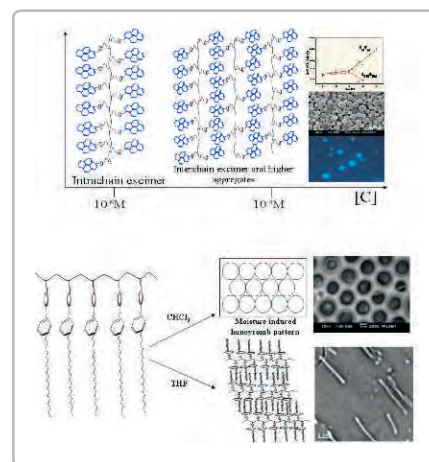
The monomers were synthesized in one pot by coupling one equivalent of isophorone diisocyanate (IPDI) with one equivalent of cardanol/pyrene followed by coupling with one equivalent of hydroxyethyl methacrylate (HEMA). They were polymerized free radically using benzoyl peroxide (BPO) as the initiator and were characterized by NMR, FT-IR and the molecular weights were determined by gel permeation chromatography (GPC). The unique polymer design had sites for self-organization via hydrogen bonding of the side chain urethane units,  $\pi$ - $\pi$  stacking interactions of the aromatic units as well as interdigitation of the long  $C_{15}$  alkyl side chains in the case of the cardanol based polymer.

The structure of the polymers is shown in scheme-1. The pyrene based polymer exhibited the characteristic pyrene excimer emission at 476 nm in THF in dilute condition arising from intrachain interactions but at higher concentrations, interchain interactions also occurred resulting in stable ground state aggregate formation. Drop cast films of the sample from tetrahydrofuran (THF) as solvent showed vesicles whereas those drop cast from THF/ $H_2O$  9:1 solvent combination formed microspheres or compound micelles as observed in the TEM



Scheme -1. Structure of pyrene and cardanol-based urethane methacrylate polymers

images. The cardanol based polymer, exhibited microsphere formation in THF, with most of the spheres having an opening on the surface, as confirmed by SEM. The TEM images of dropcast film from THF showed the coexistence of spheres and tubes. On the other hand, the polymer formed honeycomb patterns from chloroform ( $CHCl_3$ ). Scheme-2 shows the schematic representation of the different types of morphology observed in  $CHCl_3$  and THF.



Scheme-2 (Left) Schematic representation of Inter and intramolecular excimer formation as well as spherical morphology obtained for pyrene based urethane methacrylate comb polymer and (Right) 3D honeycomb pattern formation by breathe figure mechanism from chloroform and self-assembly into multiple morphologies like spheres and tubes from THF observed for cardanol based urethane methacrylate comb polymers.

## Selected publications:

- ✦ *J. Phys. Chem B*, 2009, 113, 11887
- ✦ *J. Polym. Sci. Polym. Chem.*, 2009, 47, 2996

## Functional polymers



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Polymeric heterogeneous supports for removal of metal ion contamination

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Contamination of water by heavy metal ions such as arsenic, chromium, nickel is becoming serious issue due to their associated ecological and health toxic effects at lower concentrations. The metal ions being carcinogenic affect the gastrointestinal tract, cardiac, vascular system and central nervous system. Metal ion removal technologies currently practiced are activated alumina sorption, polymeric anion-exchange and iron oxide coated sand (IOCS) particles. Among these techniques, adsorption is generally preferred for the removal of metal ions because of its high efficiency, easy handling, and availability of different adsorbents. We have synthesised different chelating polymers for removal of toxic heavy metals. The important criteria in designing these chelating polymers is fast complexation as well as reusability. Although techniques for enhancing metal selectivity are easily developed, achieving regularly shaped polymers with sufficient porosity is a drawback.

Epoxy functionalised beaded porous supports of varying pore morphologies were synthesised by copolymerisation of glycidyl methacrylate and allyl glycidyl ether with crosslinkers such as ethylene dimethacrylate and divinyl benzene using a new high internal phase emulsified suspension methodology. This type of HIPE methodology comprises of polymerizing water in oil in water type of emulsions. Surfactant type, surfactant ratio, ratio of discontinuous phase and stirring speed plays an important role in designing the surface properties and morphology of the beads, which effects the efficiency of the beads to be used as adsorbents. All these parameters were studied to synthesise beads having maximum uptake of metal ions. The HIPE beads are more uniform than the corresponding suspension polymerised beads and are characterised by the presence of large cells (cavities) interconnected by a series of smaller pores (windows), thereby enabling each to interact with those adjacent to them (Figure 1). The amount of surface functional groups available for metal binding is also an important criteria for complexation. In HIPE technique there is large amount of water is dispersed in the continuous monomer phase. Therefore, while stabilising the water droplets in the monomer phase large amount of epoxy groups avoid coming to the interface of oil and water, rather they remain in the oil (monomer) phase and are buried in the matrix of polymers. Particle size of majority of the beads observed lies in the range of 0.5 to 100 microns. This is a narrower particle size distribution as

compared to suspension polymerisation where one generally ends up with large beads having a wider particle size distribution (10-2000 micron) at the same stirring rate. The reason for this lies in HIPE methodology. Unlike suspension polymerisation, the particle size in HIPE is determined by the initial rate of stirring. In our method we have used *quasi-dynamic* emulsion polymerisation. Here, the polymerisation proceeds in confined droplets, which are already formed at the beginning. Stirring speeds determine the particle size. It is established that an increase in agitation speed causes a reduction of droplet size formed. The droplet size formed is primarily governed by its growth time prior to detachment, which is effectively reduced at higher shear stress as a result of higher agitation speeds. This indicates that smaller droplets are produced at higher stirring rates. Here, the beads were synthesised at fairly high shear rates so the particle size is low and distribution is narrow.

The cell size and windows were controlled by variations in mixing speed, surfactant (emulsion stabiliser), monomer composition and water/monomer ratio. The epoxy functionalities were derivatised with oligoethyleneimine, characterised by IR and EDAX and evaluated for binding of As (III) and As (V) anions at different pH. It was also observed that as the cross-link density increases, the percentage of PEI attached to poly(GMA-EGDM) and poly(AGE-EGDM) beads decreases, due to decrease in epoxy content. Particle size of the beads is also an important parameter influencing the efficiency of metal adsorption.

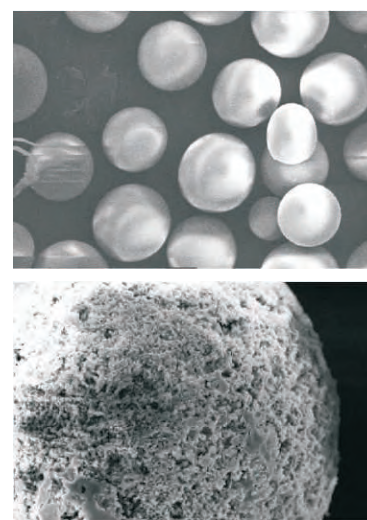


Figure1: SEM micrographs of poly (GMA-EGDM) beads synthesised by HIPE suspension methodology at different magnification: a) 500X b) 10000X.



Maximum As (III) adsorption capacity of PEI-attached poly(GMA-EGDM) in alkaline region was found 262 mg/g and that of poly(AGE-EGDM) was 266 mg/g. Maximum As(V) adsorption capacity of PEI-attached poly(GMA-EGDM) in acidic region was found 225 mg/g and that of poly(AGE-EGDM) was 234 mg/g. Figure 2 shows the arsenic adsorption studies of polymers with variation in crosslink density at different pH conditions. The protonation and deprotonation of the acidic and basic groups of the metal complexation ligand, its adsorption behaviour for metal ions is influenced by the pH, which affects the surface structure of sorbents and the interaction between sorbents and metal ions.

The regenerability of the polymer beads is very important to reduce the process cost. Regeneration of the adsorbed arsenic ions from the beads was also studied. Desorption was performed by using 1.0 M HNO<sub>3</sub> and very high desorption ratios were achieved. These desorbed poly(HIPE) beads can be used for a number of cycles for arsenic removal. During desorption, the coordination spheres of chelated heavy metal ion is disrupted and subsequently arsenic ions are released from the solid surface into the desorption medium.

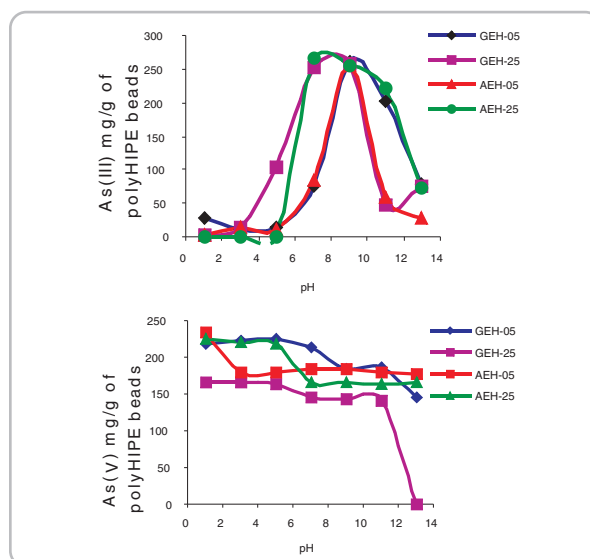


Figure 2 : As (III) and As (V) absorption studies on the polymers synthesised at different pH



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## Membrane science and technology

**PEM membrane for fuel cell**

NCL has been engaged in developing Fuel cell based on high temperature proton exchange membranes; in coordination with other CSIR laboratories (CECRI and NPL). PBI based membrane preparation ( $15 \times 20 \text{ cm}^2$ ) for the working stacks of different capacities and development of new generation PBI membranes are the main goals of the activity. Improving electrochemical performance by optimizing MEA preparation parameters on smaller scale ( $2 \times 2$  to  $5 \times 5 \text{ cm}^2$  active membrane area) is being done at NCL in coordination with the Physical Chemistry division. Exploring the applicability of PBI in other areas such as supercapacitor is also being pursued.

**Gas permeation**

Though high rigidity of PBI could be useful in maintaining its gas selectivity at higher temperature, its low permeability imposes limitations. With an objective of improving gas permeation properties, *N*-substitution of PBI is being performed. Ionic liquids (IL) are known to exhibit high  $\text{CO}_2$  sorption capacity. There are inherent limitations to employ this crucial phenomenon in performing  $\text{CO}_2$  separation using IL-based membranes. Thus, polymeric forms of ionic liquids (PFIL) are being prepared to investigate  $\text{CO}_2$  sorption and membrane formation ability.

**Ultrafiltration**

Towards exploring high chemical stability of PBI family in preparation of acid, base and solvent resistant membranes, ABPBI based membranes were prepared and analyzed for their performance. The supported membranes using PP nonwoven support exhibited molecular weight cut-off (MWCO) of  $\sim 6000$  (Fig. 1).

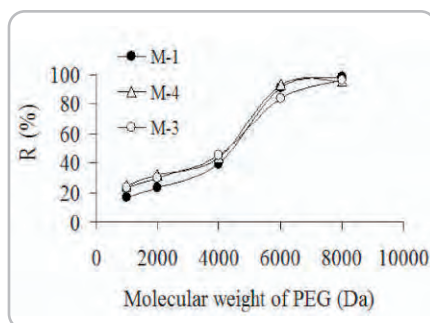


Fig. 1. PEG Rejection of ABPBI based membranes prepared using PP support (M-1, M-2: 6 % dope solution concentration and water / NaOH as the nonsolvent; M-3: 4 % dope solution conc. and water as nonsolvent)

**Selected publications:**

- ✦ *Polymer*, 2009, 50, 1403
- ✦ *J. Applied Electrochemistry*, 2008, 38, 583; 2009, 39, 1097
- ✦ *Chemical Engineering Journal*, 2009, 147, 97
- ✦ *J. Membr. Sci.*, 2009, 320, 159

These membranes exhibit stability towards 25 N  $\text{H}_2\text{SO}_4$ , 2.5 N NaOH and various solvents like DMF, DMAc, dioxane, toluene, hexane, chlorinated solvents and alcohols.

The MWCO of these membranes could be successfully elevated by using polyester nonwoven fabric as support and optimizing membrane preparation parameters, as given in Fig. 2 below.

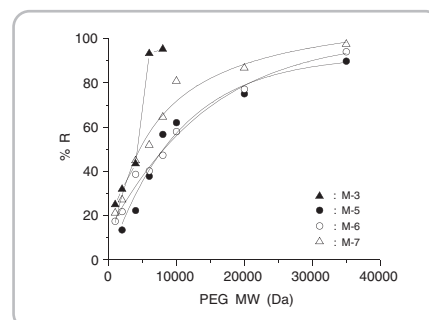


Fig. 2. PEG Rejection of ABPBI based membranes prepared using PP and polyester supports (M-3: membrane with PP support, M-5, M-6 and M-7: membranes prepared with polyester supports).



## Polymers from renewable resources



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Studies on biomass science and technologies, carbohydrate polymers, and biodegradable polymers

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**Background / objectives**

Biomass derived polymers such as cellulose, hemicellulose and lignin constitute one of the most important class of renewable and sustainable feedstock for the production of polymeric materials, chemicals, solvents and fuel. Considerable research efforts, encompassing diverse disciplines such as polymers, microbiology, genetic engineering, enzyme catalysis, chemical and process engineering have been utilized into developing viable technological solutions for new materials based on renewable resources. Poly(hydroxy butyrate), poly(lactic acid)s, poly( $\alpha$ -amino acid)s, poly(aspartic acid)s and aliphatic poly(ester)s derived from 1,4-butane diol and succinic acids are some examples of materials made from renewable resources in recent years. In addition, natural polymers such as modified starch and cellulose have been examined as biodegradable polymeric materials. Chitin / chitosan is another abundant biomass polymer derived from ocean sources, and its structure and properties make it an ideal functionalized polymer for further development into niche as well as bulk polymers. Technologies for obtaining these individual polymers in a pure state, as well as derivatising it to value-added polymers, and utilizing the pretreated biomass for obtaining polymeric materials, chemicals, solvents and fuels which can replace existing technologies utilizing petrochemical feedstocks is a goal of this laboratory.

Development of the science and technology of biodegradable polymers synthesized from natural polymers as well as from synthetic polymers on which are chemically anchored biodegradable natural moieties is another related area of research being pursued in this laboratory. Mechanisms pertaining to the microbial action are being investigated, as this will enable further developments in this field.

**Work done and discussion**

In the area of biomass chemistry and technology, isolation technologies of pure polymeric constituents – cellulose, hemicellulose and lignin – of plant biomass materials was carried out using a variety of techniques. The polymers thus derived were characterized for their structure, morphology, molecular weights, properties, and reactivities. In an analogous research, pretreatment methodologies were investigated with these biomass materials to render them hydrolysable by cellulase and xylanase enzymes; the sugars thus obtained are excellent platform chemicals for transformation, chemically or biochemically, into series of other value-added chemicals, solvents, specialty chemicals, and fuel. In particular, the biofuel ethanol programme was pursued vigorously, and a specific pretreatment was devised to enable enzyme hydrolysis.

In the area of chitin/chitosan, Chitin was crosslinked using diisocyanatohexane (HDI),

trimellitic anhydride (TMA), and dibromodecane (DBD), then deacetylated in strong aqueous alkali. This led to a product with amine functional groups on the exposed surface of the crosslinked chitin, which could be utilized for complexation with heavy metals. Thus, a key feature of the crosslinked derivatives prepared was that only the hydroxy groups were utilized in the crosslinking reaction, and the acetamino groups of chitin were hydrolyzed only after the crosslinking was accomplished. This ensured that all amino groups of the chitosans thus produced would be available for metal complexation, and not partially used up in crosslinking. This proposed advantage was proved by the similar binding observed for heavy metals such as Hg (348-372 mg/g), Cu (91-119 mg/g), Zn (71-92 mg/g), Mn (3-10 mg/g), Cd (121-160 mg/g), and Pb (32-86 mg/g) using these crosslinked polymers (max. and min. values taken from Table 1) whereas the control polymer (uncrosslinked chitosan powder) had complexation values for Hg (348-361 mg/g), Cu (100-106 mg/g), Zn (81-92 mg/g), Mn (4-7 mg/g), Cd (135 mg/g), and Pb (25-59 mg/g). Additionally, in a case where chitosan was crosslinked with HDI, the amino groups were consumed in the crosslinking reaction, and the metal complexation capacity has found to be decreased for Cu (91-109 mg/g), Cd 133 mg/g and Zn (71-77 mg/g) while remaining nearly the same for Hg (362 mg/g). The literature value for Cu complexation is 59.67 mg/g for chitosan crosslinked with glutaraldehyde. The crosslinked derivatives have the added advantage of insolubility even in low pH aqueous media, making their repeated re-use possible. Further, these crosslinked derivatives could be used in a powder form, and the additional step of preparing beads was found to be not necessary for ease of separation of the crosslinked powder by filtration. The binding capacity of various crosslinked chitin and deacetylated derivatives for Cu, Cd, Hg, Zn, Mn, and Pb was in the region of 100, 140, 360, 88, 5 and 60 mg/g (rounded off values) of polymer, respectively, very close to the values obtained for uncrosslinked chitosan. For Cu ions, the Langmuir equation was found to be the best fit for HDI crosslinked deacetylated chitin and TMA crosslinked deacetylated chitin. The morphological studies conducted using WAXRD are in close agreement with the metal complexation data, showing complete loss of original chitosan peaks for the heavily complexed derivatives, and minor changes for the weakly complexed metals.

Biodegradable elastomers based on synthetic polymers styrene-butadiene-styrene and chlorosulfonated polyethylene were undertaken by anchoring of monomeric sugars onto the backbone of the polymers using a variety of synthetic tools such as click chemistry. The work has thrown new light on the types of sugars which cause easy biodegradation by microbes.

**Selected publications:**

- \* *Trends in Carbohydrate Research*, 2009, 1, 10
- \* *Carbohydrate Polym.*, 2008, 71, 66; 2007, 67, 576

## Polymers from renewable resources



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Value added chemicals starting from cashew nut shell liquid

### Members:

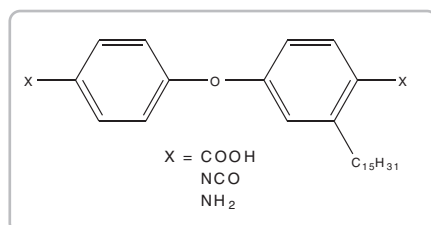
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### Objective

To synthesize condensation monomers, such as diacid, diamine, and diisocyanate, and thermosetting resins, viz., cyanate esters, bismaleimides, epoxies, and propargyl ether resins starting from cashew nut shell liquid (CNSL) - an inexpensive and abundantly available renewable resource material.

### Work done and discussion

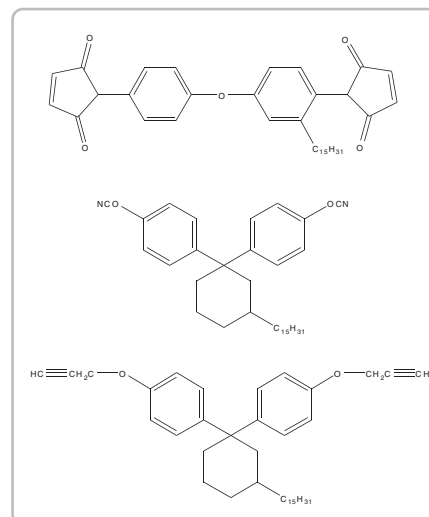
A range of condensation monomers, such as, diacid, diamine, and diisocyanate were synthesized starting from CNSL making use of simple organic transformation reactions (Figure 1).



The highlighting features of these condensation monomers are the presence of flexibilizing ether linkage and pendant pentadecyl chain, both of which contribute to improvement in processing characteristics of the high performance polymers derived therefrom.

Organo-soluble and film forming polyamides, polyimides, poly(amide imide)s and polyazomethines were synthesized by polycondensation of the difunctional polymers obtained from CNSL. These polymers represent an important class of processable high performance polymers which have potential applications as membrane materials for gas separation.

New thermosetting resins viz., cyanate esters, bismaleimides, epoxies, and propargyl ether resins containing pentadecyl chains which acts as an internal plasticizer were synthesized (Figure 2). These thermosetting resins exhibited improved processing characteristics.



CNSL was utilized as a starting material for the synthesis of condensation monomers and thermosetting resins. Polymers derived therefrom possessed an attractive combination of properties such as improved processability and good thermal stability.

Polymers from renewable resources



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Dnyaneswar Rasale, JRF  
Mallinath, PA-II

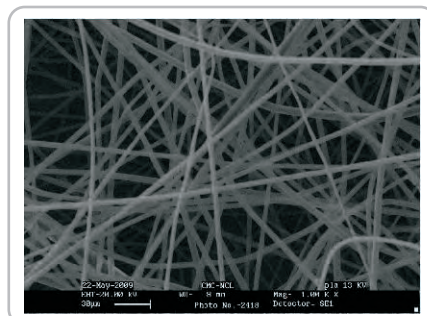
Collaborators:

- ✦ M. Jayabalan, SCTIMST, Thiruranathapuram
- ✦ Rathna GVN, NCL

Polymer synthesis

Polymer supported catalyst was prepared using styrene-divinyl benzene by suspension polymerization, inverse emulsion polymerization. The salts containing transition metals such as Pt, Pd etc. was incorporated in it, and *in situ* and out side reduction were carried out. These prepared catalysts were used for exchange of hydrogen isotopes between gaseous hydrogen and liquid water on a trickle bed reactor. The Pt loaded Styrene-divinyl crosslinked copolymer showed ten-fold better catalytic activity in the trickle bed reactor in comparison with the existing catalyst used in the literature. The surface area and pore volume obtained as 200gm/m<sup>2</sup> and pore volume 0.25gm/c.c. The diameter of the sphere is 2mm.

Synthesis of Biocompatible and Biodegradable Polymer and copolymers particularly based on L-lactic acid (from renewable resources) were carried out. The antibacterial and antifungal drugs were conjugated with polymer backbone covalently selecting appropriate click chemistry. The drugs, particularly azithromycin, was linked to Poly (L-Lactic acid) and L-lactide acid copolymers. The prepared homo and copolymers were successfully electro spun using various solvents and combination of solvents.

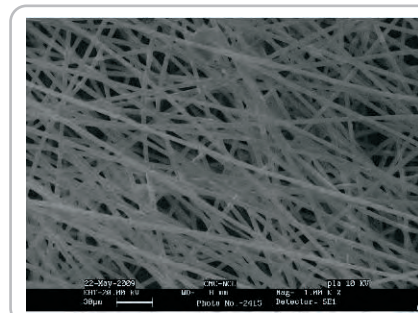


Electrospinning of poly (L, L-Lactide)s

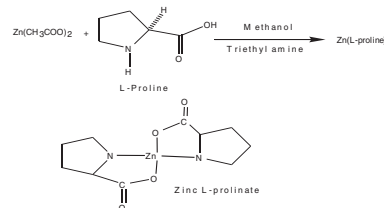
Homo and copolymerization of L,L-lactide in presence of zinc prolinat

Zinc L-prolinat and Zinc D-prolinat catalyst were prepared and used for PLA polymerization L-LA-caprolactone copolymerizations  
Biodegradable random and block copolymers L, LA-ε-CL were synthesized using ring opening polymerization of ε-caprolactone and L, L-lactide in presence of Zn(L-prolinat)<sub>2</sub> catalyst. Scheme 1 shows preparation of a catalyst. Scheme 2 and Scheme 3 show the mechanism of PLLA/PCL random and block copolymers. PLLA/PCL block copolymer was synthesized by ROP by addition of ε-caprolactone and L, L-lactide. Break seal techniques were used in all the experiments of copolymerization reaction. Zn (L-prolinat)<sub>2</sub> caused partial racemization. The isolated copolymer

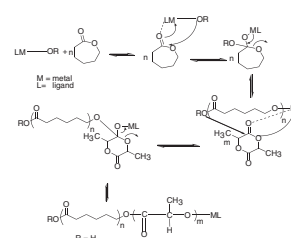
possesses a reasonable composition matching with feed ratio. Results showed that linear copolymer with M<sub>w</sub> ~ 9,000-30,000 can be prepared with Zn (L-prolinat)<sub>2</sub> catalyst. Block copolymer of ε-caprolactone with L, L-lactide resulted M<sub>w</sub> ~ 52,000.



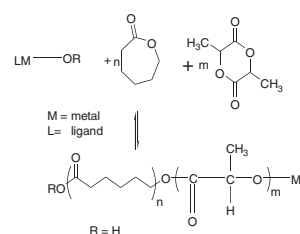
Electrospinning of poly (D,D-Lactide)s



Scheme-1



Scheme 2



Scheme 3

Polymers from renewable resources



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Biocompatible and biodegradable polymers for vital applications

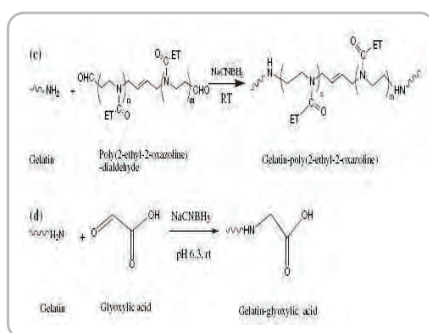
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Collaborators:

- ✦ Jui Chakraborty, CGCRI, Kolkata
- ✦ Sutapa Gosh, IICT, Hyderabad
- ✦ Jyoti P. Jog, NCL
- ✦ B. Garmaik, NCL

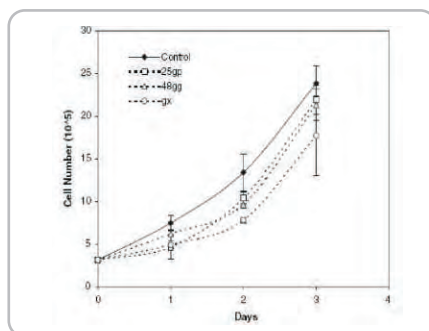
Globally, biodegradable and biocompatible polymers are catching more attention over petro-based polymers due to health and environmental concerns. The natural polymers that are biodegradable and biocompatible are being modified or blended with biocompatible synthetic polymers to compete with the properties of petro-based polymers. The modified polymers with improved properties have vital applications in biomedicine [scaffolds, membranes, nanofibers, implants, sutures, drug carriers], waste water treatment [metal extraction], food packing, etc.



Chemical modification of gelatin with polyoxazoline and glyoxylic acid

Chemically modified protein as drug carriers

Gelatin, egg albumen were conjugated with polyethylene glycol [PEG] polyoxazoline and glyoxylic acid to enhance the biocompatibility and the conjugated gelatin matrix was immobilized with antibacterial drug, chlorhexidine. The drug release studies were done in pH.7.4 and 4.5 at 37°C. Faster drug release was observed in buffer of pH 4.5 over pH 7.4 due to ionization and interaction between polymer and drug. The cytotoxicity studies indicated that gelatin conjugated with polyoxazoline or glyoxylic acid was more biocompatible than the unmodified



Cytotoxicity studies for with and without chemically modified gelatin.

Selected publications:

- ✦ *J. Material Science: Materials in Medicine*, 2008, 19, 2351
- ✦ *Proc of Platinidia, 7th international conference, Delhi* 2009, 7, 68

crosslinked gelatin.

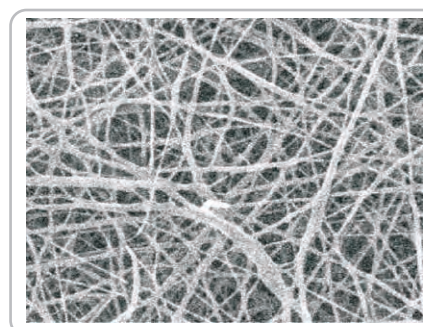
Non-woven nanofiber mats

(a) *Biomedical applications (scaffolds, wound dressings, bone implants)*

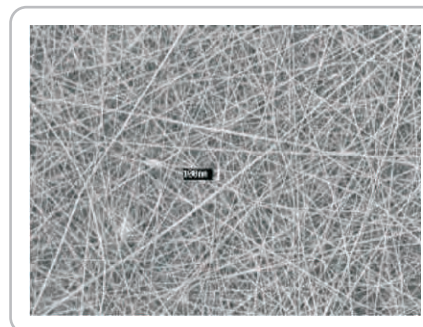
Non-woven nanofiber mats are gaining more attention because nanofibers provide intrinsic advantages such as, high surface area, flexibility, enhanced hydrophilicity, biocompatibility and bio-recognition.

Non-woven nanofiber mats of egg albumen and poly (vinyl alcohol), [PVA] were developed using electrospinning apparatus. Egg albumen did not produce nanofibers at any given concentration. However, nanofibers were developed when egg albumen was blended with biocompatible synthetic polymer poly (vinyl alcohol). From DSC analysis the Tg of PVA recorded 76°C where as the blends of egg albumin with PVA decreased to 52°C. This decrease in Tg indicates that PVA and EA are compatible with out any phase separation.

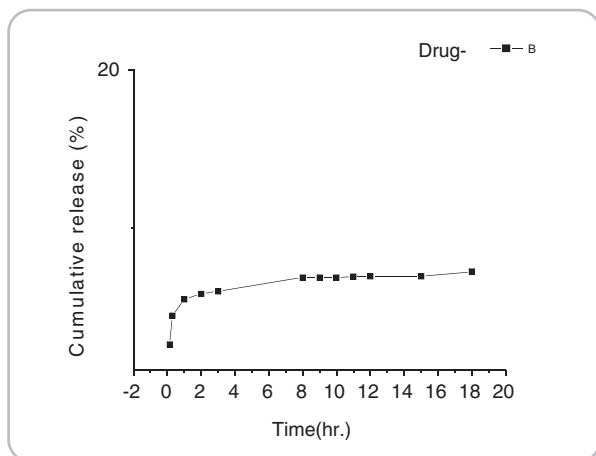
Similarly, sodium alginate was incapable of producing nanofibers at any given concentration but, when this was blended with PVA fine nanofibers were produce which on average was 100 nm in diameter. The nanofibers were loaded with 15 % diltiazem hydrochloride, crosslinked and controlled drug release studies were done in pH 7.4 at 37°C. The drug release experiment recorded only 7 % of release over 24 h because the network was highly crosslinked as result the drug was entrapped.



Drug loaded nano-fibers of sodium alginate and PVA blends



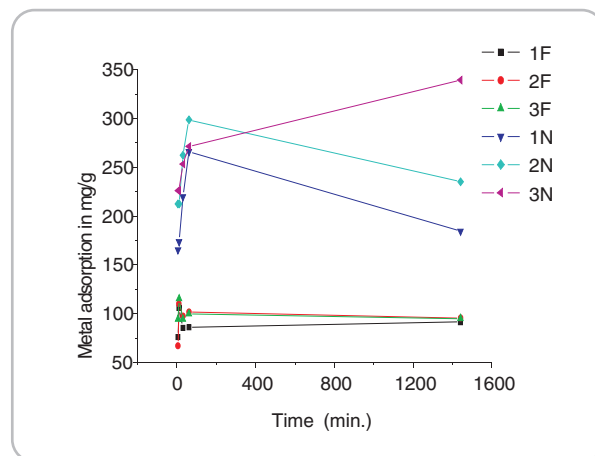
Egg albumen and polyvinyl alcohol nanofibers



Controlled drug release studies of nanofibers

**(b) Metal extraction**

Sodium alginate and PVA nanofiber mats were also evaluated to determine the efficiency to metal adsorption. The results indicated that the nanofibers adsorbed three times of more



Metal adsorption studies of films and nanofibers

metal than the films of the same composition of sodium alginate and PVA. The reason for more adsorption is increased surface area of nanofibers. The metal adsorption increased with increase in sodium alginate.

Structure-property relationships



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Exfoliation of clay layers in polypropylene matrix using potassium succinate-g-polypropylene as compatibilizer

Polypropylene (PP) is one of the most successful thermoplastic polymers and dominates the industrial applications due to its attractive combination of properties such as low density, high thermal stability, resistance to corrosion etc. and low cost. It has been shown that reinforcement with dispersed clay in the polymer matrix enhances the mechanical properties without significantly affecting the density of the polymer. Therefore, efforts have been made to efficiently disperse the clay in the PP matrix. However, such dispersions are hard to prepare in view of the non polar nature of PP. Many researchers introduced ionic groups in nonpolar polymers, thereby, improving the surface energy of the polymer to obtain exfoliated polymer/clay nanocomposites. In the present work we explore the efficiency of PP ionomers to compatibilize higher molecular weight PP in clay. For the first time we show that PP ionomers can be utilized to exfoliate and uniformly disperse the clay layers in a high molecular weight PP matrix.

Cloisite 20A was chosen as the organoclay to be dispersed in the PP matrix. Binary composites containing 95 wt% KPPSA and 5 wt% Cloisite 20A were prepared by melt mixing using DSM micro compounder at 190°C for 10 minutes with a screw speed of 100 rpm. The product was characterized by WAXD. The WAXD pattern [Figure 1 (A)] of KPPSA/Cloisite 20A showed no peak for the organoclay indicating that the organoclay was completely delaminated and exfoliated in the KPPSA matrix. PPMA/Cloisite 20A blend, however, showed a broad low intensity peak with a d-spacing of 38 Å indicating the presence of intercalated tactoids. The above result confirms that the polar ionic functional groups in KPPSA is responsible for the delamination of clay layers and KPPSA is superior to PPMA as a compatibilizer. It may be noted that the PPMA is commonly used for the preparation of PP nanocomposites.

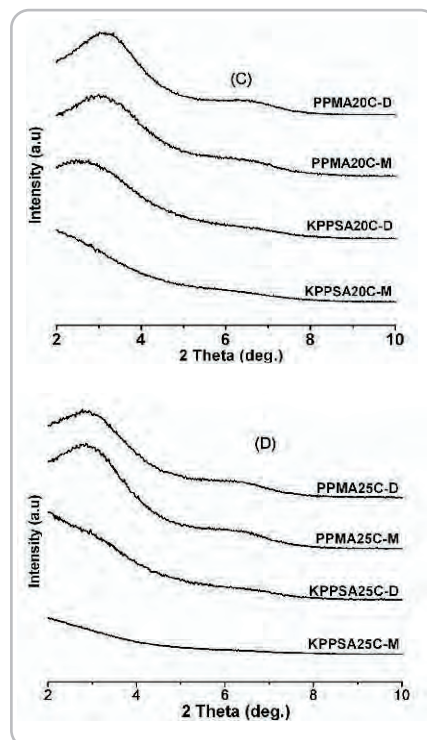
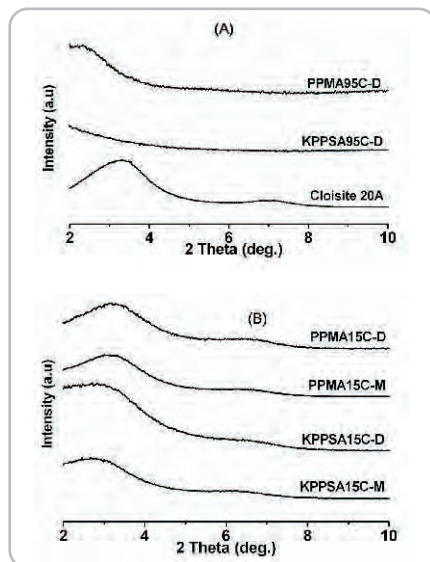


Figure 1: WAXD of nanocomposites of (A) binary composites (B) 15 wt% of the compatibilizers (C) 20 wt% of the compatibilizers (D) 25 wt % of the compatibilizers; In the sample code, the number indicates wt% of the compatibilizer, C indicates 5 wt% cloisite 20A, D for the samples prepared by direct mixing route and M for the samples prepared by masterbatch route.



From TEM micrographs of the nanocomposites prepared by masterbatch route with 25 wt% KPPSA and with 25 wt% PPMA it is evident from the TEM pictures that the nanocomposites prepared with 25 wt% KPPSA as compatibilizer show exfoliated structures where the clay layers are completely delaminated and dispersed homogeneously in the polymer matrix while the nanocomposites prepared with 25 wt% PPMA as compatibilizer showed clusters of clay layers suggesting intercalated structures.

Generally, dispersion of clay in a high molecular weight PP is found to be difficult using a compatibilizer such as PPMA. However, an ionomer such as KPPSA was found to be an efficient compatibilizer even for a high molecular weight PP resulting in the formation of exfoliated nanocomposites.



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### Polymer degradation and stabilization

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The present study is to examine the photo-stabilization effect of antioxidant on the photo-oxidation of ethylene-propylene-diene monomer (EPDM) - clay nanocomposites. The nanocomposites were obtained by solution dispersion followed by melt compounding of EPDM and organophilic montmorillonite (OMMT). They were stabilized with varying antioxidant contents. The degree of interaction of clay-polymer matrix was characterized by X-ray diffraction (XRD) and FTIR spectroscopy. Thermal stability of the prepared nanocomposites was studied by thermo-gravimetric analysis (TGA). They were irradiated in accelerated weathering chamber (SEPA 12/24) using UV-radiation ( $\lambda > 290\text{nm}$ ). Morphological changes upon irradiation were followed by Scanning Electron Microscopy (SEM). It was found that the antagonistic interaction between antioxidant and clays could be lowered by initial incorporation of antioxidant in to EPDM matrix. Hence, the photo-stability of EPDM - OMMT nanocomposite was remarkably improved by the use of antioxidant. Subsequently the physical properties of material can be retained after photo-oxidation.

A significant decrease in the rate of photo-degradation was observed. It was found that this reduction in degradation was linear with the content of antioxidant. Among all the samples, maximum stabilization was observed with antioxidant content up to 1.5%. The changes on the surface morphology have also exhibited the reduced rate of degradation.

The experimental result indicate that the photo-oxidative degradation of EPDM / OMMT nanocomposites is faster than that of pure EPDM and may generate same oxidation products under UV exposure. The acceleration of photo-oxidative degradation of EPDM / OMMT nanocomposites must be due to the clay and ions (clay modifier). The degradability increases with filler concentration. The surface morphology examination shows that degradation starts from surface and then penetrates into the matrix.

The effect of CNT into EPDM matrix was also studied and rate of photo-oxidative degradation of EPDM/CNT composites was found faster than that of pristine EPDM. This may be because of the simultaneous degradation of both CNT as well as EPDM.

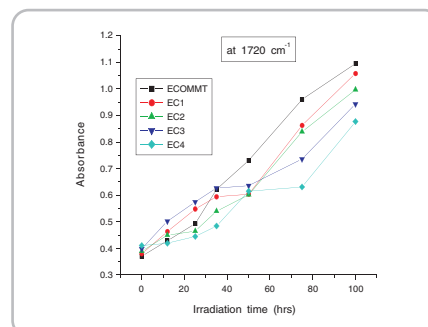


Figure 1. Evolution in the Carbonyl absorption band during the phot-oxidation of the EC-Na<sup>+</sup>, EC-1, EC-2, EC-3 and EC-4

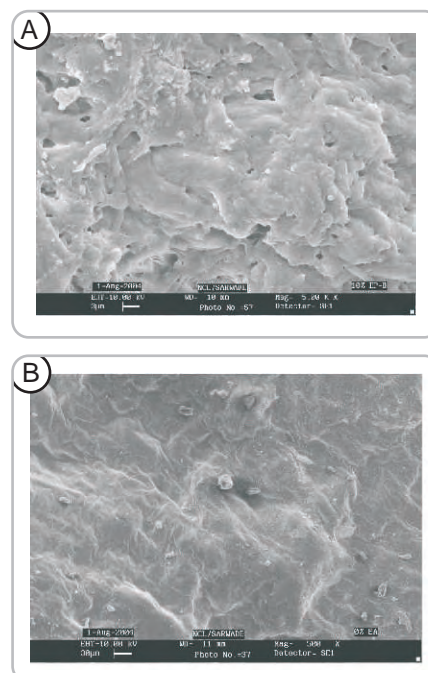


Figure 2. SEM photographs of pristine EPDM (A) and EPDM with clay and antioxidant (B) after 150h UV exposure

#### Selected publications:

- ✦ *Polymers for Advanced Technologies*, 2007, 18, 891
- ✦ *EXPRESS Polymer Letters*, 2007, 1, 748
- ✦ *Bioresource Technology*, 2008, 99, 8803
- ✦ *Polymer Composite*, 2009, 30, 855

## Carbohydrate chemistry



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Carbohydrate chemistry/ chemical glycosylation

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Shivaji A. Thadke, JRF  
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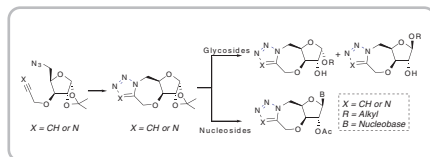
## Collaborators:

- ✦ Souvik Maiti, IGIB, New Delhi
- ✦ B. L. V. Prasad, NCL

Carbohydrate templates have emerged as new and powerful scaffolds for effecting diversity oriented synthesis to obtain natural product-like, oxygen-rich and multicyclic small molecules with high chiral content. In this context, we perform various contemporary reactions such as the Pauson-Khand reaction, Hashmi's reaction, 1,3-dipolar cycloadditions, etc. on carbohydrate templates to obtain libraries which are rich in a number of oxygen atoms and chiral centers and are multicyclic. Interesting observations from this study led us to discover a novel glycosylation protocol exploiting salient features of gold catalysts as well propargyl glycosides. Propargyl glycosides are stable, prepared easily, and orthogonal to various other glycosyl donors that are reported to date. Subsequently, 1,2-orthoesters were introduced to obtain 1,2-trans selective glycosides and oligosaccharides. The overall objectives of the group are: (i) utilization of carbohydrate templates for the synthesis of small molecule libraries with the use of diversity oriented synthesis, (ii) development of novel glycosyl donors exploiting various gold catalysts, (iii) synthesis and evaluation of designer functional materials in collaboration with materials and biophysical chemists

### Diversity oriented synthesis of 1,2,3-triazole fused multi-cyclic glycosides and nucleosides

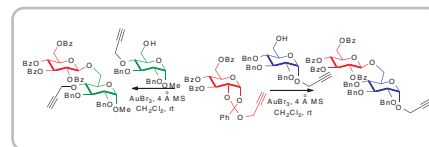
Various 1,2,3-triazole and 1,2,3,4-tetrazole fused multi-cyclic compounds were synthesized from carbohydrate derived azido-alkyne and azido-cyanide substrates. The acid sensitive 1,2-*O*-isopropylidene group of the furanosyl sugar was utilized for diversification to glycosides and nucleosides under Fischer glycosidation and Vorbruggen's conditions, respectively.



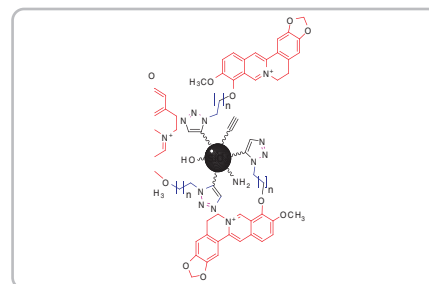
### Gold mediated glycosylations

In continuation of our studies on the propargyl glycosides as glycosyl donors, the selective activation of propargyl 1,2-orthoesters in the presence of propargyl glycosides and ethers using a catalytic amount of AuBr<sub>3</sub> was investigated. It is interesting to note that the AuBr<sub>3</sub> activated propargyloxy group of 1,2-orthoesters though there is a competing propargyl moiety present in the reaction system. The propargylated disaccharides can be utilized to synthesize pseudo-oligosaccharides, neoglycoconjugates and higher saccharides.

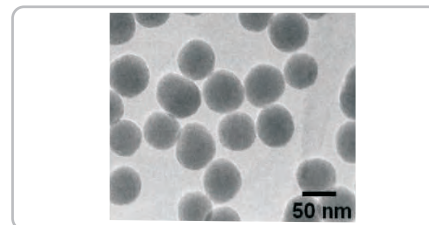
### Natural product-silica conjugates as biological probes



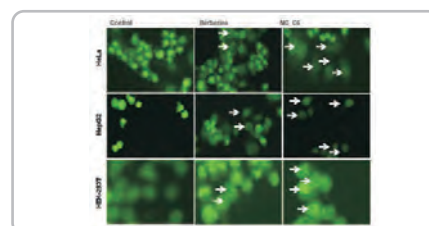
The synthesis and biological characterization of novel prototype, namely, silica nanoconjugates bearing a covalently linked berberine, a plant alkaloid known to have antiproliferative activity, was studied. The effect of synthesized nanoconjugates on the cell proliferation, cell cycle profile and apoptosis in the human cervical carcinoma cell line (HeLa), human hepatocellular liver carcinoma cell line (HepG2) and human embryonic kidney (HEK) 293T cell lines have been studied and compared with that of free berberine. Our results show that all the nanoconjugates display higher antiproliferative activity than free berberine. The ability of these nanoconjugates to inhibit cellular proliferation is mediated by the cell cycle arrest at the G1 phase. Moreover, silica nanoconjugates caused selective apoptotic arrest with a higher efficiency than free berberine followed by apoptotic cell death.



Silica-Berberine nanoconjugates



Morphology of nanoparticle after Capping



Apoptotic cells morphology under Florescence microscopy

## Selected publications:

- ✦ *Org. Biomol. Chem.*, 2008, 6, 779
- ✦ *Chem. Commun.*, 2008, 4282
- ✦ *Langmuir*, 2009, 25, 2339
- ✦ *Curr. Sci.*, 2008, 95, 1327



## Carbohydrate chemistry



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Chemistry of cyclitols

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**Collaborators:**

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**Objectives**

To develop regioselective / enantioselective reactions for cyclitols and their derivatives which aid the synthesis of organic compounds necessary to understand cellular signal transduction and related biological processes.

**Work done and discussion**

A general method for the completely regioselective protection of the three secondary hydroxyl groups of orthoester derivatives of *myo*-inositol, utilizing the subtle differences in reactivity exhibited by its alkali metal alkoxides due to differences in their ability to form chelates, was developed. Similarly, the reaction of inositol derived diols and triols (without the orthoformate bridge) with alkyl halides or sulfonyl chloride could be directed to a hydroxyl group having a vicinal *cis*-oxygen atom, in the presence of lithium ions due to

its ability to form chelates. That metal ion - inositol derivative chelates were involved during the regioselective reactions mentioned above was complemented by the observation that *myo*-inositol derived crown ethers in which two of the oxygen atoms in the crown ether moiety have 1,3-diaxial orientation showed the highest selectivity for binding to lithium (picrate) among the alkali metals (picrates). The O-alkylation methods mentioned above provide convenient access to orthogonally protected *myo*-inositol derivatives. The advantage of using *myo*-inositol orthoesters and their derivatives is that they can be obtained as single products in high yields from commercially available *myo*-inositol, unlike inositol derived acetals, which necessitates the separation of several regioisomers. Acyl transfer reactions in crystalline inositol derivatives were studied to understand their mechanism and utility in the context of objectives mentioned above.

**Selected publications:**

- ✦ *Carbohydr. Res.* 2009, 344, 1159
- ✦ *Tetrahedron*, 2009, 65, 2703
- ✦ *Acta Cryst. C*, 2009, C65, o54
- ✦ *Chem. Eur. J.* 2009, 15, 261



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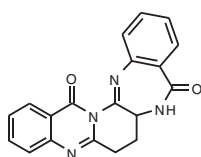
Synthesis of bioactive-natural products

#### Members:

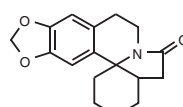
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U. A. Kshirsagar, SRF  
P. B. Wakchaure, SRF  
M. A. Singh, JRF  
P. S. Deore, JRF  
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Total synthesis of bioactive natural products occupies keystone position in organic chemistry. The real challenge lies in designing these molecules using highly efficient and practical routes. Past several years, we have been busy in total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural

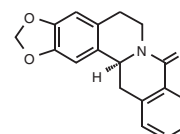
products and natural product hybrids using cyclic anhydrides as potential precursors, employing variety of new synthetic strategies. The list of nitrogen containing natural products synthesized during the past year includes auranthine, Erythrina alkaloid, gusanlung D, isoindolo- $\beta$ -carboline and nuevamine.



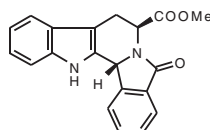
Auranthine



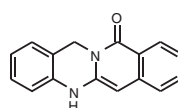
Erythrina alkaloid  
(Basic Skeleton)



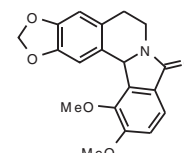
Gusanlung D  
(proposed)



(+)-Isoindolo- $\beta$ -carboline



Isoquinolinoquinazolinone  
(Unnatural)



(+)-Nuevamine

#### Selected publications:

- ✱ *Tetrahedron*, 2009, 65, 5244; 2008, 64, 1786
- ✱ *Tetrahedron: Asymmetry*, 2009, 20, 220
- ✱ *J. Org. Chem.*, 2008, 73, 6936



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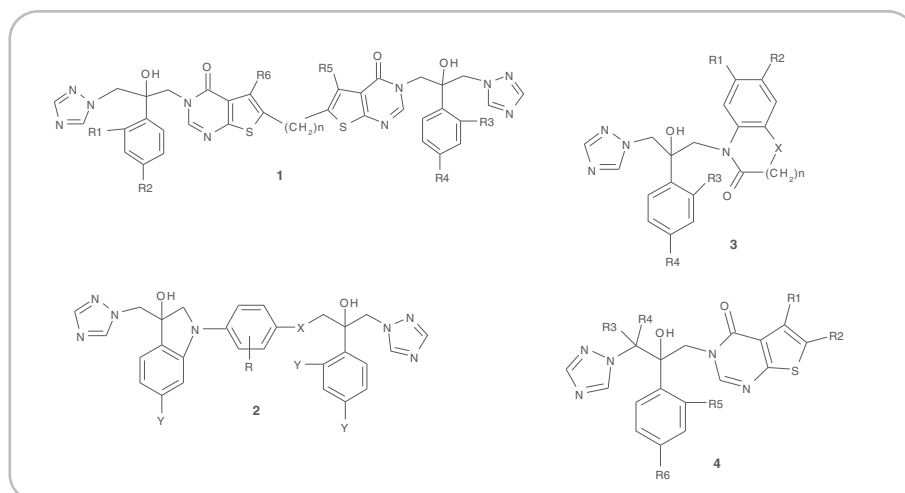
**Members:**Suleman Maujan, SRF  
S. Sawargave, SRF**Collaborators:**

- ✦ S. P. Chavan, NCL
- ✦ FDC Ltd, Mumbai
  - M. A. Chandavarkar
  - Ramki Iyer
  - Vinay Anant Joshi
  - S. R. Vaiude

## Development of novel antifungal agents

Synthesis of novel antifungal agents effective against resistant fungi has attracted the attention of synthetic organic chemists as there is emergence of resistant fungi, and the number of patients with fungal infections has been increasing in recent years. Fluconazole is an important member of the family of azole antifungals as it is orally active and has low toxicity. But its extensive use has resulted in the emergence of fluconazole-resistant fungal strains. We have undertaken synthesis of fluconazole analogues effective against resistant strains and our research has resulted in synthesis of novel antifungal compounds which are being studied in detail.

The dimeric compounds with general structures **1** were synthesized and screened against various strains of fungi to evaluate their potential as antifungal agents. Various hybrid molecules having general structures **2** were also synthesized to study their antifungal activity. More number of compounds with general structure **3** were synthesized and a patent was filed for this class. A number of molecules synthesized in the present work exhibited significant antifungal activity against *Candida albicans* and the compounds are being studied further. The compounds with general structure **4** exhibited significant antifungal activity and one of the compounds (TNF-04) has been selected for detailed biological studies at FDC Ltd, Mumbai.

**Selected publication:**

- ✦ *Ind Patent, Appl. No. 2306/MUM/2008 (24-10-2008)*



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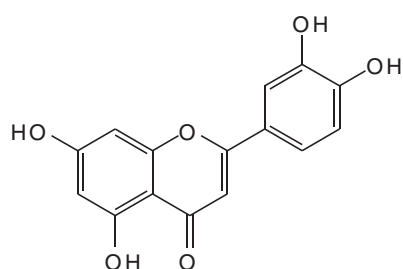
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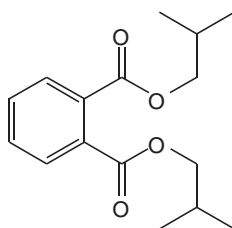
#### Natural products chemistry

After repetitive use of various chromatographic techniques, that is, column, preparative TLC and flash chromatography on EtOAc extract of the *Detarium senegalense* (powdered bark), we isolated two new compounds, one flavonoid, luteolin (**1**) and phthalic acid ester (**2**). Although luteolin (**1**) has been reported from other genus/species but it was first reported from this genus as well as species. Similarly, phthalic acid ester (**2**) is a completely new compound from this genus and species.

Further, we have isolated four secondary metabolites from the EtOAc extract of *D. senegalense*. Their further purification and structure elucidation is at present being carried out.

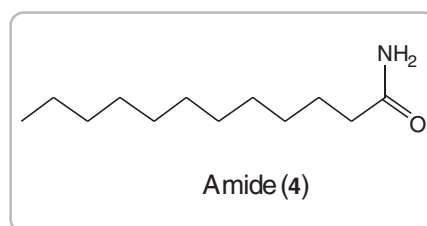
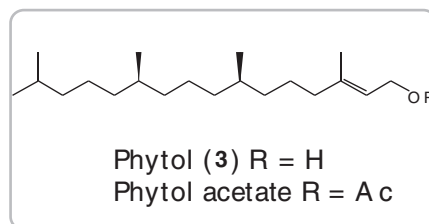


Luteolin (**1**)



Diisobutyl phthalate (**2**)

Chemical examination of the DCM extract of aerial parts of the plant, *Lagascea mollis* using various chromatographic techniques afforded two new secondary metabolites which were identified as a diterpene, phytol (**3**) and an amide (**4**) by their spectral data as well as chemical transformations. Both these compounds are new from this plant species. Further isolation of compounds from DCM extract as well from other extracts of *L. mollis* is underway.



#### Selected publications:

- ✦ *Synlett*, 2007, No. 5, 745
- ✦ *Mendeleev Commun.*, 2007, 17, 247
- ✦ *Synth. Commun.*, 2008, 38, 128; 1518
- ✦ *Tetrahedron Lett.*, 2008, 49, 2598

## Methodologies, asymmetric synthesis and organometallics



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Synthesis of biologically active compounds, development of novel antifungal agents

## Members:

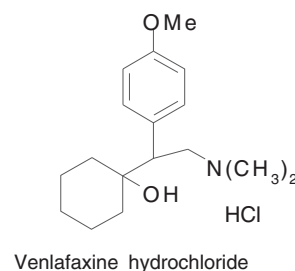
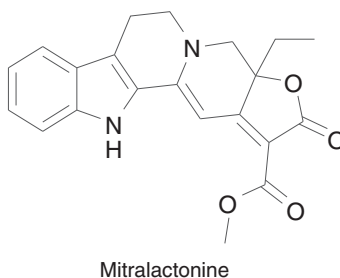
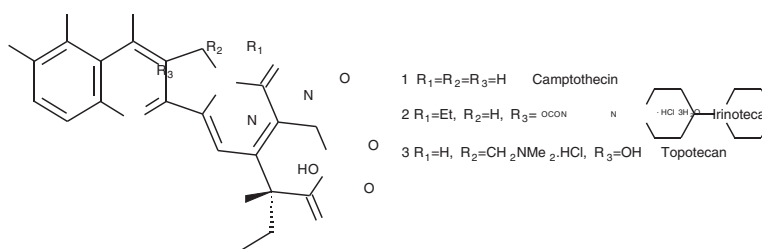
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- ✗ U. R. Kalkote, NCL
- ✗ FDC Ltd, Mumbai
  - M. A. Chandavarkar
  - Ramki Iyer
  - Vinay Anant Joshi
  - S. R. Vaiude

Synthesis of biologically active compounds is the main focus of our group. Synthesis of biologically active compounds includes synthesis of compounds of societal relevance. Conscious efforts are made to synthesise these compounds from a practical point of view. In this regard the emphasis is also laid on developing green protocols or routes for the synthesis of

natural and non-natural products. Synthesis of some of the important molecules such as anticancer compound camptothecin, mitralactonine pipecolic acid, Tamiflu as well as synthetic route towards optically active drug Venlafaxine has been undertaken. Similarly, synthesis of terpenic molecules which include cuparenone, heritol as well as himachalene have also been initiated.



## Selected publications:

- ✗ *Tetrahedron Letters*, 2007, 48, 643; 535; 965; 6561
- ✗ *Syn Commun.*, 2007, 37, 1503; 2337; 3143; 3901; 2008, 38, 3143
- ✗ *Synlett*, 2007, 2635; 2008, 2781
- ✗ *Eur J. Org Chem.*, 2007, 37, 3143



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Application of ionic liquids on dye sensitized solar cells, and metal extractants

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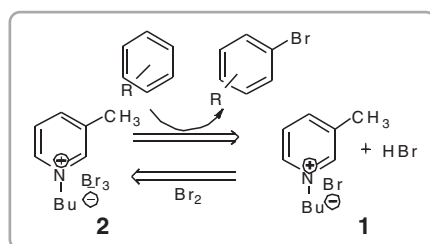
#### Collaborators:

- ✦ Igor V. Pletnev, Moscow State University, Russia
- ✦ Prof. Michael Graetzel, Institute of Chemical Science and Engineering, Lausanne, Switzerland

#### Synthesis of novel ionic liquids and their applications

Ionic Liquids were introduced as alternative green reaction media because of their unique chemical and physical properties of non-volatility, non-inflammability, thermal stability and ease of recyclability. In recent years there has been considerable interest in developing green chemistry for organic synthesis due to environmental demand and sustainability. Today ionic liquids have marked far beyond this border and find wide applications. Recently we have synthesized novel imidazolium and pyridinium based ionic liquids for a variety of organic transformations. Ionic liquids can act as reagent as well as solvent media.

1-Butyl-3-methylpyridinium tribromide, [BMPy] $Br_3$  proves to be a highly efficient, regioselective reagent/solvent for nuclear bromination of various anilines and phenols. The synthesis and characterization of the room temperature ionic liquid [BMPy] $Br_3$  (2) is described below. The bromination was carried out in the absence of organic solvents and in most cases the only extraction solvent needed was water. The spent 1-butyl-3-methylpyridinium bromide (1) was easily recycled.



The new room temperature ionic liquid (RTIL) bromine analog, which is safer and easier to use, was synthesized and characterized. It displayed improved selectivity and better reaction conditions, as compared to current bromination techniques. This new functional RTIL 2 may be classified as 'green' for the following reasons: (a) it eliminates toxic bromine vapors, (b) the bromine carrier 1 can be easily recovered and recycled, and (c) it avoids the use of organic solvents. Furthermore, 2 afforded good-to-excellent yields for a wide variety of anilines and phenols at room temperature. Novel crown ether based imidazolium ionic liquids for metal extractions studies are in progress. Application of ionic liquids as solvents for dye sensitized solar cells is also explored and has lot of advantages.

#### Synthesis of thiosugars

Thiosugars are carbohydrate analogues in which one or more oxygen atoms are substituted by a sulfur atom both in pyranoid and furanoside structures. In recent years, these compounds have attracted considerable interest from chemists and biochemists because of their biological activity. For example mono and oligosaccharide thiosugars have become increasingly important targets due to their potential value as enzyme inhibitors and therapeutic agents such as for diabetes, and antiviral and antineoplastic treatments. A good glycosidase inhibitory activity was found for five and six membered ring analogues of thiosugars.

All the strategies described in the literature to obtain are multi-step reaction sequence, generally through a novel ring opening/recyclization protocol of suitably modified D-sugars (e.g. D-glucose) derivatives.

As a part of doctoral degree programme in our laboratory we are presently dealing with a new organo-catalytic protocol for the synthesis of five and six membered thiosugars. In this regard, we have synthesized two starting materials such as  $C_2$ -symmetric diol (chiral auxiliary) and a miscellaneous mercapto compound. These starting materials have been synthesized using several synthetic steps. The  $C_2$ -symmetric diol and mercapto compound can be used for carbon-sulfur bond forming reaction which will give rise to thiosugars backbone. The thiosugar backbone will be further used for organo-catalytic reaction for the synthesis of thiosugars.

#### Selected publications:

- ✦ *Synthetic Commun.*, 2007, 37, 261
- ✦ *Tetrahedron Letters*, 2009, 50, 1007

## Methodologies, asymmetric synthesis and organometallics



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Development of simple synthetic method for organometallic dioxo molybdenum complexes for catalytic oxidation reactions

Generally organometallic molybdenum complexes are prepared by using corresponding metal carbonyl  $[\text{Mo}(\text{CO})_6]$  as precursor. However, in multi step synthesis of the final complex due to partial decomposition in each step, the yield of final product is very low. When the Mo carbonyl complex is used for oxidation reaction using hydrogen peroxide or TBHP, it forms corresponding oxide complex. Hence the objective was to prepare the organometallic Mo complex using  $\text{MoO}_3$  as cheap and readily available precursor and to reduce the number of steps for preparation of catalytically active species.

Cyclopentadienyl molybdenum dioxo acetylide complex was prepared from  $\text{MoO}_3$  via preparation of  $\text{MoO}_2\text{Cl}_2$  and reacting it further with NaCp followed by Sonogashira coupling with  $\text{PhC}\equiv\text{CH}$  in presence of CuI

and amine as solvent. The complex  $\text{CpMoO}_2(\text{C}\equiv\text{CPh})$  was characterized by FTIR and NMR spectroscopy. This synthetic route has allowed use of simple, inexpensive and easily available precursor such as  $\text{MoO}_3$  for preparation of organometallic complex in very few numbers of steps in the synthesis. Due to less number of steps involved in the synthesis the overall yield of the complex is improved. The formation of corresponding oxo peroxo complex,  $\text{CpMoO}(\text{O}_2)(\text{C}\equiv\text{CPh})$  after addition of hydrogen peroxide was confirmed by FTIR spectroscopy. Oxidation of aromatic alkanes such as ethyl benzene to acetophenone was carried out with very high conversion and very high selectivity for acetophenone. A variety of alkanes have been oxidised to corresponding carbonyl compounds with very high selectivity and very high conversions.

**Selected publications:**

- ✦ *J. Mol. Catal. A.*, 2008, 285, 111
- ✦ *Tetrahedron Letters*, 2008, 49, 3616
- ✦ *Tetrahedron Letters*, 2009, 50, 2885



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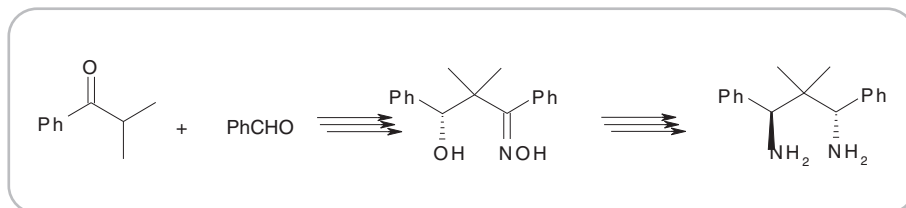
Organic chemistry / asymmetric synthesis

In continuation of our work in the area of enantioselective catalysis, we have been simultaneously engaged in three activities, namely, synthesis of new chiral ligands, addition of organometallic reagents to carbonyl compounds, and our new venture in micellar catalysis. A very brief description is provided below.

#### New chiral ligands

Chiral diamines have proved to be very

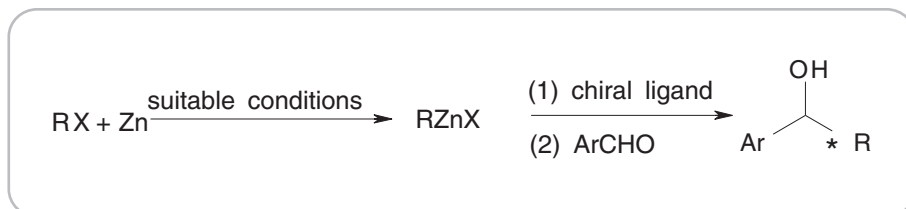
useful in asymmetric synthesis as auxiliaries as well as ligands. Although a variety of 1,2-diamines are well documented, only a few 1,3-derivatives have been reported. We believe that conformationally rigid chiral 1,3-diamines could prove to be very efficient molecules for asymmetric synthesis. In continuation of the scheme reported last year, the following diamine was synthesized. Its resolution and synthetic application is being explored.



#### Alkylation of carbonyl compounds

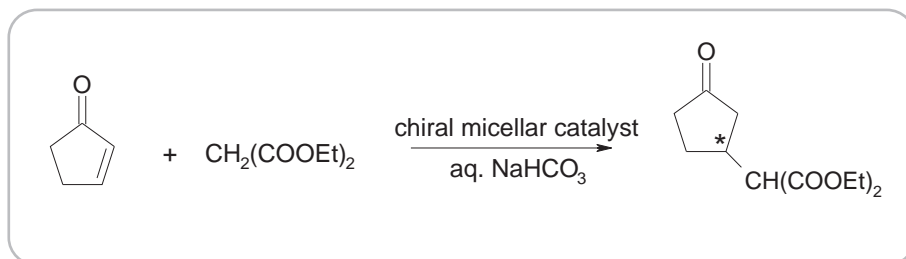
Enantioselective addition of organometallic reagents to carbonyl compounds has been a long standing problem for organic chemists. Direct addition of organolithium or Grignard reagents is very difficult to manipulate due to high reactivity of the reagents. An alternate that emerged in recent times is the catalyzed

addition of less reactive dialkylzinc reagents. However, the choice of reagents is restricted to only a couple of commercially available ones. We have been pursuing this rather difficult target with a hope that an array of organozinc reagents could be made available and reacted catalytically.



Very recently, we have undertaken explorations in the area of micellar catalysis. We believe that chiral micellar catalysts will

be the way to perform many enantioselective reactions in water. Encouraging results have been obtained so far for Michael addition.







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## Process development of methylnaltrexone

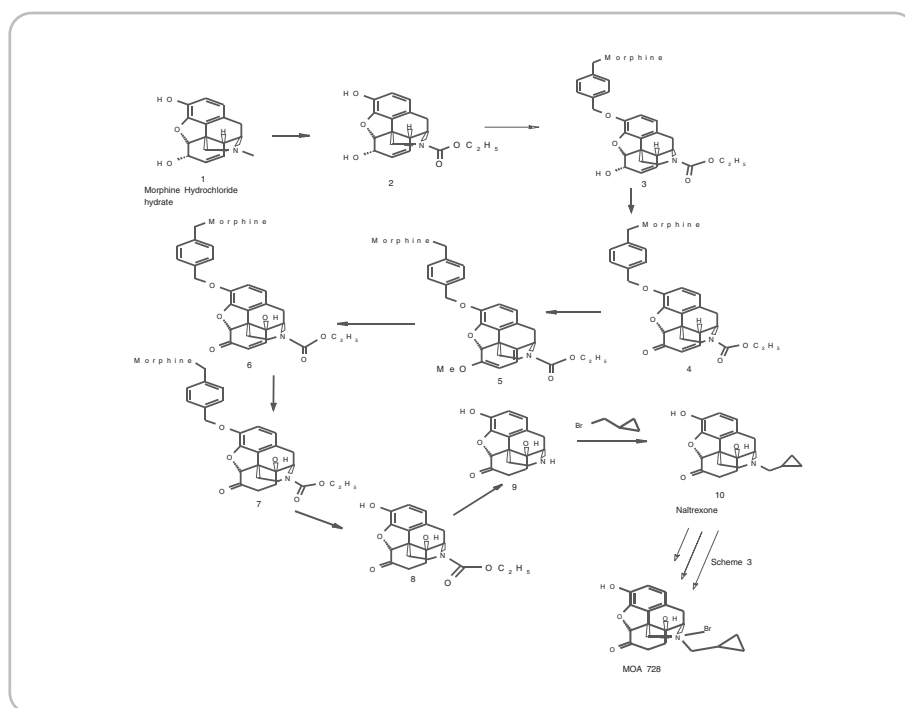
Opioids are widely used in patients with moderate to severe acute and chronic pain, but gastrointestinal side effects such as nausea and constipation can often be debilitating. Opioid-induced bowel dysfunction (OBD) is mediated by mu opioid receptors in both the central nervous system and bowel wall, but the 'peripheral' bowel effects may be more important. Methylnaltrexone (MNTX) is a derivative of naltrexone that does not cross the blood-brain barrier. It acts as a selective antagonist at peripheral opioid receptors without reversing central effects such as analgesia. In preclinical and human volunteer studies, parenteral and oral MNTX consistently reversed OBD at doses that produced minimal side effects. Intravenous MNTX also reversed opioid inhibition of bladder function, suggesting a possible role in the treatment of opioid-induced urinary retention. Two phase III studies showed that s.c. administration of 0.15-0.3 mg/kg MNTX induced laxation in patients with advanced medical illness given chronic opioids. Additional studies of MNTX targeting postoperative ileus also show promise. An NDA submission is anticipated in early 2008.

Synthesis of Naltrexone was planned from morphine as described in scheme:

Morphine was treated with ethylchloroformate in presence of a mixture sodium carbonate and sodium bicarbonate in toluene to obtain >85% carbamate derivative with 97% HPLC purity.

Carbamate derivative (**2**) on reaction with  $\alpha, \alpha'$ -dibromo *p*-xylene in presence of potassium carbonate in toluene yielded bis derivative (**3**) >70% yield with 78% HPLC purity. Bis derivative **3** on PCC oxidation gave bis keto compound **4** in >90% yield in 90% HPLC purity. Bis keto **4** was treated with Cobalt (II) acetate, sodium acetate in ethanol at reflux temperature with continuous air bubble for 70 hrs to yield 14-hydroxy derivative **6** in 75% yield (HPLC purity 78%) which on selective reduction with Pd/C obtained **7** with 95% HPLC purity, and which on debenzoylation with Pd/C yielded **8**, which on decarbonylation in sulphuric acid gave demethylated compound **9** in 60% yield with (78% HPLC purity). On reaction of **9** with cyclopropyl methyl bromide in presence of potassium carbonate yielded naltrexone (**10**) in 75% yield with >94% HPLC purity.

Here naltrexone was reacted with  $\alpha, \alpha'$ -dibromo *p*-xylene in presence of potassium carbonate in toluene yielded bis derivative of naltrexone **11** in 88% yield with >90% HPLC purity. Bis naltrexone derivative **11**, on reaction with methylbromide in piperidine at 60 °C for 72 hrs gave methyl bis naltrexone bromo derivative (**12**) in 65% yield with 89% HPLC Purity which on treatment with Pd/C gave methylnaltrexone bromide (MOA 728) in 85% yield with 94% HPLC purity.





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Asymmetric total synthesis of biologically active natural products

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Ankush D. Bhise, SRF  
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#### Collaborator:

✦ P. K. Shukla, CDRI,  
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#### Background/ Objectives

The theme of the work is to develop new synthetic methodology and simple, flexible and diversity oriented approach for the enantioselective synthesis of biologically active natural products. Our research in this area is mainly focused on asymmetric synthesis of naturally occurring lactones, amino alcohols and cyclic ethers.

#### Asymmetric synthesis of naturally occurring amino alcohols, lactones and cyclic ethers

My research group is mainly involved in the total synthesis of a wide variety of biologically useful compounds mainly employing the AD/AE/AA or Jacobsen

hydrolytic kinetic resolution as the source of chirality and ring closing metathesis as one of the key steps. These target molecules include decastrictine D, medium sized cyclic ethers such as (-)-cis-lauthisan and (+)-isolaurepan. Similarly tethered amino hydroxylation protocol was used to synthesise amino alcohols such as phytosphingosine. Recently we developed a general protocol for the construction of *syn*- and *anti*-1,3-polyols which is based on sequential aminoxylation, HWE reaction of an aldehyde and reduction via proline catalysed reaction. Its usage was demonstrated successfully by the synthesis of a pheromone component, lactone.

#### Selected publications:

- ✦ *Synlett*, 2009, 1367
- ✦ *Organic Letters*, 2009, 12, 2611
- ✦ *Tetrahedron*, 2009, 65, 2226
- ✦ *Tetrahedron Lett.*, 2009, 50, 3425

## Methodologies, asymmetric synthesis and organometallics



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Design, synthesis and biological evaluation of natural product like small molecules/Asymmetric synthesis of pharmaceutically important compounds

## Objectives

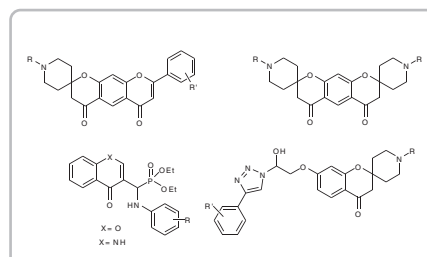
- Design and synthesis of novel *chromone* based structures and their chemical modification leading to a collection of small molecules for biological evaluation
- Asymmetric synthesis of pharmaceutically important compounds

## Work done and discussion

Nature has always been an important source of lead compounds for the development of new therapeutic agents. By modifying a biologically active natural compound, libraries of structurally similar but non-natural, synthetic analogues are created such that the molecular complexity is kept to a minimum whilst improvements are made to the desired pharmacological activity. To address this, we have chosen a chromone nucleus as a *privileged* structural unit for our library generation. In the present work, we successfully prepared natural product-like small molecule hybrids, homodimers, aminophosphonates etc based on chromone scaffold system and generated compounds are being screened for potential biological activity.

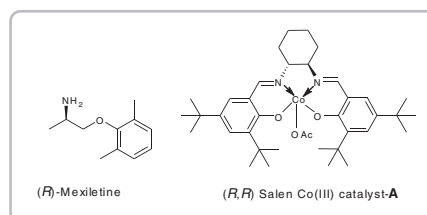
In continuation of our work in the area of asymmetric synthesis of pharmaceutically

important compounds, we developed a practical and highly enantioselective synthetic route to an antiarrhythmic drug MexitilR using Jacobsen's hydrolytic kinetic resolution method as a key step.



Representative examples of natural product-like chromone variants synthesized

In continuation of our work in the area of asymmetric synthesis of pharmaceutically important compounds, we developed a practical and highly enantioselective synthetic route to an antiarrhythmic drug MexitilR using Jacobsen's hydrolytic kinetic resolution method as a key step.



## Selected publications:

- ✦ *Tetrahedron*, 2007, 63, 1872
- ✦ *Synth. Commun.*, 2008, 38, 3875
- ✦ *Tetrahedron Lett.*, 2009, 50, 2643
- ✦ *US patent*, 2007, 7,227,039



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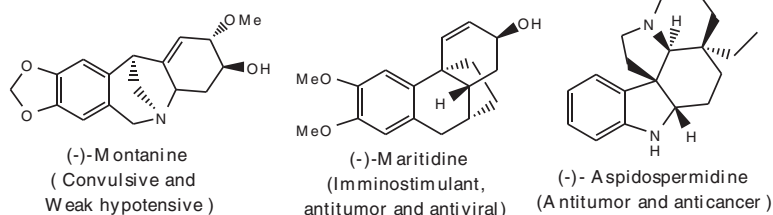
Total synthesis of complex bioactive natural products and azasugars

### Background / objectives

During the year, our research activities centered on the development of novel C-C bond formation reactions and their application in the synthesis of many of structurally complex molecules having promising biological properties. The group

and synthesized by employing PET initiated carbocyclisation of amine radical cation to electron rich olefins.

4. Synthesis of 1,10b-*epi*-7-Deoxypancratistatin and its amine analogue using Suzuki cross-coupling and

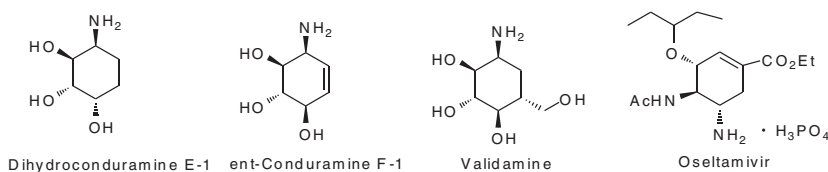


has also focused attention on the synthesis of new conformationally restricted aza sugars which are known as glycosidase inhibitors.

1. Intramolecular [3+2]-cycloaddition of non-stabilized AMY in the synthesis of polycyclic alkaloids.

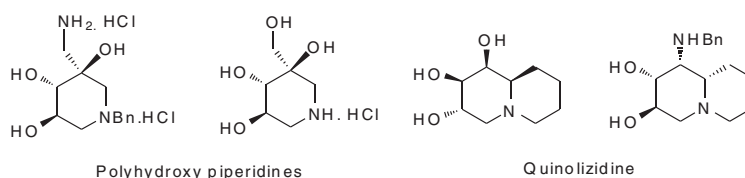
intramolecular aza-Michael addition reaction were accomplished.

The cytotoxicity of the new deoxypancratistatin derivatives have been studied against human cancer cell lines and were found to be poorer than the natural isomers.



The formal synthesis of Pancracine (Montanine type of alkaloids) and the total synthesis of Maritidine have been accomplished and the total synthesis of Aspidospermidine is in progress.

5. Suzuki cross-coupling/reductive debenzoyloxycarbonylation sequence has been developed for the syntheses of [C]annulated isoquinolines.



### Selected publications:

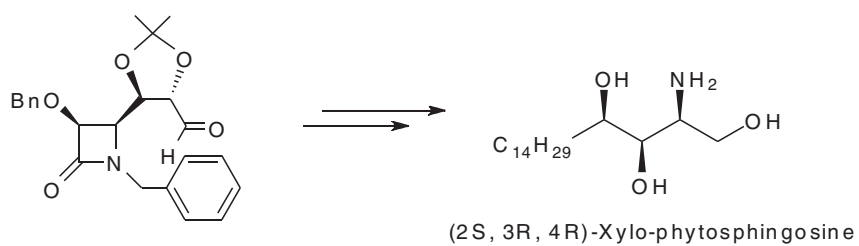
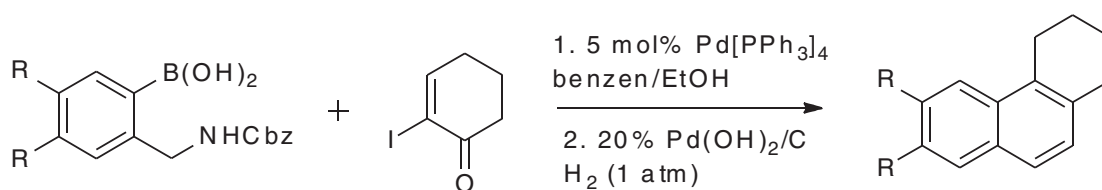
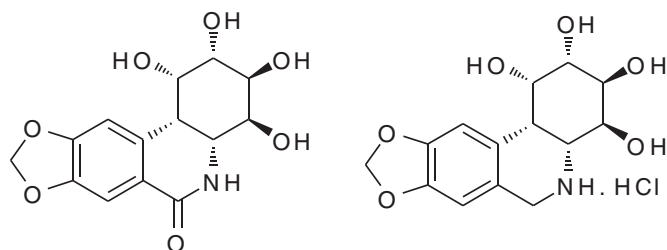
- *Org. Lett.*, 2005, 7, 3713; 2008, 10, 3611; 2009, 11, 2547
- *Org. Biomol. Chem.*, 2009, 7, 3300
- *Eur. J. Org. Chem.*, 2008, 5839
- *J. Org. Chem.*, 2008, 73, 8128

2. The syntheses of dihydroconduramine E-1 and ent-Conduramine F-1 were successfully accomplished using asymmetric desymmetrization of meso-*tert*-butyl 2,3-bis(phenylsulfonyl)-7-azabicyclo [2.2.1]hept-2-ene-7-carboxylate. The synthesis of Validamine and Osettamivir is in progress.

3. A library of glycosidase inhibitors (polyhydroxy aza-sugars) has been designed

The method was successfully applied to the syntheses of range of both substituted and unsubstituted cycloalkene-fused isoquinolines.

6. Enantiomerically pure (2S,3R,4R)-D-xylo phytosphingosine has been synthesized in 36% overall yield in seven steps from known  $\beta$ -lactam derived from D-mannitol triacetone.





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Organic syntheses, synthetic carbohydrate chemistry and transition metal catalysis

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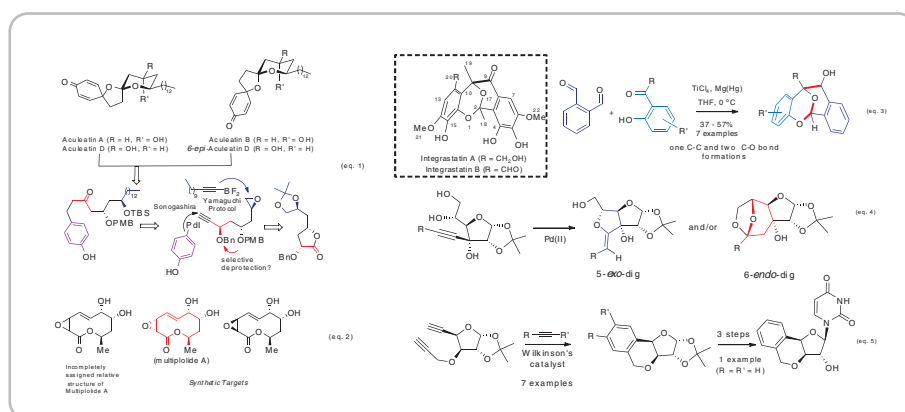
### Collaborators:

- ✦ B. L. V. Prasad, NCL
- ✦ Rajesh G. Gonnade, NCL
- ✦ P. K. Shukla, CDRI, Lucknow

In the wake of the failure of the combinatorial libraries in delivering a magic bullet, attention has focused back on the complexity and diversity of nature's small-molecules in the new drug discovery programmes. Concepts funded upon the designing around, and of the synthesis of natural products and natural product such as small molecules have provided a direct entry of 'total synthesis programmes' into medicinal chemistry research. Development of synthetic methods that are efficient and the design of strategies that are modular with a flexibility window is a prerequisite for the synthesis of natural products is derived and inspired compound collections. Synthesis of a wide array of such complex molecules requires the flexibility in terms of the reagents/substrates to be employed and more importantly the reactions that address the skeletal diversity from similar as well as simple intermediates. The development of such tools demands integration of powerful mechanistic thinking and innovative substrate design which form the basic criterion of our research programmes. We also intend to extend these simple and novel approaches for small

The adopted strategy features ring-closing metathesis (RCM) as the key reaction and screening of a set of substrates for the feasibility of RCM in general and for the requisite *E*-configuration of ring olefin in particular. Selective protecting group manipulation prior to the assembly of the central macrocyclic core was instrumental in installing the epoxide functionality on a fully deprotected nonenolide at the end of synthesis.

A facile one-step approach for the central tetracyclic core of integrastatins by employing low-valent titanium mediated pinacol cross coupling reaction has been documented. The present approach is characterized by consecutive formation of three bonds affording topologically complex tetracyclic compounds (eq.3). This adds another facet to the pinacol reaction with a potential to be extended for other structurally complex molecules by judicious substrate design. Pd-mediated cycloisomerization of 3-C-alkynyl-allo- and ribofuranose derivatives was investigated in detail to understand the influence of electronic factors on the



molecule libraries which can find application in crystal engineering and material chemistry.

We have recently described the concise assembly of aculeatin D. Central to the success of our approach is a dual-end disconnection of the aculeatins core leading to three segments in which the two terminal segments are easily available and are amicable towards alterations for the synthesis of aculeatin like small molecule libraries (eq. 1). A flexible approach for the total syntheses of possible multiplolide A diastereomers establishing the relative and absolute configuration is documented (eq.2).

regioselectivity in ring closure reaction also to provide a simple access to highly functionalized tetrahydrofuran fused bicyclic acetals and enol ether derivatives (eq.4). A general synthesis of chiral isochromans via [2+2]-cyclootrimerization of a sugar template as the key reaction was reported. One of the derived isochromans was converted into a tricyclic nucleoside by simple synthetic manipulations (eq.5).

Another area we have started recently deals with the synthesis of C-glycosides for medicinal and material applications. In this context we have developed a general and stereoselective approach for the synthesis of

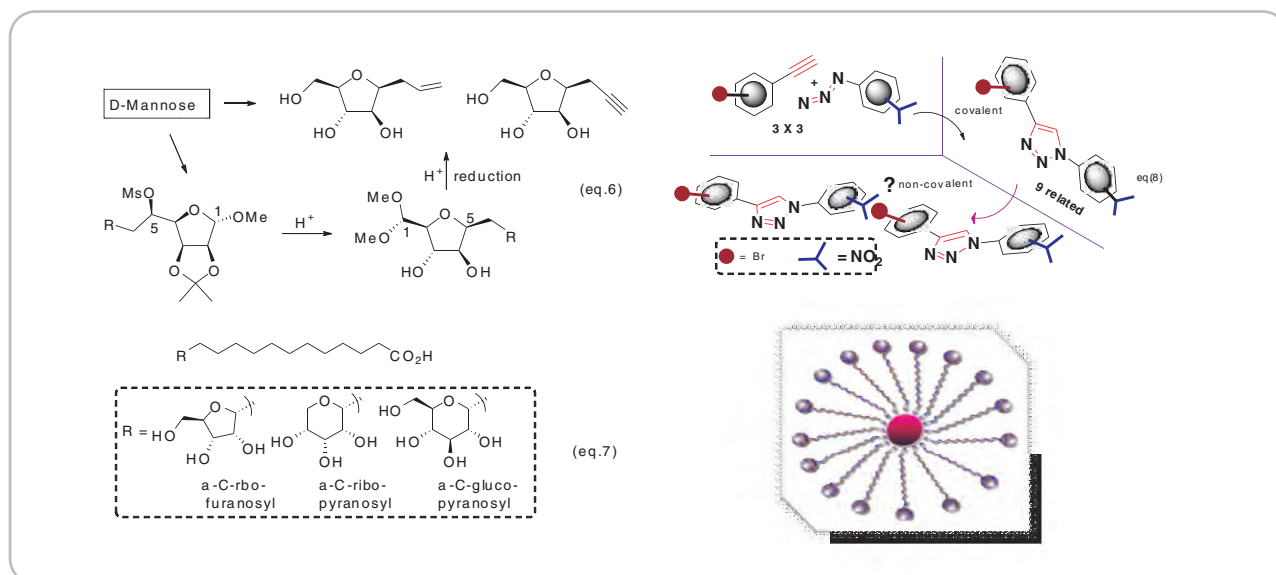
### Selected publications:

- ✦ *J. Org. Chem.*, 2008, 73, 3817; 3915
- ✦ *Chem. Commun.*, 2008, 3151
- ✦ *Tetrahedron Lett.*, 2008, 49, 6227
- ✦ *Cryst. Engg. Comm.*, 2009, 143



$\beta$ -configured *C*-allyl and *C*-propargyl-D-arabinofuranosides (eq.6). We have employed the cross metathesis reaction to prepared 12-  $\alpha$ -*C*-glycosyl dodecanoic acids containing either

$\text{NO}_2$  functional groups and evaluation of the occurrence of bifurcated Br/ $\text{NO}_2$  synthon was demonstrated (eq.8). We have noticed a helical assembly of molecules through C-H/O



ribopentofuranose, ribopentopyranose, or glucohexopyranose (eq.6). *C*-glycosides of ribose could reduce and cap the Ag NPs in water without any aggregation.

The potential of Cu(I) catalysed azide-alkyne 'click reaction' as a simple synthetic tool to build a collection of crystalline isomeric compounds with modular positioning of the Br and

interactions in 2- $\text{NO}_2$  series, and the self-complementary patterns in the crystal structures of 3- $\text{NO}_2$  series. These investigations promises the design of materials that require a reversible alternative for covalent bond by employing exclusively weak hydrogen bonding interactions like C-H/O/N to form either 2D sheets or 3D-helical networks. The simple chemistry described could be also used to evaluate the efficiency of other weak supramolecular synthons.



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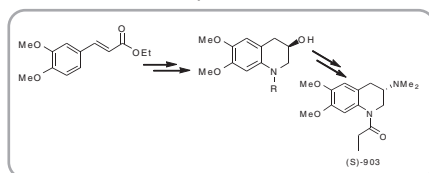
Asymmetric synthesis of bioactive molecules and development of new synthetic methods

Our focus lies in the application of both organo- and metal catalysts in the synthesis of bioactive molecules and designing newer methods involving proline and its derivatives as catalysts for effecting organic transformations. We are currently involved in the following projects:

- Catalytic asymmetric aminobromination of alkenes, alkynes and imines and
- Development of a high temperature proton conducting solid polymer electrolyte based hydrogen sensor

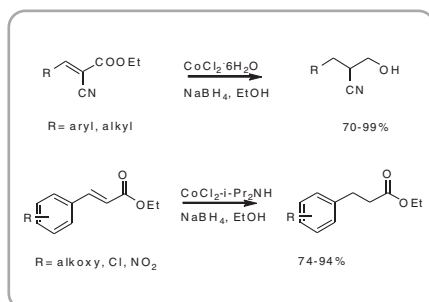
#### Synthesis of 1-[(S)-3-(dimethyl-amino)-3,4-dihydro-6,7-dimethoxy-quinolin-1(2H)-yl]propan-1-one, (S)-903

A new method for the construction of chiral 3-substituted tetrahydroquinoline derivatives based on asymmetric dihydroxylation and  $\text{CoCl}_2$ -catalyzed reductive cyclization of nitro cyclic sulfites with  $\text{NaBH}_4$  has been described with high optical purities. This method has been successfully applied in the formal synthesis of PNU 9566E and anachelin H chromophore.



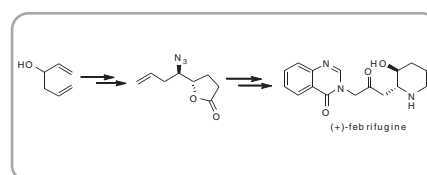
#### Cobalt (II) chloride hexahydrate-diisopropylamine catalyzed chemoselective reduction of carboxylic esters

The cobalt-catalyzed reduction of unsaturated  $\alpha$ -cyano carboxylic esters using sodium borohydride ( $\text{NaBH}_4$ ) leads to the corresponding saturated cyano alcohols in high yields. In particular, the new catalytic system cobalt(II) chloride-diisopropylamine in combination with  $\text{NaBH}_4$  showed excellent activity in the chemoselective reduction of a variety of carboxylic esters to their corresponding alcohols in good to excellent yields under mild conditions.



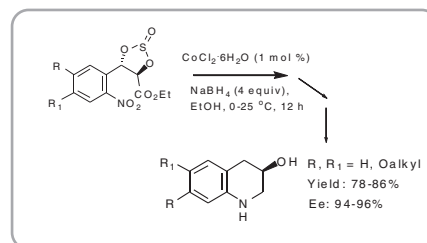
#### A concise enantioselective synthesis of (+)-febrifugine

A short enantioselective synthesis of (+)-febrifugine, a potent antimalarial alkaloid, has been described based on the regioselective asymmetric dihydroxylation of a 1,4-dienic ester as the key step. The strategy also involves chemoselective [3,3]-sigmatropic rearrangement of 1,5-hexadiene-3-ol and intramolecular lactamization of azidolactone for the construction of piperidine core.



#### Synthesis of tetrahydroquinolin-3-ols via $\text{CoCl}_2$ -catalyzed reductive cyclization of nitro cyclic sulfites

A concise enantioselective synthesis of (S)-903, an inotropic agent was described in nine linear steps and 95% ee based on asymmetric dihydroxylation of cinnamate ester and Co-catalyzed multifunctional reduction of several functional groups leading to the construction of core tetrahydroquinolin-3-ol, as the key steps.



#### Selected publications:

- *Tetrahedron: Asymmetry*, 2009, 20, 84, 335
- *Synthesis*, 2009, 4, 660
- *Organic Letters*, 2009, 11, 803





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Structure-function study of selected plant and microbial proteins

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- ✦ S. M. Gaikwad, NCL
- ✦ L. S. Kumar, NCL
- ✦ M. V. Rele, NCL
- ✦ Yogesh Shouche, NCCC, Pune
- ✦ M. V. Krishnasastry, NCCC, Pune
- ✦ Prof. J. K. Pal, Univ. of Pune

Research towards structure determination of lectins with complex sugar specificity from *Cicer arietinum* and *Moringa oleifera* have been continuing. More of different crystal types from different crystallization conditions have been grown and characterized. Efforts at getting heavy atom derivative have continued. Biophysical characterization of *Moringa oleifera* lectin has been published.

Refinement of the structures of recombinant penicillin G. acylase from *Alcaligenes faecalis* in two crystal forms has been continued.

Analysis of polymorphism in protein crystals has continued. More proteins with several polymorphs have been identified using a database search.

Modelling and study of the structure of an amylase from the rice pest, *Scirpophaga incertulas* walker, and its interaction with a wheat inhibitor have been initiated. Similarly, study of the human eukaryotic initiation factor 2 $\alpha$ , in collaboration with University of Pune, has been started.

## Study of human mitochondrial genetic disorders

Mitochondrial DNA samples collected from paediatric patients with clinical or morphological features of mitochondrial encephalopathies have been further studied. Samples have been studied for complex I defects by measuring activity levels of respiratory chain enzymes. Analysis of reactive oxygen species (ROS) and antioxidant defences in such patients have revealed a specific increase in superoxide dismutase activity.

## Selected publications:

- ✦ *Int. J. Biol. Macromol.*, 2008, 42, 203
- ✦ *J. Fluoresc.*, 2008, 18, 479
- ✦ *Free Radical Res.*, 2008, 42, 415
- ✦ *Carbohydr. Res.*, 2008, 343, 1163



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NMR for structural characterization

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- ✦ C. S. Gopinath, NCL
- ✦ M. I. Khan, NCL
- ✦ Nandini Devi, NCL
- ✦ R. A. Joshi, NCL
- ✦ S. P. Joshi, NCL

### Selected publications:

- ✦ *J. Am. Chem. Soc.*, 2008, 130, 17743
- ✦ *Chem. Commun.*, 2009, 3446
- ✦ *J. Phys. Chem. C*, 2009, 113, 8557
- ✦ *Org. Biomol. Chem.*, 2009, 7, 2458

Our research activities focus in two broad areas

- Structure and dynamics of novel organic and bio-organic molecules, and
- Studies of organic-inorganic hybrid materials using liquid and solid-state NMR

We have extensive collaboration with different research groups in NCL and outside. Some of the ongoing projects are described below.

### I. Structure and dynamics of novel organic and bio-organic molecules

#### (a) 1,2,4- and 1,2,3-Triazole hybrids

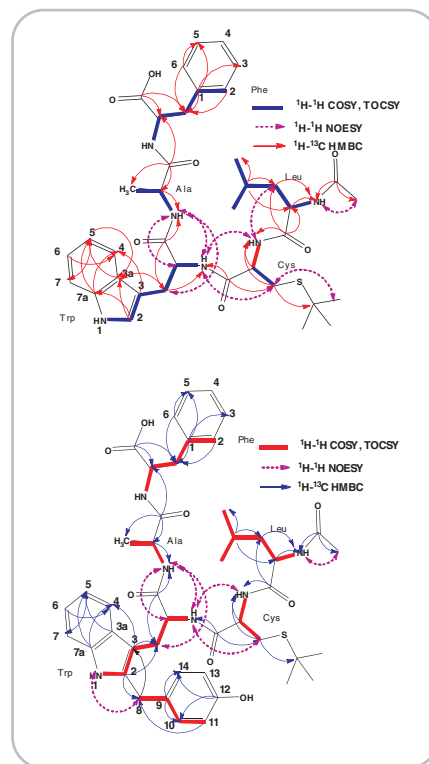
In continuation of our work on propargylation of 1,2,4 triazole thiols, a series of new hybrid systems containing 1,2,4 and 1,2,3 triazoles rings has been synthesized and characterized by multinuclear solution and solid state magnetic resonance approach. These hybrid triazoles are potential candidates for many biological activities as both 1,2,4 and 1,2,3 moieties are known to possess a variety of activities such as anti HIV, anti bacterial, anti-histamine, antifungal etc. The results provided information about stacking of the triazole rings in some of the hybrid systems in solution and solid state.

#### (b) Synthetic foldamers

A series of new foldamers with diverse structural motifs have been analyzed. The 3-dimensional structural information obtained from NMR studies, using a combination of various  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{15}\text{N}$ , 1D and 2D NMR experiments, were also compared with the X-ray structures, where ever possible, and with structures predicted with Molecular Dynamics calculation. The relative strengths of hydrogen bonds, which drive the folding, have also been estimated by NMR spectroscopic techniques. Some of systems studied included  $\alpha$ - $\beta$  hybrid peptides containing anthranilic acid and proline, foldamers with binol, spiro(biindane), naphthalene and bi phenyl naphthalenes.

#### (c) Oligo-peptides

Multi nuclear and two dimensional NMR approach has been used for the structural elucidation of peptide isolated from *Streptomyces* sp NCIM2081. NMR provided unambiguous evidence for the co existence of two inseparable novel modified thiol protease inhibitor penta peptides with very similar structures. The peptides were identified as AcNHLeu-Cys(S-tBu)-Trp-Ala-Phe and AcNHLeu-Cys(S-tBu)-Trp (2- $\text{CH}_2$ - $\text{C}_6\text{H}_4$ -OH)-Ala-Phe. The peptide mixture isolated was found to inhibit the tumor cell migration without having any cytotoxicity activity.



NMR correlation charts of the inseparable penta peptide mixture isolated from *Streptomyces* sp NCIM2081

#### (d) Insight to the formation of Pt nanoparticles

Dispersion of platinum precursor (Chloroplatinic acid) in surfactant (CTAB) modified polymer (P123) to different extents and using these composite materials as templates for the formation of mesoporous silica such as SBA-15 lead to the formation of different shapes of platinum nanoparticles. An insight to the formation of these nanoparticles was obtained from a detailed NMR investigation of the Chloro platonic acid-CTAB-polymer system. It is observed that the  $[\text{PtCl}_6]^{2-}$  precursor interacts with the cationic head group of the surfactant and facilitates the isolation of precursors within the composite template leading to the formation of nanoparticles moulded by the walls of the mesochannels when calcined. We have demonstrated that at very low concentrations, nanoparticle morphology can be controlled and fine tuned by easily varying extent to which platinum-CTAB complex precursor is allowed to agglomerate in the composite micelle template prior to the formation of the siliceous meso channels and these modifications could be achieved with the same concentration of platinum. These factors are crucial in nanoparticle synthesis especially for catalysis, since



highly dispersed low weight percentage of noble metals supported on oxides are ideal materials as heterogeneous catalysts.

#### (e) Polymer surfactant interactions

The interaction of polymers with surfactants which are highly cooperative and often reflected in macroscopic solution properties such as viscosity has been studied by various  $^1\text{H}$  and  $^{13}\text{C}$  NMR techniques. The addition of surfactant to polymers can alter the properties of both the individual systems due to the synergic effect. This has greatly stimulated interest in polymer/surfactant systems and in the understanding of polymer/surfactant interactions. Some of the systems that are being studied by NMR Overhauser spectroscopy and Diffusion Ordered spectroscopy include interaction of poly(*N*-isopropylacrylamide) with various surfactants (SDS, CTAB, Tween20), interaction pluronics such as P123 with surfactants, phase properties of polymeric surfactant-water-organic system etc.

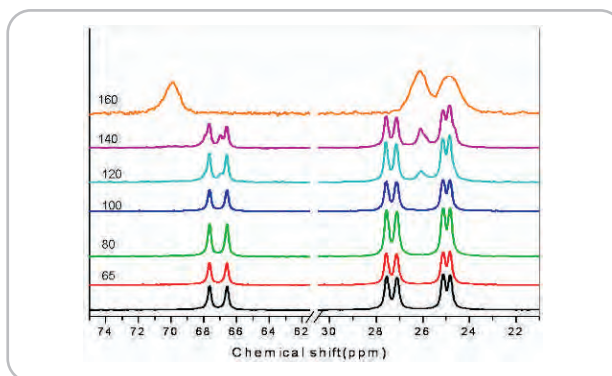
#### (e) Studies on pharmaceuticals and natural products

Impurity profiling is one of the major requirements of the pharmaceutical industry. Multi nuclear magnetic resonance approach has been successfully employed in the structural elucidation of impurities formed during the preparation of API for various pharmaceutical industries. Impurity profiling of a number of compounds has been performed by a combination of 1D and 2D multi NMR approach similar approach has also been used for structural elucidation of many natural products. In addition, solid state NMR techniques have also been used for identification of polymorphs of APIs in pharmaceuticals.

## II. Studies on inorganic-organic hybrid materials

### Studies on $\text{MgCl}_2$ -alcohol adducts

The discovery of  $\text{MgCl}_2$ -supported  $\text{TiCl}_4$  catalyst has revolutionized the area of synthesis of polyolefines using Ziegler-Natta catalyst. It is also known that the characteristics of the polymer depend heavily on the nature of  $\text{MgCl}_2$  support.  $\text{MgCl}_2$  forms stable adducts with Lewis bases such as alcohols, ethers, esters, ketones, etc. with varying stoichiometry. We have been looking at the possibility of using various  $\text{MgCl}_2$ -alcohol adducts as Ziegler-Natta catalyst supports. It is essential to characterize these materials thoroughly for a proper understanding of their stoichiometry and hence their properties. 1D and 2D NMR methods based on multinuclear ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{25}\text{Mg}$ ) solid state NMR techniques were applied to characterize adducts of  $\text{MgCl}_2$  with different alcohols (isopropanol, butanol, isobutanol, benzyl alcohol etc.) prepared under different conditions. The results provided more insight to their stoichiometry, phase purity and temperature dependant phase and stoichiometry changes.



$^{13}\text{C}$  CP/MAS and Temperature dependant phase changes of  $\text{MgCl}_2 \cdot 4\text{iPrOH}$  adduct

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Solid state and supramolecular structural chemistry



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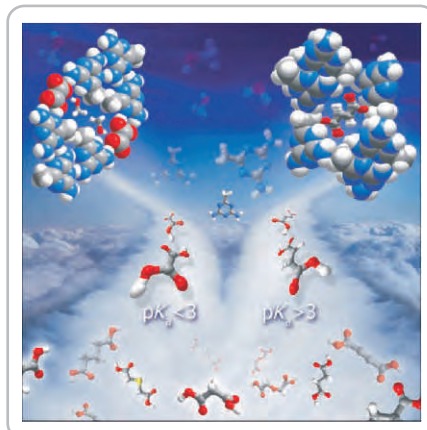
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- ✦ Prof. Judith A. K. Howard, University of Durham, U.K.
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- ✦ Prof. Roland Boese, University of Essen, Germany

Design, synthesis and applications of novel supramolecular assemblies with designer characteristics comprising of organic, organic-inorganic and biological molecules will form the focus of the object. The assemblies will be characterized by single crystal X-ray diffraction method and we plan to evaluate physical properties such as conductivity, magnetic susceptibility and chemical properties such as catalysis and adsorption phenomenon etc. The information gained will be utilized to improve the desired structural characteristics of new materials and possibility of their utilization in the electronic devices and biosensors, depending upon the properties exhibited by the materials.

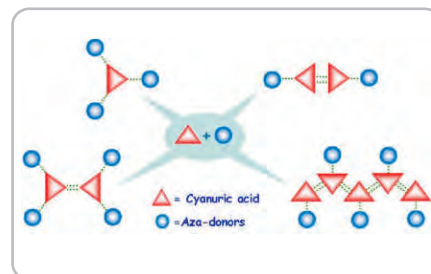
Molecular adducts of 2,4-diamino-6-methyl-1,3,5-triazine have been prepared with various aliphatic dicarboxylic acids. The molecular complexes, thus, formed by co-crystallizing the triazine with oxalic, malonic, succinic, fumaric, acetylene dicarboxylic, glutaric, thiodiglycolic, diglycolic, and adipic acids have been found to give two types of host-guest assemblies that have voids or channels in a three-dimensional arrangement. The different types of host-guest arrangement appear to result from differences in the acidity of the dicarboxylic acids, that is, acids with  $pK_a < 3.0$  give host networks that consist of the triazine and the corresponding acid with water or solvent molecules of crystallization present as guests. On the other hand acids with  $pK_a > 3.0$  exist as guests in voids in a host network formed by the triazine. These variations are depicted in the cover illustration of this work appeared on *Chemistry- A European Journal*.



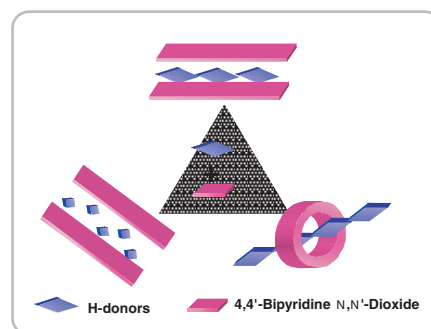
## Selected publications:

- ✦ *J. Mol. Struct.*, 2009, 937, 81
- ✦ *New J. Chem.*, 2009, 33, 57
- ✦ *Chem. Eur. J.*, 2008, 14, 6967
- ✦ *Tetrahedron Lett.*, 2008, 49, 3666

The preparation and structure elucidation of cocrystals formed by cyanuric acid (CA) with aza-donor compounds 4,7-phenanthroline, 1,7-phenanthroline, phenazine and 1,3-bis(4-pyridyl)propane, has been carried out, as depicted pictorially in the adjacent drawing, to rationalize the formation of supramolecular patterns of different degree of bond orders. Thus, it has been established that while CA forms different types of self-assembling modes-monomers, dimers and infinite tapes in the presence of the aza-donors, primarily through N-H...N and C-H...O hydrogen bonds.



Molecular adducts of 4,4'-bipyridine-N,N'-dioxide with various H-donors such as cyanuric acid, trithiocyanuric acid, 1,3,5-trihydroxybenzene (phloroglucinol), 1,3-dihydroxybenzene (resorcinol) and 1,2,4,5-benzenetetracarboxylic acid have been prepared and characterized by single crystal x-ray diffraction methods to identify the major interactions between the ligands in the assemblies as N-H...O, N-H...S, O-H...O and C-H...O, in the form of *homomeric* and *heteromeric* patterns of the constituents either as a single or as cyclic hydrogen-bonded motifs. In three dimensions, the ensembles of molecules yield planar sheets, ladders and pseudorotaxane type assemblies.





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Structural surprises of myo-inositols: Polymorphism and a role of weak interactions

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- Prof. T. N. Guru Row, IISc, Bangalore.
- Prof. (Mrs.) S. Y. Rane, University of Pune

Research activities of our group focus on the broad areas of polymorphism, solvatomorphism, solid-state reactions, structural phase transitions and the study of various non-bonding intermolecular interactions in collaboration with Dr. M. S. Shashidhar of Organic Chemistry Division. We investigated several cases of polymorphism, solvatomorphism, crystal-to-crystal phase transitions and solid-state acyl transfer reactions exhibited by several *myo*-inositol derivatives. Some of the results of the ongoing work are described below.

#### Conformational polymorphism, 1D-isostructurality and dipolar (ether) O•••C=O short contact

Research to understand polymorphism is becoming increasingly important in drugs, pigments, agrochemicals and high energy materials due to high consistency required in the physicochemical properties of these solids.

Isostructurality implies similarity in the crystal structures of different compounds whereas polymorphism means the existence of different crystal forms of the same compound. These two phenomena represent the two extremes of molecular assembly. However, fascinating cases of polymorphs which lie between these extremes having one- and two-dimensional isostructurality are much less common.

Crystal structure analysis of polymorphs with common structural features could give insight into various modes of molecular association during nucleation that can be used as computational criteria for 'crystal structure prediction'.

Although conformational polymorphs cannot have isostructurality as they are formed due to different molecular conformations, we found an interesting case of one-dimensional isostructurality (except for tosyl group orientation) in conformational polymorphs of sulfonated *myo*-inositol orthoester derivatives that exhibit remarkably conserved molecular association via (ether) O•••C=O short contacts.

The *myo*-inositol orthoacetate derivatives, namely, racemic 2,4-di-O-acetyl-6-O-tosyl-*myo*-inositol 1,3,5-orthoformate and its orthoacetate analogue produced conformational polymorphs. In these polymorphs, the tosyl group adopted different conformations due to the rotation about the O-S bond.

A significant variation in the torsion angle for the tosyl group (~56°) was observed

between the crystals of two polymorphs of the orthoformate derivative, which exhibited an intramolecular dipolar S=O•••C=O (sulfonyl-carbonyl) short contact whereas only slight variation (~3°) in the tosyl group orientation is observed in case of the orthoacetate analog.

An interesting feature in all conformational polymorphs is the formation of an isostructural string (despite the differences in the orientation of the tosyl group) linked *via* dipolar (ether) O•••C=O contacts, which is further stitched by other weak interactions to form different layers in their crystal lattice.

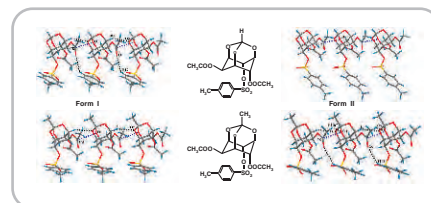


Fig. 1 Figure showing one-dimensional isostructurality in the molecular association mainly via dipolar (ether) O•••C=O short contact is a consistent feature in the dimorphs of different orthoester *myo*-inositol derivatives irrespective of their different tosyl group conformation.

#### Crystal-to-crystal thermal phase transition, 2D-isostructurality and morphotropism

Crystal-to-crystal transformations take place more often when molecules aggregate *via* weak intermolecular interactions, as they can rearrange themselves forming a new lattice with another set of weak interactions.

Such inter conversion amongst polymorphs is an important aspect of research, particularly in functional solids, in order to understand the relationship between structure and function. Amongst these, single-crystal-to-single-crystal phase transformations provide valuable information about the flexibilities and movement of molecules in the crystal lattice.

Intrigued by the phenomenon of the disappearing chiral polymorph of the achiral hexa-*O*-benzoyl-*myo*-inositol, we investigated the polymorphic behaviour of structurally analogous hexa-*O*-toluoyl-*myo*-inositol. This compound crystallized in the triclinic form (*P*-1, Form I) and exhibited single-crystal-to-single-crystal irreversible phase transition centered at ~250°C.

Transformation of these crystals to monoclinic (*P*<sub>2</sub>/n, Form II) form was revealed by DSC and X-Ray diffraction studies. Crystal structure analysis revealed that the molecules in both the forms are linked via bifurcated C-H•••O interactions to

#### Selected publications:

- *CrystEngComm*, 2009, 11, 143, 1022
- *Chem. Eur. J.*, 2009, 15, 261
- *J. Mol. Struct.*, 2008, 892, 246



make almost identical centrosymmetric dimers. The neighbouring dimers are bridged via C-H...O and aromatic  $\pi$ ... $\pi$  stacking interactions to create two-dimensional isostructural assemblies.

The difference in the two crystal forms arises from linking of the centrosymmetric dimers along the third dimension; the dimers are centrosymmetrically bridged in the triclinic form while they have *n*-glide relationship in the monoclinic form.

Comparison of structures of dimorphs further revealed that they are actually an excellent case of morphotropism. Morphotropism refers to the non crystallographic rotation and translation of common motifs.

In the present case the dimorphs are related by morphotropism of their dimers in molecular organization. The thermal crystal-to-crystal transformation involves the non-crystallographic rotation and translation of the dimer which led to the conversion of triclinic form to monoclinic form.

This observation suggests that the differences between crystal structures of isostructural polymorphs and transitions amongst them could be well understood from the studies of morphotropism. This study could further help in delineating the factors that govern nucleation and crystal growth as well as an

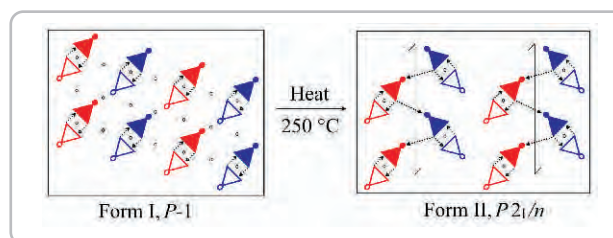


Fig. 2 Topological patterns of the molecular organization during phase transition.  
(A) linear arrangement of centrosymmetric dimers in triclinic (*P*-1) and  
(B) packing pattern generated in monoclinic (*P*<sub>2</sub>/*n*) after non crystallographic rotation (180°) and translation of dimers.



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Bioinformatics

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### Collaborator:

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High throughput gene expression profiling using DNA microarrays provides an opportunity to link disease phenotypes with molecular changes within a cell. In addition to contributing to a mechanistic understanding of the disease, such data can also be used to identify biomarker profiles (that is gene expression profiles) for prediction of phenotype of an unknown sample. This can aid medical diagnosis and prognosis in cases where histological or other tests are inconclusive. The accuracy of microarray based sample classification depends on the algorithm employed for selecting the features (genes) used for classification, and the classification algorithm.

We evaluated the performance of over 2000 combinations of feature selection and classification algorithms in classifying cancer datasets to identify the best performing algorithms. SVM for ranking genes + SMO shows excellent classification accuracy using a small number of genes across three cancer datasets tested. Notably, classification using 15 selected genes yields 96% accuracy for a dataset obtained on an independent microarray platform.

### Selected publications:

- ✦ *BMC Bioinfo*, 2008, 9:380
- ✦ *Int J Bioinfo Res Appl*, 2009, 5: 417



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Molecular scaffolds

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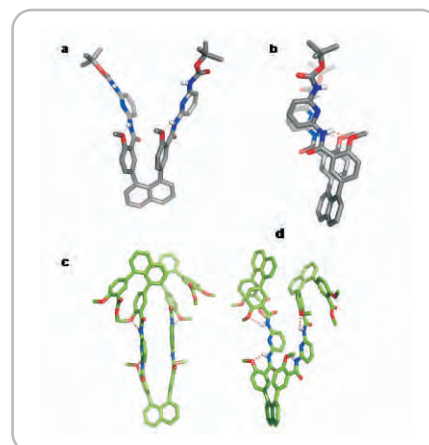
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### Novel synthetic oligomers (foldamers)

The major thrust of our research focus over the years has been to generate synthetic scaffolds capable of displaying diverse secondary structural features of peptides and proteins. These *de novo* designed molecules with diverse backbones find potential applications in molecular recognition, drug design, and material sciences. Owing to the predictable and stable conformation, abiotic backbones have been proved to be attractive targets in foldamer research. Although the majority of them display helical conformations, a common feature observed in biomolecules, sheet and rod conformations can also be attained with a proper tuning of the backbone. In this context, development of structural architectures different from those classically observed would be of considerable interest.

For instance, we have been able to report recently the synthesis and conformational studies of a novel class of abiotic hybrid oligoamides with cofacial structural architecture. The peri-positioning of phenyl

rings at the 1- and 8- positions of the naphthyl ring leads to an almost parallel orientation of the aryl rings to each other and to their nearly perpendicular orientation to the naphthyl ring. This makes the 1,8-diarylnaphthyl unit an excellent template for building cofacial structures, as we have demonstrated recently.



**Figure 1:** Structure of cofacial oligomers: X-ray crystal structure (upper panel) and *ab initio* model (lower panel).

#### Selected publications:

- ✦ *Chem. Commun.*, 2009, 3446; 2008, 712, 2541
- ✦ *J. Am. Chem. Soc.*, 2008, 130, 17743



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Role of molecular dynamics in protein-RNA recognition



#### Collaborator:

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#### Background

Protein-RNA interactions are fundamental to many cellular processes, including assembly and function of ribosomes and spliceosomes, post-transcriptional regulation of gene expression etc. The first step in understanding the protein-RNA recognition process is to determine three-dimensional structures of the protein and the RNA and follow the structural changes which occur in both partners on complex formation, particularly, at the binding interface. The three dimensional structures of several RNA binding proteins, their RNA targets and intermolecular complexes have been determined recently and is an active area of research. The structural studies have provided important insights into the conformational features and location of the contacts which permit protein-RNA binding. Many of these studies have also provided evidence for protein-RNA interface dynamics thereby making it clear that knowledge of static structures alone is not sufficient to fully understand the protein-RNA recognition event.

Three dimensional structure determinations of protein-RNA complexes by NMR are fairly recent; hence studies on dynamics involving these complexes are rare. The few dynamics studies available focus only on changes in motions in the protein on binding to RNA. Our interest is in examining dynamics changes in both interacting partners and establishing how molecular motions influence the thermodynamical aspects of the interaction.

#### Work done and discussion

Recently we carried out a detailed  $^{13}\text{C}$  NMR relaxation study of the role of RNA dynamics in the interaction of the Smaug recognition element stem-loop RNA (SRE-RNA) and the sterile alpha motif domain of *Saccharomyces cerevisiae* Vts1p (VTS1p-SAM). This study has provided important insights into the molecular motions taking place in the RNA and the changes that occur on interaction with the protein.

The work has been extended to examine molecular motions in the protein and changes resulting from interaction with the RNA.  $^{15}\text{N}$  NMR relaxation measurements have been carried out on the VTS1p-SAM domain in its free and SRE-RNA bound states.

Detailed quantitative analysis of the  $^{15}\text{N}$  relaxation rates in the free and bound states of the VTS1p-SAM domain was carried out by employing the Lipari-Szabo model free approach. Interesting changes in protein dynamics in the pico-nano second time scale

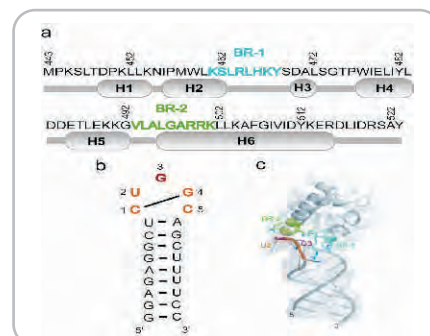


Figure 1. Schematic representation of the sequences of (a) VTS1p-SAM domain (b) SRE-RNA and (c) secondary structure of the complex. The residues and nucleotides which form the binding interface are indicated in colour.

and micro-milli second time scale resulting from interaction with the SRE-RNA are observed in the VTS1p-SAM domain.

The interaction of VTS1p-SAM domain and SRE-RNA occurs by shape specific recognition and combines elements of specificity and non-specificity. VTS1p-SAM domain recognizes a general consensus sequence of the form XNGY(N) for the RNA loop, where N is any nucleotide and X and Y form a Watson-Crick base pair. Only the

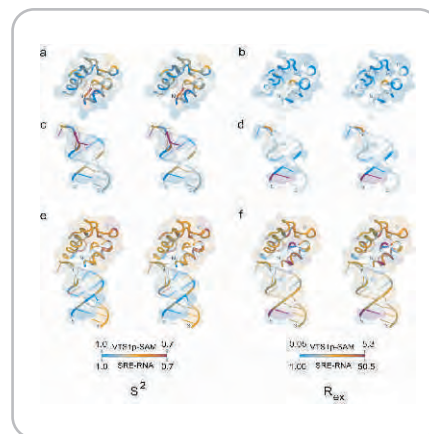


Figure 2. Representation of internal motion parameters for backbone  $^{15}\text{N}$  sites of VTS1p-SAM and aromatic  $^{13}\text{C}$  sites of SRE-RNA in the free and bound states. (a)  $S_2$ , (b)  $R_{ex}$  for VTS1p-SAM and (c)  $S_2$ , (d)  $R_{ex}$  for SRE-RNA in the free state. (e)  $S_2$  and (f)  $R_{ex}$  for both components in the bound state. Different scales are used since measurements for VTS1p-SAM domain.

central G nucleotide and the shape of the RNA fold induced by the base pairing is specifically recognized. Deletion of the nucleotide indicated in parentheses does not alter binding affinity indicating that penta- or tetra loop RNAs can bind to the VTS1p-SAM domain. Dynamics studies show that in its free state the VTS1p-SAM domain is mostly rigid with no significant motions in the fast and slow time scales. This is consistent with the idea of a conformationally pre-organized



binding surface on the protein which can accommodate the RNA loop. On interaction with the CUGGC loop of the SRE-RNA, a majority of the residues achieve increased flexibility in the bound state. Interestingly, residues belonging to the binding surface which are associated with the specific recognition of the central G nucleotide in the RNA loop, show significant restriction in mobility following binding. In contrast to the increased rigidity of residues involved in specific interaction with the central G nucleotide, those protein residues of the binding surface which are involved in non-specific interaction with other nucleotides in the RNA loop show increased flexibility in the bound state.

As in the case of pico-second to nano-second time scale motions, interaction with RNA also results in an overall increase

in micro-second to milli-second time scale motions in most residues of the protein. The only exceptions are the residues in the binding region which are involved in specific recognition of the central G nucleotide of the RNA. The dynamics studies clearly indicate that the parts of the binding interface associated with specificity of recognition is accompanied by increased rigidity whereas the parts interacting in a non-specific manner attain increased flexibility on binding. This is perhaps functionally relevant since non-specific interaction requires nucleotides of different sizes and hydrogen bonding strengths to be accommodated at the binding surface of the protein. Thus molecular motions play a role in modulating the binding affinity for different combinations of loop nucleotides allowing a general consensus sequence of the form XNGY(N) for the RNA loop in the recognition of SRE-RNA by the VTS1p-SAM domain.



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Organic biomolecular chemistry

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### Background / objectives

The main emphasis of the research in our group is to develop strategies for treatment of diseases at the level of genes rather than at the level of proteins. This novel approach, known as antisense therapeutics, uses oligonucleotide analogues (DNA/RNA) as drugs and is applicable to fearsome diseases of viral, genetic or cancerous origins where small molecular therapies remain ineffective. Our work addresses the most important challenges concerning the practical applications of oligomers in this research area such as specific and strong RNA recognition, intracellular stability, cell-delivery, ease of synthesis and safety.

We chose to replace the sugar-phosphate backbone in DNA by electrically neutral, non-canonical peptide backbone as in the case of peptide nucleic acids (PNA). The introduction of structural variations in 2'-5' linked sugar-phosphate oligomers to improve biostability and activity is also an important research goal and several modifications to control conformational preferences of the sugar rings were planned in order to arrive at a structure that is compatible for strong RNA binding.

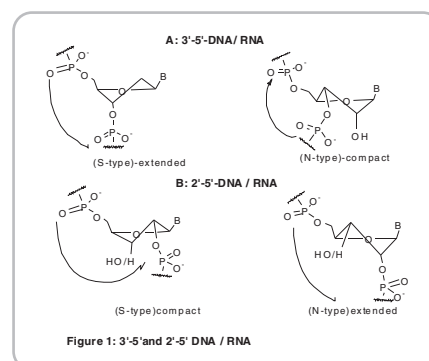
### Work done and discussion

The sugar phosphate backbone was replaced with a backbone that alternates with natural  $\alpha$ -amino acids with nucleoside derived  $\beta$ -amino acid. The easy access to the nucleoside- $\beta$ -amino acid was achieved using Tempo-BAIB oxidation of primary alcohol group of 3'-deoxy, 3'-amino thymidine to yield a nucleoside  $\beta$ -amino acid. Sequential alternating couplings of nucleoside- $\beta$ -amino acid with natural  $\alpha$ -amino acid yielded a non-canonical peptide backbone comprising alternate  $\alpha$ - $\beta$  amino acids. This backbone with sequentially attached array of nucleobases was able to recognize specific complementary DNA and RNA sequences. We further studied the effect of backbone chirality while exchanging the L-amino acid by D-amino acid. The dimer blocks

containing D-proline, L-proline and prochiral glycine exhibited very interesting CD-curves. The CD data obtained shows differential base stacking features that may have implications in recognition of DNA/RNA sequences.

The oligonucleotides joined by 'non-genetic' 2', 5'-linkages were found to bind to complementary single-stranded RNA but to bind weakly, or not at all, to single-stranded DNA. The 2'-5' phosphodiester linkages are also known to be stable to nucleases. Both these attributes make them to be the right choice for development as antisense oligonucleotides for direct testing in cell assays. We are working towards finding out the structural preferences of these oligomers in the context of preferred 3' versus 2'-endo/exo sugar ring conformations by introducing appropriate locked sugar conformations.

The conjugation of AS oligomers to cell-penetrating peptides (CPP) is a method of choice in antisense as well as siRNA techniques for the drug-delivery inside the cells. The known methods in the literature involve tedious continuous synthesis or other convergent methods that require orthogonal protection strategies. We are currently working on the synthesis of intrinsically guanidylated PNA oligomers for better cellular uptake. Also studies towards the synthesis and cellular uptake of conformationally constrained novel peptides are undertaken.



### Selected publications:

- ✦ *Chem. Commun.*, 2009, 6646; 2008, 706
- ✦ *J. Org. Chem.*, 2008, 73, 1508
- ✦ *Nucleic Acids Symposium Series*, 2008, No. 52, 191



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Design and synthesis of novel drug conjugates containing 1,2,3-triazole

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**Collaborators:**

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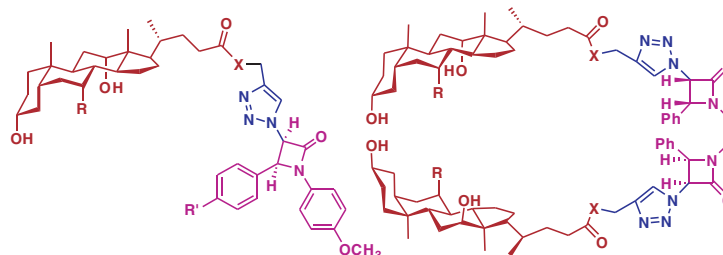
Due to their large, rigid, and curved steroidal skeletons, chemically different hydroxy groups, enantiomeric purities, and unique amphiphilicity, together with availability and low cost, bile acids are a valuable group of compounds from the pharmaceutical point of view. A common feature of bile acid-derived antimicrobials is their potential to exhibit facially amphiphilic nature, due to polar hydroxyl groups on one face and nonpolar hydrophobic methyl group on the other.

$\beta$ -Lactams are a large class of antibiotics. Microorganisms have developed resistance against most of the traditional  $\beta$ -lactam antibiotics due to their wide-spread overuse. 1,2,3-Triazole moieties are attractive connecting units with metabolic stability and are capable of hydrogen bonding useful for binding to biomolecular targets. Bile acids are considered very useful in the preparation of new pharmaceuticals because of their inherent chemical and biological properties. By combining these three different units we have synthesized 1,2,3-triazole linked  $\beta$ -lactum-bile acid conjugates as monomers as well as dimers and studied their biological activities. Most of the compounds exhibited

significant antifungal and moderate antibacterial activities.

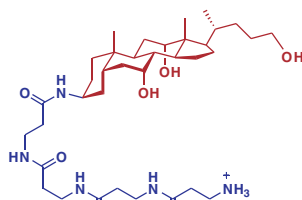
Fluconazole based novel mimics containing 1,2,3-triazole were also synthesized, maintaining its pharmacophore. *In-vitro* as well as *in-vivo* antifungal activity of these new molecules was evaluated. Two molecules showed better activity than fluconazole but were found to be little more toxic. A patent has been filed on this work.

Squalamine, a steroid-polyamine conjugate has attracted considerable attention because of its potent antimicrobial activity against a broad spectrum of micro-organisms. Several peptides such as polymixin B have been identified that increase the permeability of the outer membranes of Gram-negative bacteria. Based on these molecules and literature survey, novel bile acid-tetrapeptide conjugates of glycine and  $\beta$ -alanine were designed and synthesized. While relatively inactive by themselves, these compounds interact synergistically with antibiotics such as fluconazole and erythromycin to inhibit fungal and bacterial growth respectively at 1-24 g/mL.

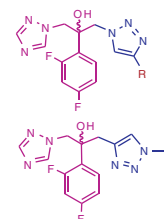


X, = O/NH; R = H/OH and R' = H/Cl

Bile acid- $\beta$ -lactum conjugates



Steroid-peptide scaffolds



R = Bile acid/long chain alkane/H  
Fluconazole conjugates

**Selected publications:**

- ✦ *Bioorg. Med. Chem. Lett.*, 2008, 18, 2043; 5512; 2009, 19, 759
- ✦ *Org. Biomol. Chem.*, 2008, 6, 3823
- ✦ *Indian patent*, 2008, NF 054



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Biocatalysis and biosynthesis

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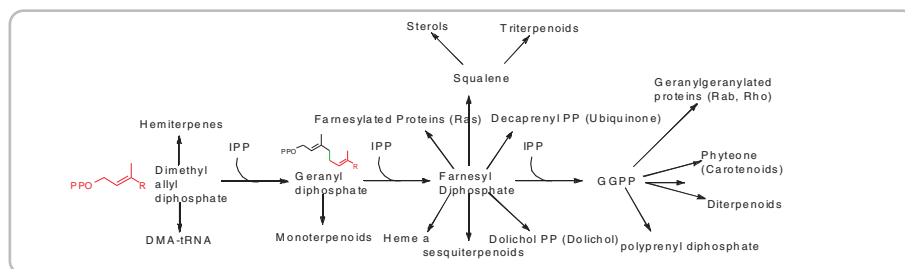
**Collaborators:**

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- ✦ Bora, NEIST, Jorhat

**The research in our group focuses on two major areas:**

(1) Elucidation of biosynthetic pathways for Isoprenoids: The isoprenoid biosynthetic pathways provide intermediates for the synthesis of a vast variety of structurally and chemically diverse natural products that

serve numerous biochemical functions in living systems. We are interested in elucidation of isoprenoid biosynthetic pathways with special emphasis on establishing the mechanisms of the enzyme-catalyzed transformations and how the enzymes promote the reactions.



Scheme 1. Biosynthesis of various isoprenoids

(2) Biocatalysis: In this area we focus on the application of biocatalysts such as microorganisms and isolated enzymes for the production of biologically important molecules or their intermediates in enantiomerically pure form. Further the activity of an enzyme(s) will be modified by recombinant DNA technologies.

from culture collections) to carry out the stereo- and regio-specific redox reactions with wide substrate specificity. We found that several fungal strains were able to carry out the quantitative stereo- and regio-specific reduction of double bonds, hydroxylations on non-activated carbon atoms, and chiral resolution of esters. The work is progressing towards the construction of DNA libraries which will be used to screen for the genes which encode these novel oxidoreductases and lipases.

**Work done and discussion**

We have been engaged in screening the microorganisms (isolated from soil as well as

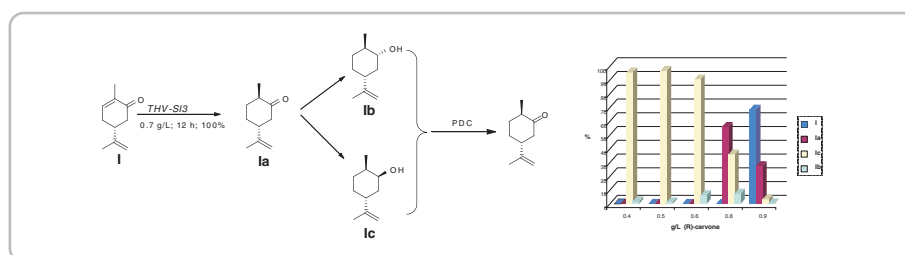


Figure 1: Biotransformation of R-carvone by fungus

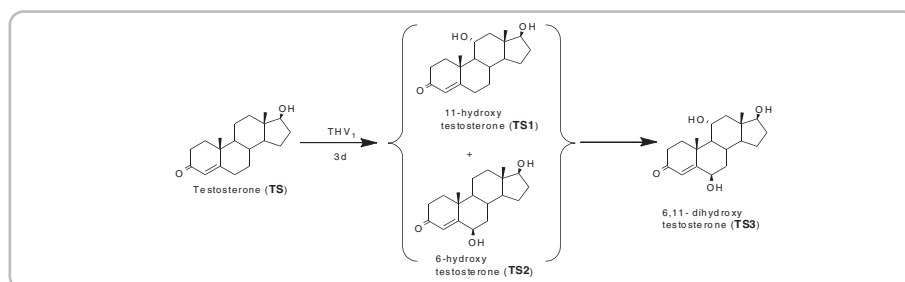


Figure 2. Biotransformation of testosterone by fungus

**Selected publication:**

- ✦ *J. Am. Chem. Soc.*, 2008, 130, 1966

We have standardized method and carried out thorough study on the metabolic profiling of the limonoids in neem seed kernel at different developing stages, sandalwood (*S. album*) and *Ocimum sanctum*. Work is

progressing towards the construction of cDNA libraries for the isolation and characterization of terpene synthases and downstream enzymes in isoprenoid biosynthetic pathway.

## Process development



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Process development for vinyl benzoate and vinyl-2-ethyl hexanoate

### Background

The transition metal complex catalyzed transvinylation of carboxylic acid with vinyl acetate monomer is of significant interest for synthesis. Various transvinylation processes are available in literature in a batch type, with low catalyst turn-over number, equilibrium process and poses problem during the product isolation. M/s Celanese is looking for the process development of the two monomers, Vinyl benzoate (VB) (CAS No. 769-78-8) and vinyl-2-ethyl hexanoate (V-2-EH) (CAS No. 94-04-2), which Celanese intends to use in various applications.

- A unique reactive distillation (RD) facility was created in India.
- A generic continuous process for quantitative transvinylation of carboxylic acids using transition metal complex catalyst and vinyl acetate monomer was operated at MEHK PVT LTD, Thane with complete recycle of excess of reactants, catalysts etc with large turnover number.
- The capacity of plant at commercial scale is one ton/day. About two tons of vinyl benzoate and vinyl-2-ethyl hexanoate are produced at MEHK.

### Objectives

- To develop commercially viable route for vinyl benzoate and vinyl-2-ethyl hexanoate.
- Selection of route, process development, scale-up and demonstration.

### Work done and discussion

- New continuous process based on transvinylation using carboxylic acid and vinyl acetate monomers in the presence of transition metal complex catalyst has been developed.
- Quantitative conversion of acid on recycle basis.
- No side product formation.
- Zero effluent process, that is, green process.
- Total recycle and recovery of catalyst possible.
- Large turn-over number of catalyst about 20-25 kg/gm of catalyst.
- The purity of product obtained in the commercial unit was more than 99.95%.
- The entire exercise of concept to commercialization was completed within one year.



Commercial plant for production of vinyl esters by MEHK Chemicals Pvt. Ltd, Thane



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Prediction of the thermodynamic properties

### Prediction of the enthalpy of formation of free radicals

The importance of and need for *apriori* estimation of the standard state enthalpy of formation of organic free radicals cannot be overstated. Benson's group additivity (GA) method for estimating free radical enthalpies seems to be quite suited to routine practical work giving fairly accurate results. The main handicap in more routine use of the GA method is the lack of availability of the group additivity values (GAVs) that are used in the estimation process. One of the objectives of this project has been to remove this handicap. In an earlier paper (2006) we had re-estimated 7 GAVs pertinent to the alkyl radicals, and 22 GAVs pertinent to the oxygen-containing radicals (many of these for the first time) following two different methodologies and compared the predicted DELHF values with experimental data, wherever available. Recently, we have extended the database of GAVs to those pertaining to unsaturated, aromatic and haloalkyl radicals, nitrogen and sulfur-containing radicals, and successfully used these GAVs (about 100) to estimate the DELHF values for a number of radicals which can be shown to be constructed using one or more of the radical groups. A second long term objective has been to adopt suitable computational chemistry approaches to get around the need of any experimental data (though much less extensively in the above approach) to estimate the GAVs and also to get around the use of the empirical structural correction factors occasionally used in the GA method.

A new approach has been defined and carried out to combine the power of computational chemistry that has become more routinely available to the desktop of an average engineer with the organization and insight that one inherits from the traditional GA method minus the empirical factors. The upshot has been the demonstration of a capability to make *a priori* prediction of the enthalpy of formation of a large number of saturated alkyl radicals (especially those that are relatively highly branched) for which experimental data are scarcely available. The predictions appear to be quite close to experimental data where available, and are also quite comparable to values calculated by the GA method or those by the so-called difference method.

### *Apriori* prediction of the vapor-liquid equilibria by molecular simulation

In connection with the recent development of new green and environmentally friendly processes, gas-expanded (especially, carbon dioxide expanded) organic solvents or, even better, ionic solvents are being tried out as the preferred media for liquid phase oxidation, hydroformylation, hydrogenation, etc. One of the key requirements for modelling and design of such processes has been the thermodynamic and the transport properties such as oxygen and CO<sub>2</sub> solubilities, volume expansions, diffusivities in these new media. While traditional equation of state methods has been used wherever feasible, these methods are clearly limited by the requirement of binary interaction parameters which in turn presupposes experimental VLE data at high pressures that are not always available.

We have initiated a project on exploring the use of molecular simulation (Monte Carlo and molecular dynamics) techniques for *apriori* and consistent prediction of the relevant vapour-liquid equilibria and other thermophysical properties of the liquid phase. Our initial studies suggest that effective methodologies can be set up and useful volumetric and thermodynamic properties data for several CO<sub>2</sub>-expanded organic solvents (for example, aliphatic alcohol, ketone, nitrile, carboxylic acid, aromatics, etc) can be generated. In addition it has been shown that the changes in the oxygen solubilities in some of these gas-expanded solvents (*vis-à-vis* the neat solvents), can also be predicted by simulation. These data would be useful in the process design of proposed processes based on some of these neoteric solvents.

## Process modeling and simulations



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Studies in complexity: Applications of nonlinear dynamics, chaos and turbulence

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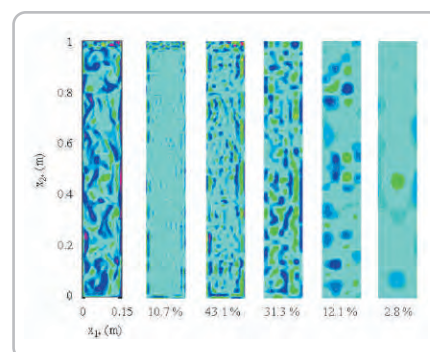
## Collaborators:

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- ✦ Prof. JB Joshi, ICT, Mumbai
- ✦ Sagar Deshpande, ICT, Mumbai

The group has been carrying out advanced research in the interdisciplinary area of nonlinear dynamics with a view to understand the properties of chaotic and turbulent systems. The approach has been a top-down practical approach that analyses temporal / space-time monitored process data for process multiscale features that are inherently present within it. Pattern recognition, feature extraction and mechanism elucidation in these systems need to be strengthened by devising newer formalisms of analysis. It has specially been the endeavour of the group to bring out powerful algorithms that unravel the multiscale features of complex systems by especially using new mathematical tools.

Planar information of velocity from 2D particle image velocimetry (PIV) and large eddy simulation (LES) data have been studied using multiresolution wavelet transform (WT) formalisms, that is, discrete and continuous WT. Identification of dominant energy containing structures and their characterization in terms of fractal spectra has been carried out for industrially important equipment exhibiting turbulent behaviour. These include annular centrifugal contactor, jet loop reactor, ultrasound reactor, channel flow, stirred tank and bubble column reactor. The characterization of their dynamics based on denoising the data and studying the local energy along the WT scales shows sensitive variation and this helps in identifying the size and shape of structures. A dependency is seen between mixing time and the higher order moments of length scale distribution, namely, skewness

and kurtosis and a generalized correlation has been built up for important types of equipment and associated flow parameters. The correlation is not only based on the knowledge of reactor geometry and operating conditions but also on the flow structures via their statistical parameters. Wavelet transform modulus maxima (WTMM) methodology has been used to study the evolution of structures and their interaction in a reduced dimensionality by evaluating the fractal spectra. Classification studies have been carried out using principal component analysis (PCA) of the fractal spectra. The results obtained show clear classes for the six types of equipment and delineate regimes to obtain benchmark patterns of flow hydrodynamics based on PCA co-ordinates. This methodology offers a generalized way for the optimal design and operation of different types of reactors.



Multiscale vorticity reconstructions for bubble column reactor based on 2d wavelet transforms with percentage energy distribution

## Selected publication:

- ✦ *Chem. Eng. Sci.*, 2008, 5330



## Separation science



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Reaction kinetics and separations

**Members:**

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S. Mandal, RA

The overall objective of our work is to study application of adsorption, ion-exchange, hybrid processes, and kinetics of these reactions.

**Reaction kinetics and separations**

Our research interests encompass adsorption, ion-exchange, hybrid processes, and kinetics of reactions. In adsorptive separation studies on the adsorption of organic isomers (cresols, xylenes), ground water decontamination (removal of fluorides/selenium), desulfurization of transportation fuels (diesel, petrol), separation of acids from dilute solutions and mathematical modeling and simulation are being continued.

**Fluoride/selenium decontamination from water**

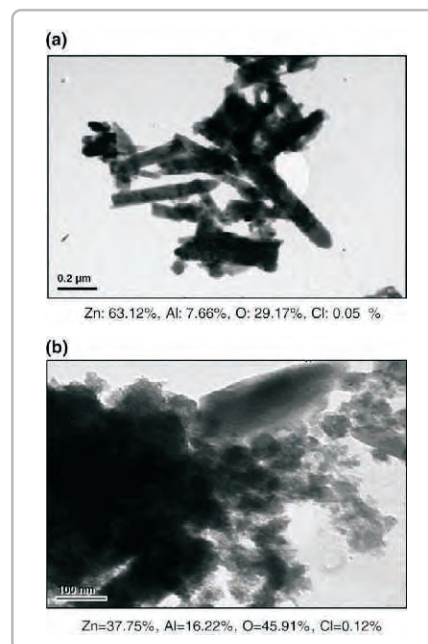
Anionic clays with varying amounts of bivalent and tri-valent metal ion ( $M^{2+}$ ,  $M^{3+}$ ) were synthesized and tested for their fluoride/selenium adsorption capacity. The influence of type of metal ions, metal ion ratio, pH of water, presence of other ions and surface charge of the LDH on the adsorption of fluoride and selenium was studied. It was possible to improve the adsorption efficiency of the clay by appropriate surface modification and use of support.

Zn-Al layered double hydroxides (LDHs) with different molar ratios Zn/Al (0, 0.17, 0.34, 0.97, 3.47,  $\infty$ ) were prepared by the co-precipitation of chlorides, characterized and evaluated for their fluoride adsorption at room temperature from aqueous solutions. The as-synthesized LDHs had a specific surface area below  $100\text{m}^2/\text{g}$ , which increased with thermal treatment up to  $500^\circ\text{C}$ . The pzc of this LDH corresponded to a solution pH of 9.7. ZA-11 with a Zn/Al ratio of 0.97 had the highest capacity for the adsorption of fluoride ions (1.14-4.16 mg/g).

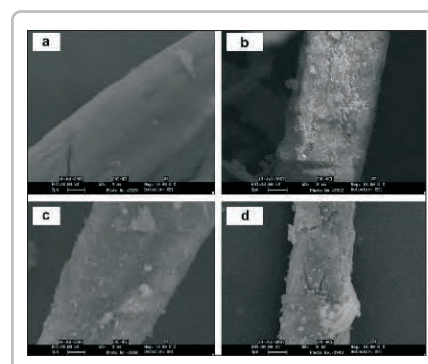
Cellulose supported layered double hydroxides (CSLDHs) were synthesized and tested for adsorption of fluoride in aqueous medium. Batch adsorption as well as fixed-bed column experiments were performed for determining the fluoride adsorption characteristics of CSLDHs. The fluoride adsorption properties of CSLDHs were found to be superior to those of reported adsorbents, including activated alumina and carbon nanotubes. Defluoridation capacity of the CSLDHs was 2 to 4 times higher than that of unsupported LDH.

**Selected publications:**

- ✦ Chemosphere, 2008, 72, 998
- ✦ Applied Clay Science, 2008, 40, 54
- ✦ Mater. Res. Soc. Symp. Proc., 2008, 1151, SS01-05



TEM images of the LDH particles along with their chemical composition obtained from SEM-EDAX analysis; (a) ZA-31, (b) ZA-11.



Scanning electron microscopic image of single fiber of CS (a) and cellulose supported LDHs, CSLDH-25 (b), CSLDH-50 (c) and CSLDH-75 (d).

## Biochemical engineering



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## Materials and surface-based approaches in proteomics

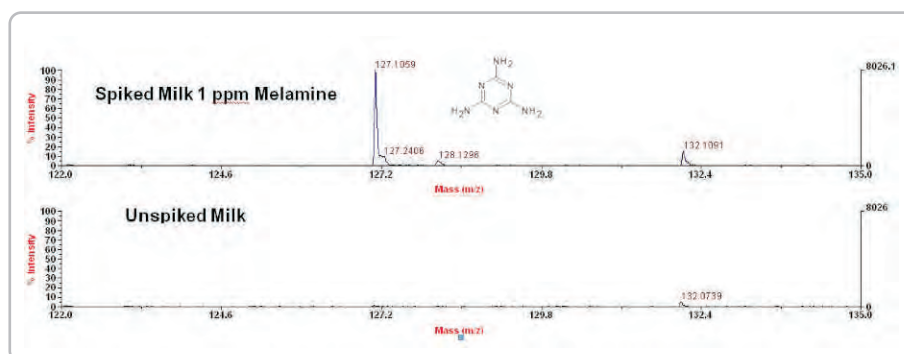
The discovery of biomarkers has immense impact on the well being of our society in diverse areas of biotechnology, especially for diagnostic and therapeutic applications. However, research in the biomarker discovery is riddled with major challenges due to the complexity of biological samples making it difficult to reap the results from the genome mapping, which has progressed considerably in the last decade. For example, a typical biological sample can contain analytes that come in a wide dynamic range of molecular masses - from small metabolites to peptides, proteins and protein complexes. In a proteomic sample, complexity also arises from posttranslational modifications, protein isoforms and differences in relative abundances. Thus, separating, isolating, analysis and quantification of biological samples, especially, proteins and peptides from a complex proteome is a challenging task. Existing strategies using poly acrylamide gel electrophoresis (PAGE) and HPLC have many inherent limitations impacting the progress of research in proteomics. There is a severe need for newer comprehensive methods as well as tools. The objective of this project is to apply materials and surface chemistry approaches for specific bioanalysis in the domain of proteomics and small molecule analysis.

We are currently developing and testing planar chromatographic techniques using capillary based (TLC) or electroosmotic force-based (EOF) approaches for the analysis of proteins and peptides. Planar

chromatography followed by mass spectrometry, in various forms has been recently demonstrated as being an alternative to the existing methods in the analysis of a proteins and peptides. This project involves design and fabrication of a suitable separation platform as well as optimization of the separation parameters and interfacing with fluorescence imaging and mass spectrometry.

**Low abundant analyte isolation and mass spectrometry of metabolites**

Low abundant analytes such as phosphoproteins and certain metabolites are a challenge to isolate and detect, yet, provide a wealth of information in a biological sample. Recently, titania-based devices have been successfully demonstrated to enrich phosphopeptides. Similarly, small molecules and metabolites are masked by matrix peaks in the mass spectra obtained by matrix assisted laser desorption ionization mass spectrometry (MALDI MS). Strategies to efficiently isolate analytes in low abundance and perform matrix-free LDI MS are being investigated in our group. In one demonstration of the usefulness of this method, we have isolated melamine, a harmful contaminant in milk products, using MALDI and LDI MS at a low ppm level (Figure). The USDA has prescribed a limit of 1ppm for infant milk products, which can be achieved by our method in addition to allowing the detection in a high throughput mode making it a practical method for analysis of contaminants in milk.



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Catalytic conversion of biomass into value-added products

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### Background / objectives

Utilization of lignocellulosic materials such as wood and agricultural wastes is essential in the context of increasing prices and finite source of fossil feedstock. While the main component of wood is cellulose (homopolymer) which constitutes almost 50% of wood material, the other major constituent (ca. 25-30%) of wood and second largest renewable feedstock derived from plant is hemicellulose. Cellulose is made up of glucose units linked together in a  $\beta$ -1:4 fashion and hemicelluloses are complex heterogeneous polymers composed of various monosaccharides such as xylose, mannose, glucose, galactose, arabinose, glucuronic acid etc. depending on the

source. Figure 1 illustrates the idea of biorefinery by which biomass can be converted into chemicals, fuels and power (energy).

Currently, a lot of research is devoted on the hydrolysis (or decomposition) of cellulose into glucose, and hemicellulose into xylose, by using various enzymes and dilute acid. But due to typical drawbacks associated with these methods, industries and academicians are looking at alternative ways for hydrolysis of cellulose and hemicellulose. Taking cue from this, study on cellulose and hemicellulose, hydrolysis catalyzed by heterogeneous catalysts was taken up.

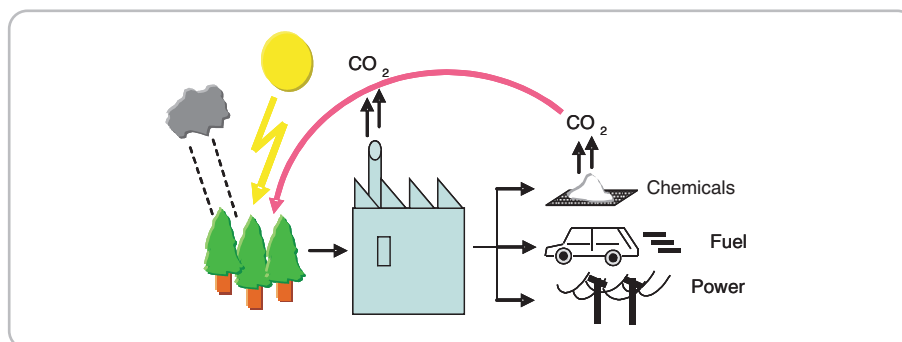
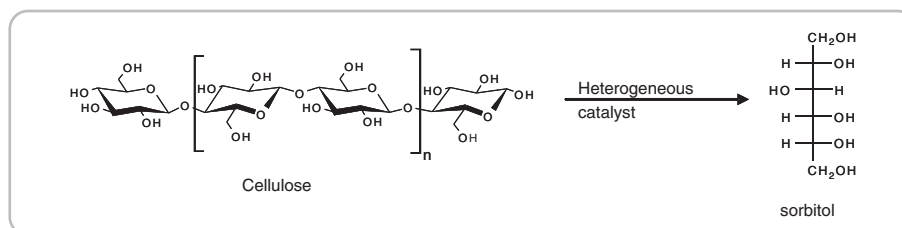


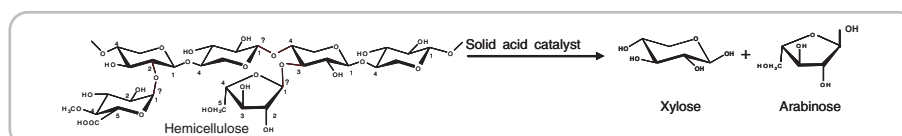
Figure 1. Biorefineryconcept

### Work done and discussion



For the conversion of cellulose into sugar alcohols (sorbitol and mannitol), supported metal catalysts were used under hydrogen atmosphere. With ~ 40% conversion and

with selectivity for sugar alcohols production of around 90% the catalysts showed good recyclability.



Work was also undertaken to convert hemicellulose into xylose and arabinose using heterogeneous catalysts. It is observed that over solid acid catalysts, formation of xylose from hemicellulose with almost 51% xylose yield is possible. Various solid acid catalysts were tested for the reaction and showed varying xylose yields

ranging from 20-50%. The effect of time, pressure, and temperature was also studied on the xylose formation. The catalysts were recyclable with almost no loss of activity. Under certain reaction conditions it was also possible to obtain furfural directly from hemicellulose with high yields.

### Selected publications:

- Chemical Record*, 2009, 9, 224
- ChemSusChem*, 2008, 1, 969



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Synthesis of novel catalysts for organic transformations and environmental catalysis

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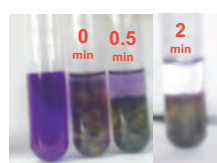
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### Inorganic gels for removal of organic dyes and organic contaminants

A simple process has been developed for the removal of the organic dyes and organic contaminants from an aqueous solution by treating it with titanium peroxide gel with or without other metal/metal oxides nanoparticles so as to degrade the colored contaminants from various industrial effluents for its safe disposal in the open environment. The coloured dyes are removed from the aqueous solution by adsorption/separation using this gel. The adsorbed dyes can be further degraded by exposing the titanium gel with the adsorbed contaminant to sunlight or by treating it with an oxidizing agent and the gel can be regenerated for its recycle. The degradation of organic contaminants from aqueous effluents can be carried out by using titanium peroxy gel resulting in the decrease in the COD value for safe disposal in the environment.

The titanium peroxy gel is prepared by very simple method using titanium alkoxide as titanium precursor, hydrogen peroxide and water at room temperature. The gel synthesis can be easily scaled up, and one kg batches have been prepared regularly in our laboratory. The removal of dyes and organic contaminants can be carried out using a slurry reactor or a down flow reactor, and the dyes and organic contaminants from the solution are separated by adsorption/filtration to obtain the colourless supernatant /filtrate. The separation of organic dyes from an aqueous solution, either by stirring in the slurry reactor or by passing over the gel packed in down flow reactor using titanium peroxy gel needs few minutes to few hours depending on the nature and concentration of the contaminants. Nearly ten different dyes as well as real industrial effluents containing dye contaminants have been removed / degraded using titanium peroxide gel.



Methyl violet



Methylene blue



Colored gels

#### Organic dyes

Methylene blue  
Methyl orange  
Methyl red  
Malachite green  
Methyl violet  
Rhodamine B  
Dimethyl yellow  
Basic violet -2  
Pararosaniline base  
Ink

### Ba-based NOx storage materials

The project aims at developing a Ba-based NOx storage material to be used as NOx storage reduction catalyst for removal of NOx from an automobile engine exhaust operating under lean condition. Especially the project aims at developing Ba-based NOx storage material with CeO<sub>2</sub> as a support because of its better performance compared to alpha-Al<sub>2</sub>O<sub>3</sub>. The objective of the proposal is to improve the performance of Ba/CeO<sub>2</sub> after hydrothermal aging at 850°C. This could be achieved by modifying the structural / textural properties of the CeO<sub>2</sub> support either by doping with some other metal oxide or by adapting a different strategy to prepare Ba/CeO<sub>2</sub> material to avoid the formation of BaCeO<sub>3</sub>. The overall objective of the project is to improve the

performance of the Ba/CeO<sub>2</sub> catalyst system for NOx storage as well as to improve its hydrothermal aging stability at 850°C.

We have developed Ba-based NOx storage catalysts which showed excellent catalytic activity for NSR and the results have been communicated to BASF and further study is going on as per BASF suggestions.

Selective catalytic reduction of NOx by hydrocarbons using mesoporous metal oxide catalysts

This is an ongoing activity for development of SCR catalyst for NOx reduction using a mesoporous metal oxide catalyst and we have developed a good catalyst composition which is showing encouraging results.

### Selected publications:

- Applied Catalysis, B*, 2009, 90, 416
- J. Mol. Catal. A*, 2009, 310, 150
- Oriental J. Chemistry*, 2008, 24, 62
- DGMK Tagungsbericht*, 2008, 169

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Band structure controlled semiconducting materials for energy conversion and photocatalytic splitting of water to produce hydrogen

**Role of lattice defects in the photocatalytic activity of vanadium-doped indium titanate for splitting of water molecules**

Thermoluminescence (TL), photoluminescence and diffuse reflectance UV-visible spectroscopy techniques were employed to investigate the doping-induced defect states and band structural properties of semiconducting indium titanate ( $\text{In}_2\text{Ti}_{1-x}\text{V}_x\text{O}_{5+\delta}$ ,  $0.0 = x = 0.2$ ) photocatalysts. Doping of vanadium caused a significant red shift in absorption edge, enabling the radiation absorption in entire visible region of

400-800 nm, and gave rise to at least two sets of closely spaced energy levels at the depth of ~1.1 and 1.3 eV in between the valence and conduction bands of the host matrix. It is concluded that the participation of these energy levels in the radiative/non-radiative recombination of photo-excited  $e^-/h^+$  pair, as shown in Fig.1, may control the availability of the electrons and holes for photocatalytic oxidation/reduction reactions. The reaction mechanism and the role of micro-structural defects in the activity of these mixed metal oxides for photo-dissociation of water molecules have been

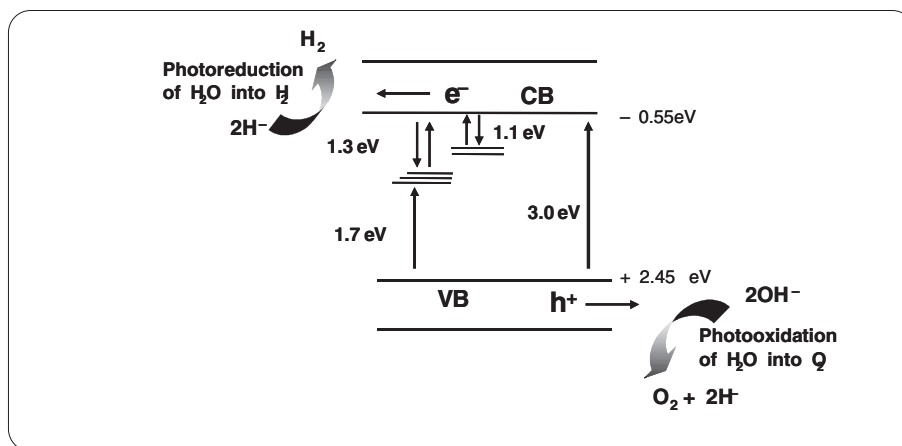


Fig.1. Band energy diagram of  $\text{In}_2\text{Ti}_{1-x}\text{V}_x\text{O}_{5+\delta}$  representing the localized energy levels that play an important role in the radiative/non-radiative recombination of the photo-excited  $e^-/h^+$  pair and in the overall activity for photocatalytic splitting of water

**Synthesis, physico-chemical and photo-physical properties of semiconducting mixed oxides**

The new series of mixed metal oxides,  $\text{In}_2\text{Ti}_{1-x}\text{Nb}_x\text{O}_{5+\delta}$ ,  $\text{InV}_{1-x}\text{Ti}_x\text{O}_{4+\delta}$  and  $\text{Ti}_{1-x}\text{In}_x\text{VO}_3$  with nominal compositions  $0 = X = 0.2$ , were synthesized and characterized systematically by using the techniques of powder XRD, UV-visible spectroscopy, IR spectroscopy and scanning electron microscopy. The synthesized materials were normally of single phase and the metal doping at A or B site resulted in a progressive red shift in the absorption edge. Studies on the defect states and the photocatalytic properties of these materials, without and after incorporation of various co-catalysts, are now in progress.

**Photocatalytic mineralization of volatile organic compounds over Au/TiO2 nanotubes: the role of sample morphology and gold nanoparticles**

Titanium dioxide nanotube (NT) samples were synthesized hydrothermally, followed by an alkaline treatment. Gold (1-2 wt %) was incorporated into these nanotubes after

calcination at different temperatures. High-resolution TEM examination revealed that 1.5 to 5 nm size gold particles were distributed both within and at the outside surface of Au/NT samples in addition to some larger size clusters (<40 nm) (Fig. 2). The temperature-programmed desorption study revealed a significant entrapment of  $\text{O}_2$  at two distinct tubular sites of NT samples, corresponding activation energy of desorption ( $E_a$ ) being around 36 and 41 Kcal  $\text{mol}^{-1}$ . On the other hand, gold nanoparticles in Au/NT served as low-energy ( $E_a = 26 \text{ kcal mol}^{-1}$ ) sites for adsorption/desorption of  $\text{O}_2$ . These adsorptive properties of  $\text{TiO}_2$  and Au were found to be particle size dependent.

Gold-containing  $\text{TiO}_2$  nanotubes (Au/NT) displayed considerably higher activity for photooxidation of acetaldehyde and benzene, as compared to gold-free nanotubes and also a Degussa P-25 catalyst. Fig. 3 exhibits representative catalytic activity of Au/NT as a function of gold content. The transient species formed during photo catalytic process were monitored by *in situ* IR spectroscopy. In the case of acetaldehyde oxidation, acetate

**Selected publications:**

- *Mater. Chem. Phys.*, 2009, 117, 399
- *J. Colloid Interf. Sci.*, 2009, 333, 263
- *J. Photochem. Photobiol.*, 2009, 203, 24
- *Catal. Today*, 2009, 141, 144

Band structure controlled semiconducting materials for energy conversion and photocatalytic splitting of water to produce hydrogen



( $\text{CH}_3\text{COO}_{\text{ad}}^-$ ) and formate ( $\text{HCOO}_{\text{ad}}^-$ ) type surface species served as reaction intermediates. Decomposition and oxidation of these species, with the help of  $\text{O}_2^-$  as well as hydroxyl ion radicals at photo-excited Au/NT interfaces, led to the formation of reaction products. The role played by particle morphology of semi-conducting material and the adsorptive properties of the co-catalyst have been discerned on the basis of these investigations.

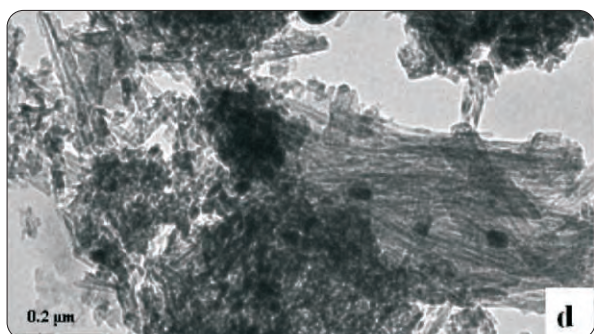


Fig. 2 TEM picture of Au (1 wt %)/TiO<sub>2</sub> nanotubes

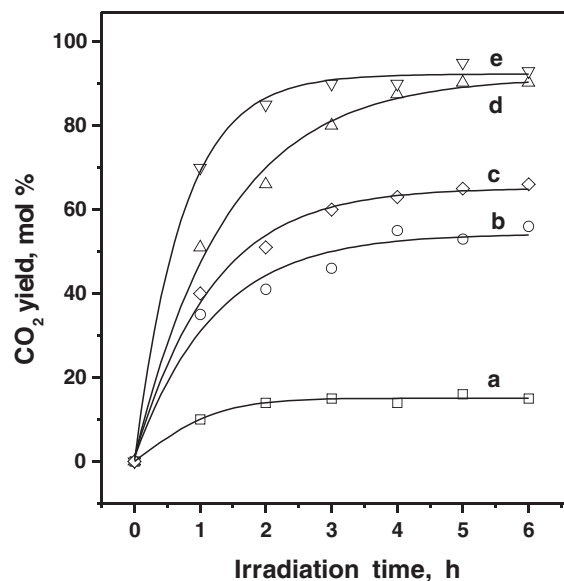


Fig.3 Plots of CO<sub>2</sub> yield when acetaldehyde (8 mol%) + air were reacted at room temperature over Degussa and TiO<sub>2</sub> nanotube (NT) samples under UV irradiation. Curve (b) Degussa P-25, (c) NT, (d) Au (1 wt%)/NT, and (e) Au (1.5 wt%) /NT. Curve (a) shows radiation induced conversion of acetaldehyde to CO<sub>2</sub> without using any catalyst.



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### Catalysis in fine chemical synthesis

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Fine chemicals are integral part of chemical industry; however, their production produces a high amount of waste when compared to bulk chemicals. The objective of our research is to develop benign routes for the synthesis of these chemicals. Conventional routes based on reagents often use hazardous starting materials and reagents. As an example of the synthesis of fine chemicals, we have shown that flavanones and aromatic ureas can be synthesized employing benign methodologies.

Hydrotalcite such as anionic clay (HTlcs) are particularly promising catalyst in the synthesis of fine chemicals due to their unique catalytic features besides easy preparation methodology involving low cost chemicals. Many times due to these advantages they are preferred over zeolite catalysts that are much expensive. In fine chemical synthesis usually substrates and products involved are polar in nature. Hence, a catalyst having proper acid-base strength of active sites is necessary to match the polarity of reactants and products. This aspect is demonstrated by following example:

The Claisen-Schmidt condensation of 2'-hydroxy acetophenone and benzaldehyde to chalcone and flavanone shows that calcined Zn-Al (6) hydrotalcite is active for this synthesis. The activity of this catalyst can be further increased by about 1.5 times by coating ionic liquid triethoxysilane-3-methyl imidazolium chloride on calcined hydrotalcite. It has been shown by  $^{13}\text{C}$  and  $^{27}\text{Al}$  NMR spectroscopic studies that IL is coated without degradation and that structural changes in calcined hydrotalcite take place when IL in amounts greater than 17.5% is coated onto CHTlc. It was observed that almost 72% alumina exists in tetra and penta coordination which seems to modify the acido-basic properties of the catalyst resulting in the enhancement of the catalytic activity at higher loading of IL. Thus, our research shows that acid-base properties of hydrotalcite like materials can be fine tuned by inter-acting these materials with ionic liquids.

Mesoporous materials are attractive supports for catalysts due to their unique structure of three-dimensional crystalline lattices with cavities. Added to this, the ability to exchange cations makes them ideal supports for heterogenizing homogeneous metal complex catalysts. The idea of making heterogenized catalysts having activity comparable to that of soluble metal complex analogues and having shape-selective property is thus feasible with mesoporous materials. NaY zeolite (and other materials, for example MCM-41) is ideal for encapsulation of transition metal complexes due to a large supercage ( $13\text{\AA}$  diameter)

having a wide pore window ( $7.4\text{\AA}$  diameter). Using this support, we demonstrate the shape selective synthesis of aromatic amines.

This research investigated the synthesis, characterization and the catalytic activity of heterogenized copper complexes for the selective amination of aryl halides. Amination reactions using homogeneous copper catalyst systems are not generally selective and it is also difficult to recover the catalyst from the homogeneous system for recycling. To overcome these difficulties, our efforts were directed towards the development of cheaper heterogeneous catalyst systems, which can be easily recovered and recycled.

Heterogenized analogues of the homogenous Cu complexes were prepared using two methods: (a) encapsulation of copper complexes in zeolite-Y, and (b) tethering of copper complexes on various supports such as zeolite-Y, silica, charcoal, or clay. The Na-Y encapsulated copper complex catalyst for amination of aryl iodide showed shape-selective formation of diphenylamine. This catalyst was stable and there was no leaching even after five recycles. Although encapsulated copper catalyst in MCM-41 for amination of aryl iodide gave selectively triphenylamine, this catalyst was not stable. The tethered  $\text{Cu}(\text{Phen})(\text{PPh}_3)_2\text{Br-PTA-Y}$  catalyst gave the best activity and selectivity towards triphenyl amine. Finally, a plausible reaction mechanism was suggested for a zeolite supported copper complex catalyst showing the pathway for shape-selective formation of diphenyl and triphenyl aniline.

Catalytic application of immobilized palladium nanoparticles for synthesis of ureas by oxidative carbonylation of amines has been demonstrated. This is the first report on oxidative carbonylation of amines to ureas using immobilized palladium nanoparticles catalyst. The palladium nanoparticles were immobilized on a NaY zeolite support through 3-aminopropyl-trimethoxysilane (APTS) as an anchoring agent. The  $[\text{Pd}]\text{-APTS-Y}$  catalyst along with NaI promoter showed high conversion and selectivity to the desired urea products over several amine compounds including an example of an aliphatic amine precursor even at 333 K. The immobilized catalyst was easily separated and recycled several times without any loss of activity. We believe that the strategically designed catalyst showed improved activity for oxidative carbonylation with respect to other reported  $\text{Pd}(0)$  catalysts possibly due to the absence of pore diffusional limitations and very good site isolation achieved by the synthesis.

#### Selected publication:

✱ *Catalysis Comm.*, 2009, 10, 1881



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Heterogeneous catalysts and catalysis / Synthesis, characterization, catalytic performance and scale-up

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**Selected publications:**

- \* *J. Physics Chemistry Solids*, 2008, 69, 2075
- \* *Materials Chemistry Physics*, 2009, 114, 344
- \* *Applied Clay Science*, 2009, 44, 255
- \* *Chemical Engineering J.*, 2009, 147, 97

**Synthesis and characterization of composite Sn-MCM-41/MFI material**

By virtue of their versatile morphological, textural and catalytic properties, Tin-containing micro- and meso- porous molecular sieves have attracted a great deal of research interest. However, the inherent diffusional limitations in the microporous molecular sieves make them less promising for the chemical transformations of various bulky organic substrates. Although, Sn-containing mesoporous materials have exhibited considerable activity in reactions such as hydroxylation, epoxidation, Mukaiyama-type aldol condensation, Baeyer Villiger, MPV and transesterification involving bulkier molecules, their low hydrothermal stability and acidity limit their potential applications. In view of overcoming these disadvantages of micro- and meso- porous materials, attempts were made to prepare Sn-containing composite micro/mesoporous material with optimal properties comprising the advantages of both micro- and mesoporous materials.

Al-free Sn- MCM-41 / MFI composite material was synthesized hydrothermally via a two-step crystallization process in presence of structure directing agent cetyltrimethylammonium bromide (CTMABr) and tetrapropylammonium hydroxide (TPAOH). The presence of both microporous and mesoporous phases were determined by XRD, nitrogen adsorption isotherm and HRTEM. Various synthesis parameters such as aging time, recrystallization time, temperature, molar ratios of structure directing agent (i.e. CTMABr/SiO<sub>2</sub>, TPAOH/SiO<sub>2</sub>), and water concentration were found to influence the physico-chemical properties of Sn- MCM-41 / MFI composite materials.

**N- Alkylation of aniline with methanol**

Mono-N-Methyl Aniline (NMA) is an industrially important product in the manufacture of paper, textile dyes, drugs, perfumes and explosives. The vapour phase alkylation of aniline with methanol to selective synthesis of mono-N methyl aniline is an advantageous route over liquid phase alkylation. Vapour phase methylation of aniline over heteropolyacid supported on clay was systematically studied and optimization of process parameters was carried out. The 20% w/w DTPA/Clay was found to be the optimum catalyst with 79% aniline conversion and 99% mono-N methyl aniline selectivity. The present observation required milder operating parameter than reported. The study was also explored to see the feasibility of 20%w/w DTPA/Clay as a

catalyst for the alkylation of aniline with other alcohols like ethanol, n-propanol, iso-propanol and n-butanol. The 20%w/w DTPA/Clay has shown decrease in activity with increase in carbon number, at the optimized process parameters.

Vapour phase alkylation of aniline for selective synthesis of N-methylaniline over lewis acidic Sn-MFI was also systematically studied. Sn-MFI (SiO<sub>2</sub>/SnO<sub>2</sub> = 50) was found to be optimum with 55% aniline conversion and 60% N-methylaniline selectivity. At lower space velocity (higher contact time) of 1h<sup>-1</sup>, aniline conversion increased to 71% at the cost of reduction in N-methylaniline (NMA) selectivity to 39% and increased in N,N-dimethylaniline (NNDMA) selectivity to 58%. The reaction follows the first order kinetics with respect to aniline having activation energy of 7.3 kcal/mol.

**Isopropylation of benzene using catalytic membrane reactor**

Selective isopropylation of benzene to cumene was demonstrated using catalytic membrane reactor (CMR) and the performance was evaluated against conventional plug flow reactor (PFR). Almost complete elimination of byproducts such as polyalkylated benzene and higher aromatics could be made possible by using CMR. These are present in significant amount when reaction is carried out with PFR. The cumene selectivity increased up to a maximum of 97.25% by CMR as against 90.05% with conventional PFR.

**Phenol hydroxylation over Sn-MFI**

Tin silicates with isolated Sn<sup>4+</sup> ions were reported to be active in the hydroxylation of phenol with aqueous H<sub>2</sub>O<sub>2</sub>. Moreover, Sn-impregnated molecular sieves and pure SnO<sub>2</sub> have shown negligible activity. Therefore, the said reaction was carried out with a view to gather more information on the nature of tin species (as a characterizing tool) and to compare the catalytic performance of different Sn-MFI catalysts prepared by different routes. Increase in concentration of isolated Sn<sup>4+</sup> ions led to increase in phenol conversion and H<sub>2</sub>O<sub>2</sub> efficiency. Nearly similar mole ratios (1.8 ± 0.2) of CAT to HQ suggested that, all the Sn-MFIs prepared by dry gel conversion method possess excellent shape selective property and the presence of well-dispersed Sn<sup>4+</sup> ions located within the channels of MFI structure. Although, not better but comparable activity has been shown by Sn-MFI prepared by dry gel conversion method with Sn-MFI prepared by conventional hydrothermal crystallization method.



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Hydroformylation using ionic liquids as solvents / Heterogenized catalysts

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- Prof. Carine Julcour, ENSIACET, Toulouse, France
- Rashmi Chansarkar, Dow Chemicals, Pune
- R. M. Deshpande, Dow Chemicals, Pune
- R. V. Chaudhari, University of Kansas, USA

Catalyst-product separation is major drawback of Homogeneous Catalysis. Non Aqueous Ionic Liquids [NAILs] represent a class of solvents, which are considered environmentally green. The aim of the work was to develop heterogenized catalysts based on ionic liquid (SILP) as well as tethered Rh complexes for easy catalyst/product separation.

### Supported ionic liquid phase catalyst

Supported ionic liquid phase catalyst (SILPC) was prepared from  $\text{Rh}(\text{CO})_2(\text{acac})/\text{TPPTS}$  and  $[\text{BMIM}][\text{PF}_6]$  supported on silica as per literature procedure. Hydroformylation of 1-octene was carried out using 50 mL high pressure autoclave and an analysis of reaction products was carried out using GC. A typical concentration-profile is shown in Figure 1. The effect of different operating parameters such as catalyst and 1-octene concentrations, hydrogen and carbon monoxide partial pressures as well as reaction temperature on the initial rate of hydroformylation was studied. Recycle experiments were performed by separating the SILP catalyst from the organic phase at the end of reaction, and adding fresh organic mixture to the SILP catalyst. Activity of the catalyst was good for 2 recycle experiments carried out. The n/i aldehyde ratio also remained constant upon recycling (between 2.3 and 2.7 after 1 hour of reaction). The ICP analysis showed small leaching of Rh (~1.5 to 3%) during the recycle experiment. SILP catalysts showed significantly higher activity compared to biphasic hydroformylation. The enhanced activity with SILPC can be attributed to the higher concentration of reagents, especially 1-octene in the proximity of active rhodium catalysts.

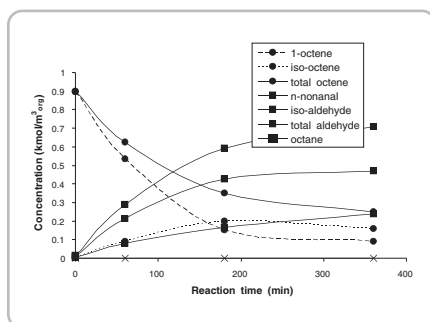


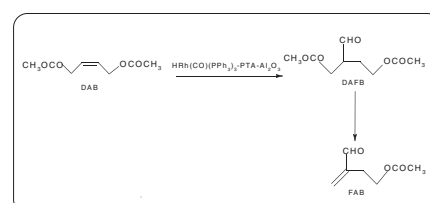
Figure 1. Typical Concentration-time profiles for hydroformylation of 1-octene using SILP catalyst. Reaction Conditions:  $\text{Rh}(\text{CO})_2(\text{acac})$ :  $15.8 \times 10^{-6}$  moles, TPPTS (without 10% oxide):  $9.46 \times 10^{-5}$  moles (P:Rh=6:1), 1-octene:  $0.973 \text{ kmol/m}^3$ , T: 353 K,  $P_T = 40 \text{ bar}$  ( $\text{H}_2:\text{CO} = 1:1$ ), total liquid volume:  $25 \times 10^{-3} \text{ m}^3$ , agitation speed: 1200 rpm.

### Selected publication:

- Industrial Eng. Chemical Research, 2009, 48, 9479

### Tethered Rh catalyst

Heterogeneous Rh complex catalysts have been prepared based on literature procedure for hydroformylation of 1,4-diacetoxy-2-butene using a tethering technique. The reaction is presented in Scheme 1. Tethered catalyst prepared  $(\text{HRh}(\text{CO})(\text{PPh}_3)_3)\text{-PTA-Al}_2\text{O}_3$  is highly active and stable for the hydroformylation of DAB to FAB, a Vitamin-A intermediate. A detailed characterization of the catalysts using  $^{31}\text{P}$  NMR, IR, ESCA, XRD, SEM-EDAX, TEM and ICP-AES analysis showed that Rh-O-W type of interaction is likely during tethering of these catalysts, and also indicates the catalysts are stable during the recycle for the hydroformylation of DAB to FAB. Various tethered catalysts were prepared from  $\text{HRh}(\text{CO})(\text{PPh}_3)_3$  using supports like alumina, calcium carbonate, carbon and used for hydroformylation of 1,4-diacetoxy-2-butene. Among the various catalysts reported tethered  $\text{HRh}(\text{CO})(\text{PPh}_3)_3$  on alumina was found to give the highest catalytic activity and stability. It was also observed that with the tethered heterogeneous catalysts, a simultaneous hydroformylation followed by deacetoxylation steps was possible, which is relevant for combining two steps in the sequence of synthesis of Vitamin-A intermediate (formyl acetoxy butene). The catalysts reported were highly stable and could be recycled number of times.



Scheme 1: Hydroformylation of 1,4-diacetoxy-2-butene



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Catalysis in liquid and vapour phase oxidation

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#### Liquid phase oxidation of toluene to benzaldehyde

Benzaldehyde is widely used in flavours such as almonds and cherry in various fragrances for soap and toiletries, chemical intermediates in manufacture of dyes perfumes, pharmaceuticals and pesticides, and photographic chemicals, as a solvent for oils, resins, cellulose ethers and fine chemicals. Benzaldehyde is produced by the hydrolysis of the corresponding side chain halogenated compounds such as benzyl chloride at a temperature range of 100°C-200°C at normal or higher pressures in the presence of excess hydrochloric acid. The hydrolysis is carried out in presence of hydrochloric acid or activated carbon treated with either sulphuric acid or metal chloride or sulphate.

A major drawback of these processes is the generation of large amount effluents and the benzaldehyde produced does not meet food grade specifications. The vapour phase oxidation of toluene to benzaldehyde is described in the patents using various transition metal catalysts at 300°C-500°C. The disadvantages of these processes are the use of high temperatures, and the formation of large amount of carbon dioxide which ultimately leads to decrease in the yield and is not environmentally acceptable. The present invention relates to an improved process for the selective liquid phase oxidation of toluene to benzaldehyde with high selectivity using a catalyst containing manganese, a Lewis acid and an organic or an inorganic halide, in the presence of organic acid, as a solvent.

A catalytic system developed consisting of manganese, a Lewis acid promoter and inorganic halide (alkali and alkaline earth metals) in presence of bromide. The catalysts showed high selectivity (50%-76%) to benzaldehyde at good conversion of toluene (5%-28%) at moderate reaction conditions.

#### Selective oxidation of propane to acrylic acid

Presently, acrylic acid is produced commercially by the oxidation of propene in two steps (i) oxidation of propene to acrolein, and (ii) oxidation of acrolein to acrylic acid using transition metal oxide catalysts. During the last decade, interest increased for the potential use of propane as a source of propene for the direct oxidation propane to oxygenates due to the abundant availability of propane and hence, economic reasons. However, activation of the C-H bond in propane is not easy due to its high strength, which requires a high energy of activation.

Literature data indicate that considerable progress has been made in the oxidation of propane to acrylic acid by molecular gas-phase oxygen. Various catalyst systems such as heteropoly acids, V-P-O catalysts, and metal oxide catalysts have been studied for the oxidation of propane to acrylic acid. Mo-V-Te-Nb-O<sub>x</sub> and Mo-V-Sb-Nb-O<sub>x</sub> mixed oxides are the most active and selective catalysts for this reaction. Among the above catalysts, mixed oxide catalyst was found to be most active, selective and stable for this reaction.

Although there are a number of research papers published using mixed oxide catalysts, there is still a need to characterize the catalysts in detail for their surface acidic and basic properties and to relate them to activity and selectivity. Therefore, it is proposed to develop new or improved mixed oxide catalysts containing alkali, alkaline or rare earth metals, by various preparation methods and conditions for the selective oxidation of propane to acrylic acid. The catalysts containing transition metals will be thoroughly characterized for their surface properties and correlated with the catalytic activity / selectivity in the process. This also includes the optimization of process parameters and to study the reaction kinetics and mechanism for the selected catalysts in oxidation of propane.

Various Mo- and V-based mixed oxide catalysts containing antimony, tellurium and alkali metals have been developed. The Mo- and V-based catalyst consisting of antimony and alkali metals is found to be highly active and selective for the selective oxidation of propane to acrylic acid. Among the alkali metal doped catalysts, highly promising catalytic performance was shown by the Cs-doped catalyst with the selectivity to acrylic acid in the range of 40%-50% with good activity. The catalyst preparation method, catalyst precursors, alkali metal concentration are found to be critical so as to achieve good activity and selectivity. It was also found that water plays an important role in the formation of oxygenated products in oxidation of propane.

#### Selected publication:

- ✦ US Patent, 2008, 7, 411, 099



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Green chemistry via catalysis

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Our group is actively engaged in designing / developing new catalysts, routes and bench scale processes for fine chemicals and pharmaceuticals with a focus to replace the conventional processes involving use of stoichiometric reagents, with catalytic processes, use of renewable feedstock and supercritical fluids.

## Highly active nanostructured Co<sub>3</sub>O<sub>4</sub> catalyst with tunable selectivity for liquid phase air oxidation of *p*-cresol

This is a first report of highly efficient heterogeneous nanostructured Co<sub>3</sub>O<sub>4</sub> catalyst (6-8 nm) having high surface area (95 m<sup>2</sup>/g) developed for selective liquid phase air oxidation of *p*-cresol under atmospheric pressure conditions. The nanostructured Co<sub>3</sub>O<sub>4</sub> was prepared from Co(NO<sub>3</sub>)<sub>2</sub> and K<sub>2</sub>CO<sub>3</sub> by a simple protocol without using any template, involving a simultaneous co-precipitation/digestion technique followed by calcination at 573 K in air.

HRTEM study of Co<sub>3</sub>O<sub>4</sub> particles indicates rod type aggregates (diameter = 4-5 nm, length = 20-30 nm) that are formed from 2-3 nm primary particles. The nanostructured Co<sub>3</sub>O<sub>4</sub> catalyst showed more than twice activity than that of the bulk catalyst. This can be attributed to the lower particle size (6-8 nm) and very high surface area (95 m<sup>2</sup>/g as against 9 m<sup>2</sup>/g of the bulk Co<sub>3</sub>O<sub>4</sub>) of the nanostructured Co<sub>3</sub>O<sub>4</sub> catalyst.

## Catalytic hydrogenation of 2-butyne-1,4-diol : Activity, selectivity and kinetic studies

Hydrogenation of 2-butyne-1,4-diol is an industrially important reaction for the manufacture of *cis* 2-butene-1,4-diol and butane-1,4-diol. In this process, 2-butene-1,4-diol is an intermediate olefinic diol, which undergoes further hydrogenation to give a saturated butane-1,4-diol.

Studies on designing various catalyst systems including colloidal as well supported palladium nanoparticles for the hydrogenation of butyne diol, role of additives, catalyst pretreatment, kinetic studies have been carried out in our group. Interestingly, almost complete selectivity to the intermediate olefinic diol was achieved with 1%Pd/CaCO<sub>3</sub>-NH<sub>3</sub> catalyst system while, platinum based catalysts eliminated the formation of side products in the hydrogenation of butyne diol. In case of continuous hydrogenation, the selectivity pattern was completely different from that found in case of batch slurry reactor and by varying the contact time, the selectivity to both butene- and butane diols could be varied over a wide range of conditions.

## The kinetics of liquid phase oxidation of *p*-cresol to *p*-hydroxybenzaldehyde

The kinetics was investigated using insoluble cobalt oxide (Co<sub>3</sub>O<sub>4</sub>) catalyst at oxygen partial pressures in the range 0.1-1.5 MPa, and reaction temperatures 333-393 K. Following rate expression was proposed considering *Langmuir-Hinshelwood (LH)* type mechanism, based on the initial rate data. A batch reactor model was also developed based on the kinetics studied and the concentration time profile predicted by the model was in good agreement with the experimental data. The activation energy for the liquid phase oxidation of *p*-cresol was found to be 39.6 kJ/mol.

$$r = \frac{wk_1K_A C_A C_B}{(1 + K_A C_A)}$$

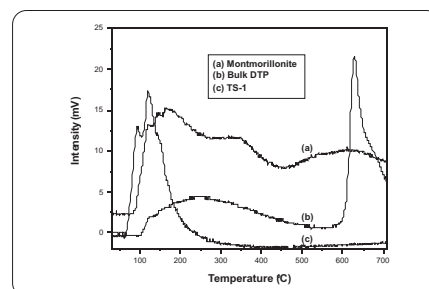
## Particle size effects of activated carbon supported rhodium catalysts on hydrogenation of naphthalene in supercritical CO<sub>2</sub>

Naphthalene hydrogenation in supercritical CO<sub>2</sub>, over activated carbon supported rhodium metal particles having dispersion between 10%-30% showed that the turnover frequencies increased with decreasing dispersion in supercritical carbon dioxide while TOF was independent of the metal dispersion in n-heptane.

## Selective hydroxyalkylation of phenols to bisphenols

Performances of montmorillonite clay, TS-1 and dodecatungsto- phosphoric acid (DTP) were compared for the hydroxy- alkylation of *p*-cresol to dihydroxydiaryl-methane (DAM).

Ammonia TPD studies of various catalysts showed that an appropriate combination of both strong and weak acid sites of montmorillonite was mainly responsible rather than only the stronger acidity of bulk DTP for its highest catalyst activity for selective hydroxyalkylation of *p*-cresol to DAM. The selectivity to DAM could be enhanced by adjusting reaction conditions such as mole ratio of *p*-cresol to formaldehyde, reaction temperature, catalyst concentration, solvent and reaction time.



## Selected publications:

- ✦ *Cat. Commun.*, 2008, 9 441
- ✦ *Appl. Catal. B: Environ.*, 2008, 79, 270
- ✦ *Chem. Lett.*, 2008, 37, 734
- ✦ *Appl. Clay Sci.*, 2009, 43, 113

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Synthesis of nanostructured bio-inorganic hybrid porous catalytic solids

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**Synthesis and characterisation of meso-porous bio-inorganic nano hybrid materials**

This project is focused on synthesising a group of bio-inorganic hybrid nano-materials that have the advantages of both the disciplines with improved credibility for applications including high performance catalysis and nanomedicine.

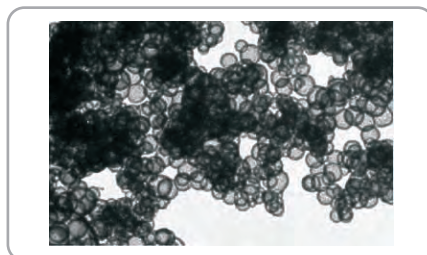


Figure 1. Bio-inorganic nano-shells of silica using liposomal templating. (average diameter ~ 100nm)

The self-assembly of organized nanoscopic structures is of great interest in both colloidal and material science. Vesicular templating offers a unique opportunity to obtain hollow submicron particles. We use a liposomal templating mechanism which is one of the recent approaches to the synthesis of silica spherical particles. The silica shells thus produced have an aqueous core of the

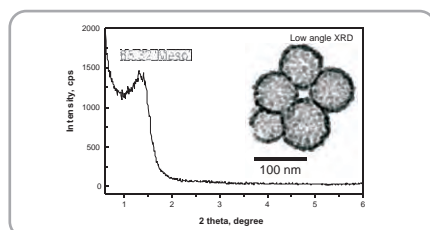


Figure 2. Low angle pXRD indicates meso-porous silica reflection (65.3 Å layer). (Inset) Isolated shells with a wall thickness ~ 12 nm

liposome in which drugs can be loaded depending on the need and covered by a silica cladding around the lipid bilayer wall of liposome. These properties and the drug release studies have proven them to be prospective candidates for drug delivery systems. The source of silica has been alkoxides such as tetraethylorthosilicate (TEOS). On the careful treatment such as controlled freeze drying make these materials lose the aqueous matter to become hallow spheres of huge surface area. Further modifications in the recipe of the inorganic cladding around the liposome lead to the formation of hallow silica spheres with the possibilities of mesoporosity. The <sup>29</sup>Si and <sup>31</sup>P solid state NMR characterization provides direct clue for the direct templating effects of the lipid bilayers into the formation of the mesoporous thin silica wall of about 13-17nm.

The synthesis of these nanoshells initially

suffered problems such as the co-formation of bulk amorphous silica, and loss of symmetry and surface deformations. The release of ethanol from the silica precursor tetraethoxysiloxane (TEOS) has been identified as a factor to destabilize the lipid membrane there by creating deformations. We demonstrated a controlled fabrication of silica nanoshells with highly symmetric shapes without surface deformation and formation of bulk silica.

**Synthesis and characterisation of silica nanotubes using dynamic templating effects**

Forming an inorganic cladding around phospholipids based liposomes has been reported as a way to make inorganic nanospheres. However, here we observed how these spherical liposomes undergo a series of dimensional transformations to form long silica nanotubes. Thus, this report demonstrates an unusual templating mechanism at ambient conditions (Fig. 1).

These silica nanotubes are observed to be around 60-90 nm in diameter and up to few microns in length. It is further interesting to observe that (a) the diameter can be fine tuned by changing the template dimension, and (b) though the template liposomes are closed vesicles by nature, the nanotubes formed out of them are generally open on both the ends. The amorphous silica wall is observed to have formed on both the inner and outer surfaces of the 'lipo-tubules' making a double wall with a thickness of about 15-19 nm. Several other factors that influence this mechanism have been studied and discussed here. The present experiment

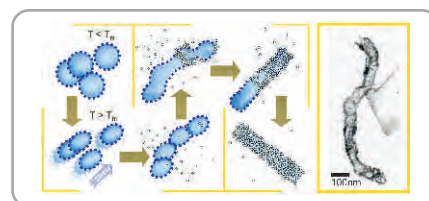


Figure 3. Transformation from nanospheres to nanotube – a schematic illustration of the proposed templating mechanism for the formation of the silica nanotube.

is, to the best of our knowledge, the first to decisively prove an earlier observation which suggests that under external electromagnetic stimulus, the ductile liposomes may form lipo-tubules. In our work, we have captured the meta-stable lipotubular structures into a solid through the above templating mechanism. However, we further report here that these dimensional transformations in the lipid bodies are possible even without such external electromagnetic stimulus.



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Synthesis, characterization of non-siliceous, siliceous organic-inorganic hybrid and triflated mesoporous materials

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The design and development of transition metal oxide based mesoporous molecular sieves (TMS) using zirconia as transition metal oxide support (Zr-TMS) were carried out by adopting suitable templating route to get high surface area with narrow pore size distributions. Further, the surface modification of Zr-TMS was done using various organic and organosilane groups such as benzylosulfonic acid (BSA), trifluoromethanesulfonic acid (TFA) and

organosilanosulfonic acid (OSA) by post synthetic route to develop a new class of highly acidic mesoporous catalysts. The proper synthesis of the catalyst was analyzed by various physico-chemical techniques such as powder XRD, N<sub>2</sub> adsorption desorption isother, FT-IR, Solid State NMR, UV-Vis, XPS etc. The activity of the catalyst was analysed for various reactions such as condensation, benzylation, acetylation, and esterification reactions.

### Catalytic activity of mesoporous Zr-TMS catalysts

S. No.	Catalyst	Reaction	Main product
1	Zr-TMS-BSA	Condensation of anisole with HCHO	4,4'-DMDPM
		Condensation of 2-Methyl furan with acetone	BMP
		Benzylation of diphenyl ether with benzoyl chloride	4-PBP
2	Zr-TMS-TFA	Acetalization of ethyl acetoacetate	Fructose
		Benzylation of biphenyl	4-PBP
		Benzylation of toluene	4,4'-DMBP
3	Zr-TMS-OSA	Esterification of glycerol	MG
		Condensation of aniline	4,4'-DADPM

Micelle-templated mesoporous and organic-inorganic hybrid mesoporous materials are important in many fields of material research, especially for hosting catalysts in confined space. Among this class, the recent discovery of periodic mesoporous organosilicas (PMOs) represents an exciting new group of organic-inorganic nanocomposites targeted for a broad range of applications ranging from catalysis to microelectronics. Compared to the earlier generation of organic-inorganic hybrid

mesoporous samples, obtained by the co-condensation reaction or by the grafting reaction, PMOs represent the right combination of organic and inorganic groups in the frame wall positions. We are focusing on organic-inorganic hybrid mesoporous material research with special emphasis over periodic mesoporous organosilica materials having various redox centers (Ti, V, Cr) suitable for oxidation reactions as well as acidic sites (Al, -SO<sub>3</sub>H) for the organic transformation of bulky molecules.

### Catalytic activity of the metal containing PMO catalysts

S. No.	Catalyst	Reaction	Main product
1	Cr-PMO	Cyclohexane oxidation	Cyclo hexanone
		Ethyl benzene	Aceto phenone
2	V-PMO	Cyclooctene oxidation	Epoxide
		Styrene oxidation	Benzaldehyde

### Acidic properties and binding states of metal triflate molecules immobilized in the channels of SBA-15 and their role in the Friedel-Crafts acylation reaction

The Zn-triflate molecules loaded (5 to 30 wt %) in mesoporous SBA-15 silicate exhibited considerably higher catalytic activity for liquid-phase Friedel Craft (FC) acylation reaction of naphthalene with *p*-toluoyl chloride, as compared to corresponding triflates of Zn, La, Ce and Y. NH<sub>3</sub>-TPD and *in situ* FTIR studies helped us in the monitoring of the acid sites and the binding mode of individual metal

triflates in the channels of functionalized SBA-15. The triflate molecules were found to be geometrically confined with no electronic binding at the zeolitic sites. At the same time, the occluded molecules caused significant physical perturbation to the hydroxyl groups of the host matrix and in turn gave rise to the formation of certain Brønsted type surface acid sites. The metal cations of triflate molecules, on the other hand, participated in the direct bonding of reactant molecules. The role of triflate-generated acid sites in the Friedel-Craft acylation of naphthalene has been elucidated.



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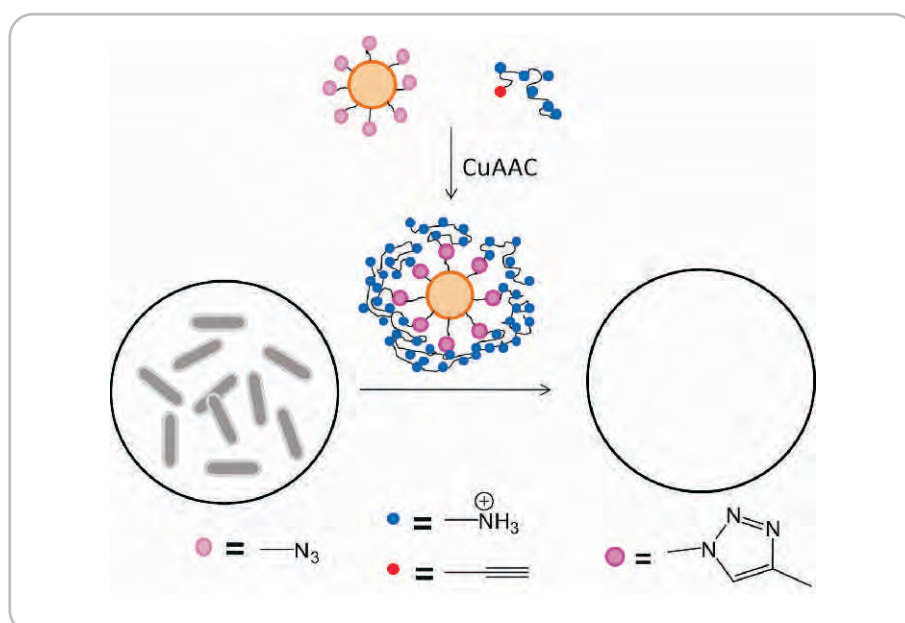
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Polypeptide polymer grafted silica nanoparticles are of considerable interest because the ordered secondary structure of the polypeptide grafts imparts novel functional properties onto the nanoparticle composite. Synthesis of polypeptide grafted silica nanoparticles such as poly-L-lysine grafted silica nanoparticles, would be of particular interest since the high density of cationic charges on the surface could lead to many applications such as gene delivery and antimicrobial agents. We have developed a "grafting to" approach using a combination of

NCA polymerization and "click chemistry" to synthesize polypeptide grafted silica nanoparticle with a high graft density of 1 chain/nm<sup>2</sup>. Poly-L-lysine grafted silica nanoparticle, synthesized by this methodology, was tested as an antimicrobial agent on both Gram-negative *E. coli* and Gram-positive *bacillus subtilis*. It was found that 50 µg/mL of PLL-silica was sufficient for a considerable (>90%) reduction of bacterial count, thus showing its potential usage as antimicrobials.



Poly-L-lysine grafted silica nanoparticles synthesized using NCA polymerization and "click chemistry" is shown to have antibacterial properties

### Selected publication:

✦ *J. Materials Chemistry*,  
2009, 22, 1409

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Sustainable catalytic routes for renewable fuels and fine chemicals

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**A. Biodiesel and biolubricants : Preparation and analysis**

*(a) A solid catalyst-based process for producing biodiesel and biolubricants*

In the past the NCL developed novel, solid double metal composition catalysts which were highly active (95%-98% conversion) for conversion of a range of oils including Jatropa, Karanja and unrefined rubber seed oil (containing up to 18% of free fatty acids, FFA) and used oils into biodiesel and biolubricants. Both transesterification (of the triglycerides) and esterification (of the FFAs) could be accomplished by this solid catalyst in a single-step.

The solid catalysts developed were reusable and active even when significant quantities of water were present (unrefined oils). Most important, the by-product glycerol obtained during the biodiesel and biolubricants manufacturing was also converted into a high cetane diesel additive thereby increasing the yield and fuel burning characteristics of biodiesel and licensed to a US-based start-up company, Benefuel Inc.

Presently the scale-up studies of a continuous process are in progress. The NCL developed necessary experimental data and Benefuel is aiming to commercialize this solid catalyst-based biodiesel technology. The solid catalyst-based process of the NCL yields 3% more biodiesel than that by conventional homogeneous alkali-based process. The quality of biodiesel and glycerin obtained are high and meet the required specifications. It is a water-free, eco-friendly process. Moreover, it is a versatile process and depending on the feedstock alcohol and requirement, the plant operation can be switched over from biodiesel to biolubricant. A proto-type pilot plant is fabricated and is being installation in USA.

*(b) Esterification of free fatty acids to biodiesel over solid catalysts*

Esterification of fatty acids to fatty acid alkyl esters (biodiesel) is a key step in the utilization of non-edible oils and animal fats as cheaper feedstocks. Design and development of highly efficient solid catalysts that can tolerate water is a challenging task. In esterifications over solid catalysts, water, a co-product limits the conversion not only due to equilibrium considerations but also by strongly adsorbing on the active, catalytic sites. In esterification, due to the different polarity and dielectric constant values of methanol and water, the strength of their interaction with the active (acidic) sites will vary. Water, with its higher dielectric constant, can

successfully compete with methanol, for adsorption on the acid sites. The apparent activation energy ( $E_a$ ) for esterification of C8.0 – C18.1 fatty acids with methanol is lower over sulfated zirconia (SZ) and Al-MCM-41 than on Fe-Zn double metal cyanide (DMC) catalyst. Over DMC, the apparent activation energy ( $E_a$ ) decreases with increasing chain length of fatty acid. A reverse trend, however, is observed over SZ

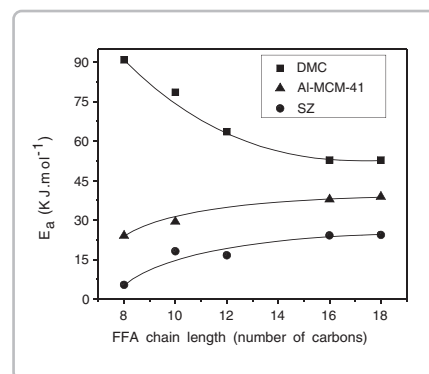


Fig. 1. Influence of chain length of fatty acid on activation energy ( $E_a$ ) for the esterification reactions over DMC, SZ and Al-MCM-41 catalysts.

and Al-MCM-41 (Fig. 1).

The variations in apparent activation energy with the chain length of fatty acid cannot be explained based only on the textural and acidic properties of the catalysts. For a given pore size,  $E_a$  is expected to increase with increasing chain length of the fatty acid as indeed observed for SZ and Al-MCM-41 (Fig. 1).

The observation of a decrease for DMC indicates that other factors such as surface polarity/hydrophobicity also play an important role. Competitive adsorption studies indicated that DMC is more hydrophobic than SZ and Al-MCM-41. Adsorption of methanol in the presence of water was found to be 10 times higher on DMC than on SZ and Al-MCM-41. The relative adsorption of methanol with respect to water (defined as the hydrophobicity index) increased in the order: Al-MCM-41 < SZ < DMC. Water therefore, competes with methanol for adsorption on the active sites and, in the process, lowers the concentration of methanol on the catalyst surface.

This effect is more in the case of Al-MCM-41 and SZ than in DMC. Adsorption of oleic acid in the presence of methanol, n-octanol and decane over different catalysts increased in the same order as their hydrophobicity index. As the chain length of the fatty acid increases, it is less miscible with water. Hence, its adsorption on

**Selected publications:**

- ✦ *Chem. Commun.*, 2009, 6484
- ✦ *Energy Fuels*, 2009, 23, 2273



hydrophobic catalyst surfaces such as DMC is expected to be thermodynamically more preferred than on the relatively more hydrophilic (and hydroxylic) SZ and Al-MCM-41.

More facile adsorption of fatty acid with increasing chain length over hydrophobic surfaces (as in the case of DMC) results in a more facile reaction and lower activation energy. This work reveals that apart from acidic and textural features, the hydrophobicity of the catalyst surface influences significantly the rate of esterification of long-chain fatty acids with methanol.

#### (c) Method for estimation of free fatty acid

A simple and fast method for estimation of free fatty acids (FFA) in vegetable oil, animal fat and biodiesel using proton NMR spectroscopy is developed. This method is non-destructive and requires only a small amount of the sample. It can also be used as an *in-situ* tool to monitor the esterification reaction of FFA to biodiesel. The FFA content is an important quality parameter which has to be determined before oil can be used for any purpose. The FFA determination is not only important for biodiesel industry but also a quick and reliable method desirable in the food industry too.

Non-edible oils and fats often contain significant amounts of phospholipids and other acidic impurities along with the FFAs. While the titrimetric method determines the total acid value in oils and fats,  $^1\text{H}$  NMR detects the FFA content exclusively. Control experiments revealed that  $^1\text{H}$  NMR can detect FFA as low as 0.5 wt%.

### B. Mesoporous titanasilicate molecular sieves for selective catalytic oxidations

Synthesis of mesoporous, titanasilicate molecular sieves containing Ti ions in lattice framework positions and capable (unlike microporous titanasilicate-1, TS-1) of selective oxidation of bulky molecules is of current interest. SBA-12 has outstanding hydrothermal stability and a three-dimensional mesoporous structure. Incorporation of Ti in its framework is difficult because under the conventional, highly acidic conditions of its synthesis, Ti exists only in the cationic form as oxy/hydroxy species. The former cannot be introduced easily into the framework via condensation processes with silica species. However, we could achieve, for the first time, the direct hydrothermal synthesis of Ti-SBA-12 containing Ti ions in framework positions.

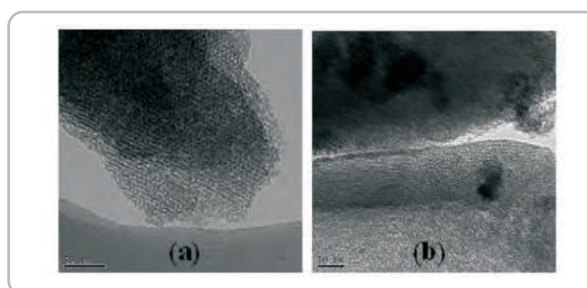


Fig 2 : HRTEM of (a) SBA-12 and (b) Ti-SBA-12 (Si/Ti = 30)

X-ray powder diffraction studies provided clear evidence for the incorporation of Ti in the framework of SBA-12. High resolution transmission electron micrographs (HRTEM) confirmed the long-range three-dimensional mesopore ordering (Fig. 2). Tetrahedral coordination of Ti as tri and tetrapodal sites in these materials were established by spectroscopic techniques.





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Surface science and catalysis

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The objective of our group was to get some insight into the molecular level aspects of catalysis as well as catalysts with surface science and other relevant approaches so that some input to its further development could be made. Also devise methods to produce new materials that might be helpful to address current problems such as photocatalysis.

#### Direct Influence of subsurface oxygen towards surface catalysis

Interactions between oxygen and Pd-surfaces have important implications,

especially towards oxidation reactions, and influence of sub-surface oxygen to oxidation reactions is the focus of the present study. In our efforts to understand the above aspects, CO oxidation reactions have been carried out with mixed molecular beam, consisting CO and O<sub>2</sub>, on Pd(111) surfaces under a wide variety of conditions (T = 400 to 900 K, CO:O<sub>2</sub> = 7:1 to 1:10). A new aspect of the above reaction observed in the transient kinetics regime is the evidence for oxygen diffusion into Pd subsurface layers (Figure 1), and its direct influence towards CO oxidation at high temperatures (≈600 K).

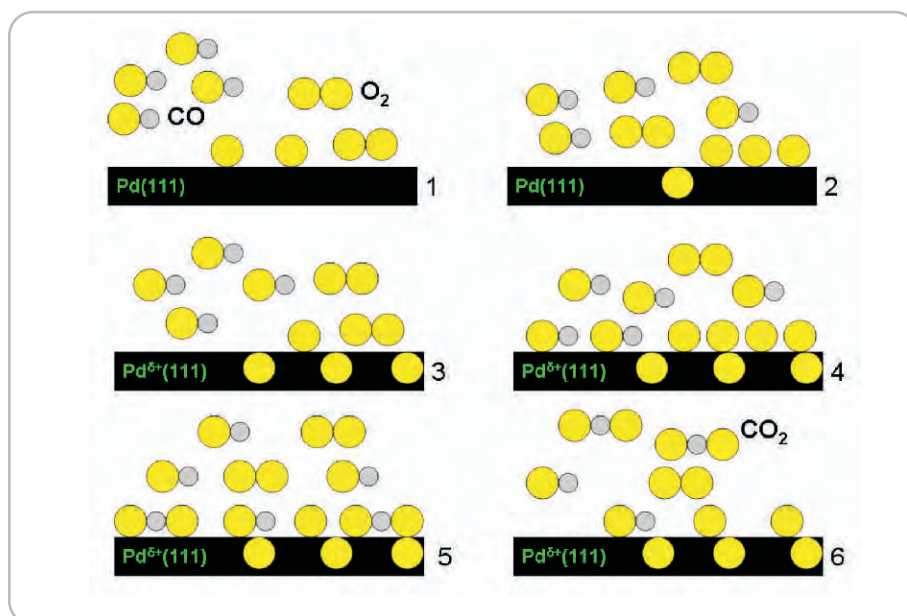


Fig. 1 Schematic model for oxygen diffusion followed by CO + O<sub>2</sub> reaction on Pd(111) > 550 K. Pd<sup>5+</sup> = mildly oxidized Pd

Interesting information derived from the above studies is necessary to fill up the sub-surface layers with oxygen atoms to threshold coverage ( $\theta_{o-sub}$ ), above which the reactive CO adsorption occurs on the surface and simultaneous CO<sub>2</sub> production begins. There is also a significant time delay ( $\tau$ ) observed between the onset of O<sub>2</sub> adsorption and CO-adsorption (or CO<sub>2</sub> production). Above studies suggest an electronic decoupling of oxygen covered surface and sub-surface layers, which is slightly oxidized, from the metallic bulk, which induces CO adsorption at high temperatures (Fig. 1) and simultaneous oxidation to CO<sub>2</sub>. An important application of the above findings is the broadening of active CO-oxidation temperature regime to high temperatures, up to 900 K, with oxygen in the sub-surfaces of Pd.

#### Combustion synthesis of nitrogen doped ZnO

ZnO is well known to form oxygen vacancies and a simple heating turns it into pale yellow/brown colour at high temperatures due to O-vacancies, and it returns to colourless material at room temperature. It is the above fact that we utilized to introduce nitrogen into the ZnO-lattice at high temperatures under combustion conditions, where significant to large number of oxygen vacancies should be available. Along with a zinc compound such as zinc nitrate, and a fuel such as urea, led to ZnO<sub>1-x</sub>N<sub>x</sub> under combustion conditions. Above conditions lead to the generation of nascent nano clusters of Zn<sub>n</sub>O<sub>z</sub> with oxygen vacancies ( $y/z > 1$ ) and *in-situ* generation of ammonia for nitridation of the above clusters were the critical steps to introduce nitrogen into the O-vacancy positions.



Indeed, a maximum of 15% bulk N-doping was achieved in  $ZnO_{1-x}N_x$  ( $x \leq 0.15$ ) by the combustion method (Figure 2), which was not possible with any of the sophisticated methods available till date. The nature of  $ZnO_{1-x}N_x$  materials has been studied by structural, spectroscopic, and microscopic methods. In spite of the harsh reaction conditions, micron size triangular crystals (Figure 2) which exhibit multifunctional

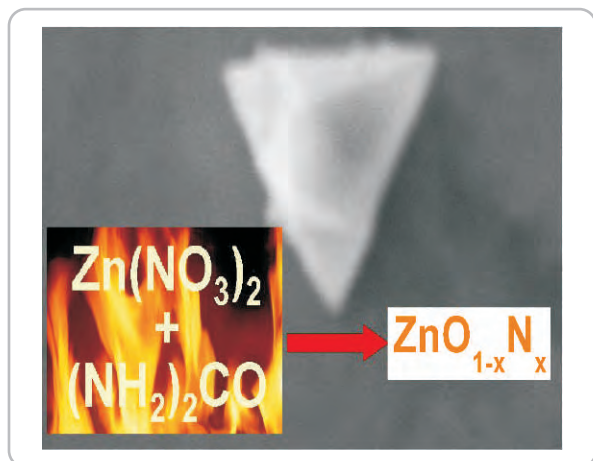


Fig. 2 Solution combustion synthesis of N-doped  $ZnO_{1-x}N_x$  from zinc nitrate and urea

characteristics (visible light absorption, room temperature ferromagnetism, high hydrophobicity, photocatalytic activity) have been observed. This method is to be extended with suitable metal ions to produce new materials with the aim of making visible light driven photocatalysts.

### Catalyst for selective production of ultra high molecular weight polyethylene

The discovery of  $MgCl_2$ -supported  $TiCl_4$  catalyst brought a breakthrough, and led to an exciting improvement in the

properties of polyolefins. The method of preparation of  $MgCl_2$  affects the catalytic properties markedly. In particular, the reaction of  $MgCl_2$  with a suitable alcohol and treated with an excess of  $TiCl_4$  can produce super active catalyst, which emphasizes the larger role of support. A new molecular adduct,  $MgCl_2 \cdot 4(CH_3)_2CHOH$  (Figure 3), has been synthesized, characterized for structural aspects, and demonstrated for super active ethylene polymerization activity. Solid state NMR results demonstrate the structural properties of the above molecular adduct, including two different sets of magnetically non-equivalent isopropanol molecules in a *cis* arrangement

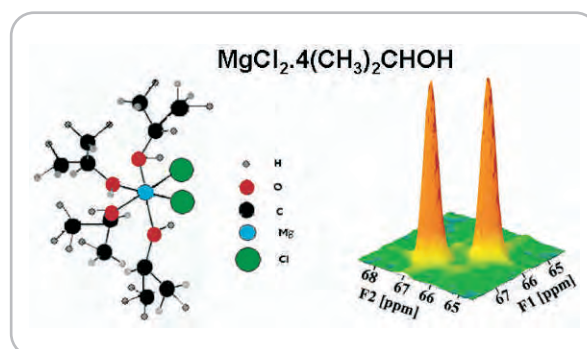


Fig. 3 Possible structure and 2D exchange NMR contour plot of  $MgCl_2 \cdot 4(CH_3)_2CHOH$

(Figure 3). With triethyl aluminium as the co-catalyst, ultra high molecular weight polyethylene (7 million) was obtained with high yield (14 kg/g catalyst or 5.75 kg/mmol of Ti) which shows that the productivity is comparable to or better than many commercial catalysts. We are also preparing  $MgCl_2 \cdot xROH$  with other alcohols to explore the polymerization aspect.



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Physical chemistry of organic reactions in unusual media

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#### Objectives

- Quantification of the origin of physical forces responsible for rate enhancement of organic reactions in unusual solvents
- Experimental measurements of solvent parameters of ionic liquids
- Development of new methodologies to improve the performance of ionic liquids for organic transformations and extraction processes
- Experimental thermodynamic measurements for delineating ionic interactions in ionic liquids
- Modelling and synthesis of select ionic liquids for electrochemical and closed fuel cycle for fast breeder reactor technology

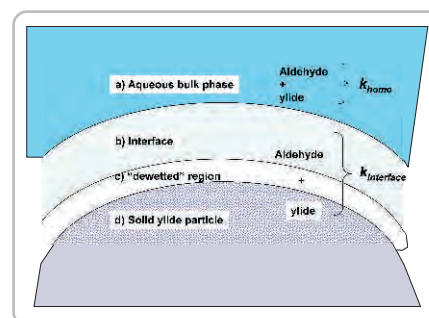
#### Work done and discussion

An unusual variation with the temperature of the salt effects in aqueous Wittig reactions observed was that hydrophobic acceleration of reactions comprising 'on water' reactants was fundamentally different from that for reactions with small non-polar solutes. The studies showed that the presence (or absence) of rate acceleration on addition of prohydrophobic salts any temperature were not the conclusive evidence for the predominance of (or lack of) 'hydrophobic effect', at least for the heterogeneous aqueous reactions. The salting effects on the kinetics of 'on water' reactions differed significantly from those observed for homogeneous aqueous reactions. The length-scale dependence of hydrophobicity must be considered before interpreting any salting phenomenon. This observation was relevant to numerous chemical processes which were known to take place at an 'hydrophobic' interface. The results have provided an indication of the complex manner in which the presence of

prohydrophobic and antihydrophobic salts is capable of influencing hydrophobicity at the interface.

Further, the role of viscosity or solvent friction in ionic liquids for an intramolecular Diels-Alder (IMDA) reaction of (*E*)-1-phenyl-4-[2-(3-methyl-2-butenyloxy) benzylidene]-5-pyrazolone was investigated. The results were analyzed on the basis of the current theoretical models and their failure to account for the observed trends is discussed in terms of 'effective' viscosity or microviscosity.

The rates of the reaction decreased with the increasing viscosity of the ionic liquids. As evident from the anionic effect, the solute-solvent specific interactions play a role in governing the kinetics of the reaction. The lower viscosities of the bistrifluoromethanesulfonimide [Ntf<sub>2</sub>]- based ionic liquids as compared to those based on tetrafluoroborate [BF<sub>4</sub>]- anion fail to result in a corresponding acceleration in the rates of the reaction. These contradictory results indicate that solvent microviscosity, rather than the bulk macroscopic viscosity, should be the criteria for selecting the ionic liquids as reaction media.



A schematic view of Interfacial Wittig reaction

#### Selected publications:

- ✦ *J. Solution Chemistry*, 2009, 38, 95
- ✦ *J. Organic Chemistry*, 2008, 73, 9075
- ✦ *Chemical Comm.*, 2008, 4445
- ✦ *Applied Catalysis A: General*, 2008, 335, 1

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Theoretical and computational methods

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**Objectives**

- Development of the methods within coupled cluster framework to calculate gauge independent magnetic properties
- Calculation of Shielding using extended coupled cluster method
- Development of code for the calculation of potential and dipole surface using decoupled approximation

**Work done and discussion**

It is known that magnetic properties are gauge-dependent. To get rid of gauge-dependence, use of London orbitals or use of large basis set is recommended. However, implementation of London orbital is complicated and needs development of a new code. We are working on this implementation for magnetizability. On similar lines we hope to implement the nuclear shielding constant. We have also developed a code based on the multi-reference based coupled cluster response approach. We have done the shielding calculations for various molecules and tested our code.

The study of the potential energy surface of a molecule in a bond breaking region using extended coupled cluster method is another interesting activity. To introduce the relaxation efficiently, partial inclusion of triples has been implemented. The decoupled approximation is developed for the energy and energy derivatives with non-iterative triples. With this we want to test for potential energy surface and dipole moment at different geometries.

**Selected publication:**

× *Inf. J. Quantum  
Chemistry*, 2009, 109,  
2191

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Electronic structure theory

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#### Implementation of Fock space coupled-cluster response approach to electric and magnetic properties

This year, further advances have been made in coding of Fock space coupled-cluster response theory, developed by our group to electric properties. The theory is based on a constrained variation approach in an effective Hamiltonian framework of multi-reference coupled-cluster theory. We have coded for first hyper-polarizability values for small to medium-sized molecules. This involved the first-order derivatives of the Lagrange multipliers. Pilot results are obtained for first hyper-polarizabilities of doublet radicals.

We have also obtained dia-magnetic susceptibilities of small open shell doublet radicals using the above version of multi-reference coupled-cluster theory.

#### Hydrogen storage materials

We are engaged in the study of hydrogen adsorption and dehydrogenation of metal hydrides and metal-organic framework. Dehydrogenation of metal hydrides and doped metal hydrides. This work is relevant in the context of hydrogen storage. Different phases of magnesium hydrides and ones doped with Si and Al have been studied. In particular, both thermodynamics and kinetics of Al and Si-substituted magnesium hydride have been studied using periodic density functional theory. One significant result obtained was that Si-doping improves hydrogen storage properties of  $\text{-MgH}_2$  both thermodynamically and kinetically.

#### Catalytic properties of beta-zeolites

We also studied the effect of cut-offs in structural parameters and interaction energies of water with Sn-beta zeolite with Ti-beta zeolite using periodic density functional Theory. We checked that the interaction energies are much more sensitive to the cut-offs compared to the structural parameters. Using this experience, we used cut-offs of about 1000 electron Volts to study the interaction of ketones and aldehydes with Sn-beta zeolite, which is known to be a very efficient oxidation catalyst.

#### Theoretical study of gold clusters

We have studied the gold clusters from Au6 to Au20 by the use of density functional theory. We have, in particular, identified the importance of relativistic effects on structure, reactivity and frequencies of gold clusters. Our study clearly pointed out the importance of relativistic effects in resolving the experimental vibrational frequencies. In general, we concluded that the relativistic effects are important in the structure and frequencies but the reactivity descriptors are much less sensitive to the relativistic effects.

#### Intermediate Hamiltonian Hilbert space coupled cluster method

We have coded Intermediate Hamiltonian Hilbert space coupled-cluster theory for study of potential energy surfaces. This is based on multi-root multi-reference based model space approach. Standard Hilbert space multi-root theories suffer from intruder state problem due to a democratic description of all roots. A more robust approach is to partition the model space into a primary and secondary space incorporating intermediate Hamiltonian, making the primary space intruder-free. Pilot applications of the approach have been carried out.

#### Effect of solvent on reactivity descriptors

The solvent effect on reactivity descriptors has been studied by using different protic and aprotic solvents.

#### Study of vibrational energy of molecules using coupled-cluster method

The vibrational energy states of molecule have been formulated using coupled cluster linear response theory in bosonic representation. The study uses Equation-of-motion based coupled-cluster theory using different truncation schemes. Convergence studies of truncation schemes of the bosonic cluster expansion have been studied for model potentials of water and formaldehyde molecules.

#### Selected publications:

- ✦ *J. Chem. Phys.*, 2008, 129, 134111; 2009, 131, 24102
- ✦ *ChemPhysChem*, 2008, 9, 928
- ✦ *J. Phys. Chem. B*, 2008, 112, 2573
- ✦ *J. Phys. Chem. C*, 2009, 113, 7101



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Development of insect tolerance in chickpea

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*Helicoverpa armigera* is a highly devastating and polyphagous insect pest of around 200 crop plants. The pest is responsible for enormous yield losses and also serves as a vector for transmission of diseases to crop plants. Conventional control methods of *H. armigera* rely on the use of chemical pesticides, which cause environmental pollution and being toxins, also lead to resistant pest resurgence. Our lab focuses on the use of plant derived proteinaceous molecules as inhibitors of the digestive enzyme for retarding the growth and development of *H.armigera*, which has potential for engineering plants for insect tolerance.

**Chickpea transformation**

Grain legumes have been considered to be recalcitrant for genetic transformation, since plant regeneration, which is a prerequisite for transgenic plant development is a major limiting factor. Like other leguminous crops, meristematic cells of apical meristem and cotyledonary node of embryonal axes of chickpea have been used for genetic transformation by earlier workers. However, the frequency of transformation has not been sufficient enough for effective biotechnological applications. Most of the earlier reports on chickpea transformation have used *Agrobacterium*-mediated method of gene transfer. However, low

success rates for recovery of plants make these protocols inefficient for genetic transformation. The recent method described in literature involves the use of the axillary meristem explant produced by removing the axillary bud and reported to give 70 % transformation efficiency in chickpea variety C-235. The efficiency and applicability of chickpea transformation protocols varies with different chickpea varieties.

Digvijay is a newly released variety of chickpea by Mahtma Phule Krishi Vidyapeeth (Agricultural University), Rahuri, which gives large-size grain, higher yields and wilt resistance in the semi-arid regions of Maharashtra. Therefore, we decided to establish a genetic transformation protocol for this variety so as to strengthen its insect resistance, and retaining its favourable agronomic traits.

We attempted several methods for checking transformation efficiency and regeneration in chickpea variety Digvijay. In all the methods *Agrobacterium*-mediated transformation of chickpea with glucouridinase gene under a 35S promoter (pRESC-GUS in GV3101 strain) was attempted. The modified methods (pre-callus transformation method, PCTM) showed good transformation efficiency as detected by GUS activity staining in Digvijay (Figure 1).

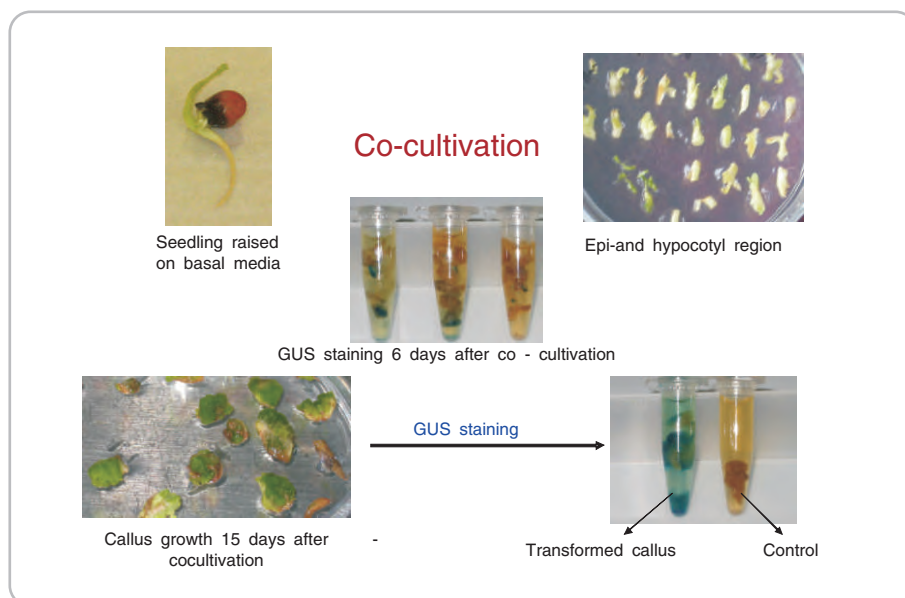


Figure 1: Chickpea transformation using pre-callus method

**Selected publications:**

- ✦ *Proteomics*, 2009, 9, 171
- ✦ *J. Insect Physiology*, 2009, 55, 663
- ✦ *Gene*, 2009, 442, 88; 431, 80

Regeneration of the transformed tissue to a plantlet is the next crucial step which also depends on the explants and the hormonal composition of the regeneration and selection media used. The above three methods that showed good transformation efficiency were further studied for regeneration. After reduction of sugar

content and increase in the agar in the media, PCTM method could regenerate only few plantlets. We are optimizing these methods using GUS staining with selected variety.

We have used reported protocol for chickpea



transformation with earlier identified winged trypsin/chymotrypsin inhibitor gene (PtWCI-5) under CaMV-35S promoter in the AGL-0/pBINAR/PtWCI-5 construct for transformation. PCR positive transformed chickpea plants were

identified with less than 3 % efficiency using WCI-5 primers. At present we are analyzing these plants for gene expression in different plant parts (Figure 2).

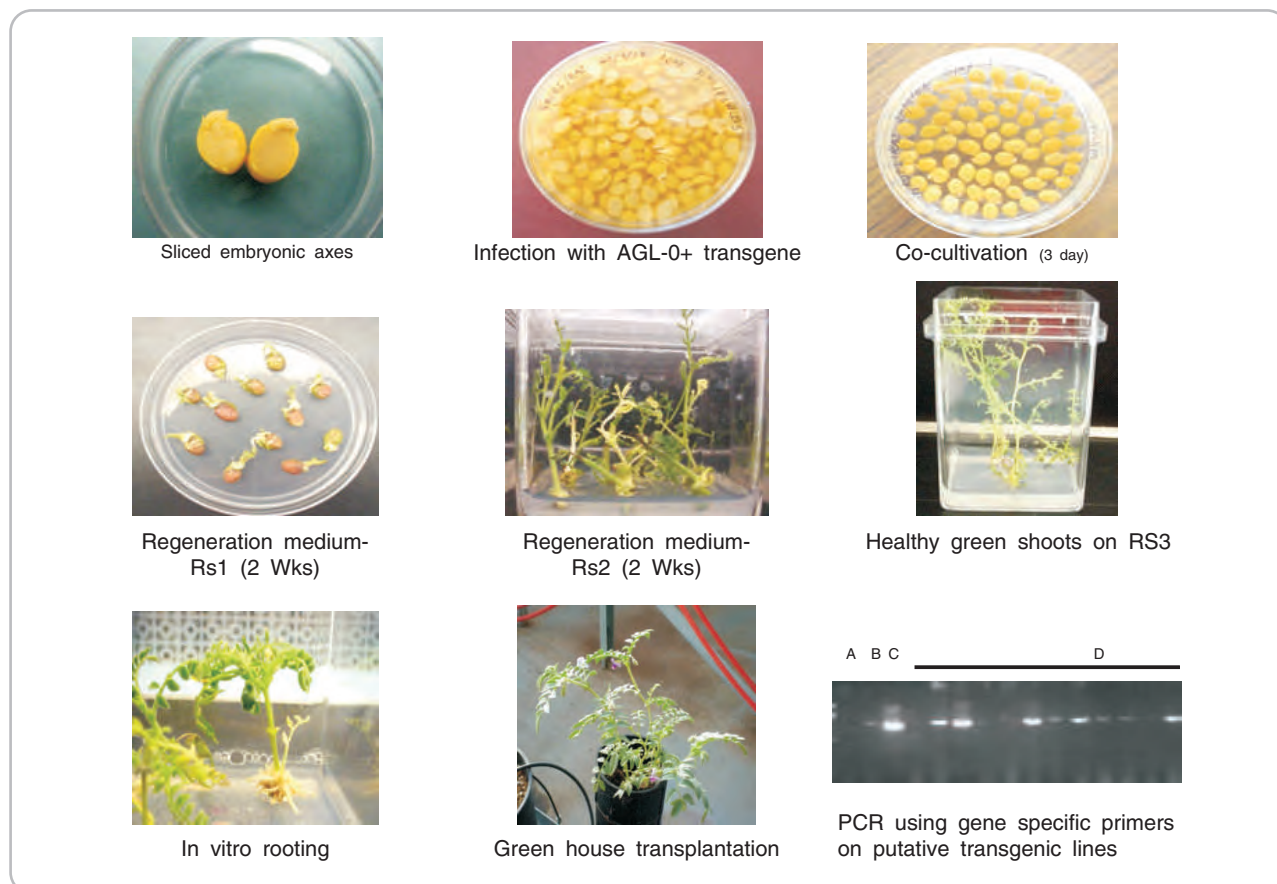


Figure 2: Chickpea transformation scheme

We have also attempted a simple method for chickpea transformation which has been successfully used previously for peanuts, *Arachis hypogaea* (Rohini and Rao 2000). The described method recommends co-cultivation of overnight imbibed, decoated and sliced seeds with *Agrobacterium tumefaciens*. After co-cultivation seedlings are transferred to vermiculite and allowed to develop radicle and plumule. We modified this transformation method for chickpea variety Digvijay by introducing pin pricks (5 to 20) in the radicle and plumule region of the embryo of 3 hour water imbibed and decoated seeds followed by co-cultivation with *A. tumefaciens* (GV3101; pRESC-GUS). Three hour imbibition of seeds in water, 12-15 number of pricks in the plumule region and 2 hours of co-cultivation could give the highest transformation efficiency as indicated by GUS staining. Without selection pressure of the selectable antibiotic GUS staining was localized in the lower region of plants and we are still optimizing the protocol to achieve transformation at the growing tip of the plumule of the embryo. As the seedlings are grown in vermiculite after co-cultivation we are optimizing the method to introduce selection pressure by painting hygromycin on the plumule. If the selection works well the growth of the transformed region of the plumule will be promoted to obtain transformed chickpea seedlings.

#### Identification of novel targets for *H. armigera* control

Apart from proteinase, amylases are another important class of major digestive enzymes in *H. armigera* which are required to assimilate nutrients and energy from consumed food. Amylase activities were detected in all the larval instars, pupae, moths and eggs in *H. armigera*. Early instars had lower amylase levels which steadily increased up to the sixth larval instar. Qualitative and quantitative differences in midgut amylases of *H. armigera* upon feeding on natural and artificial diets were evident. Correlation of amylase and proteinase activities of *H. armigera* with the protein and carbohydrate content of various diets suggested that *H. armigera* regulates the levels of these digestive enzymes in response to macromolecular composition of the diet. We also demonstrated that sorghum amylase inhibitor have strong activity against *H. armigera* midgut amylase. Work is in progress to clone and characterize these amylase inhibitor gene(s) from sorghum and test the effectiveness on *H. armigera*.



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Molecular genetic approaches for gene identification

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**Selected publications:**

- ✦ *J. Cereal Science*, 2008, 47, 587
- ✦ *Food Chem.*, 2009, 14, 363
- ✦ *Bioinformation*, 2008, 2, 461

**Molecular marker technology approach in wheat quality and rust resistance breeding**

The present programme aims at marker assisted breeding for quality enhancement and rust resistance in bread wheat. The quality traits under study include bread making quality, kernel hardness, and grain size and shape. For sustainability of wheat production in Central and Peninsular zone, which is rain Fed with predominance of leaf and stem rust, it is essential to focus research efforts on enhancing tolerance of the genotypes towards water stress conditions as well as leaf and stem rust.

*QTL identification for kernel size and shape using rye selection III x Chinese Spring:* Kernel size and morphology influence the market value and milling yield of wheat (*Triticum aestivum L.*). The objective of this study was to identify quantitative trait loci (QTLs) controlling kernel traits in hexaploid wheat. Thousand kernel weight (TKW), kernel length (KL) and kernel width (KW) were recorded for 185 recombinant inbred lines (RILs) from the cross Rye Selection 111 X Chinese Spring grown in two diverse agro-climatic regions in India for multiple years. Composite Interval Mapping (CIM) was employed for QTL detection using a linkage map with 169 simple sequence repeat (SSR) markers. Ten TKW QTLs were identified on the wheat chromosomes 1A, 1D, 2B, 2D, 4B, 5B, and 6B whereas six KL QTLs were detected on 1A, 2B, 2D, 5A, 5B and 5D. The chromosomes 1D, 2B, 2D, 4B, 5B and 5D had nine QTLs for KW. Chromosomal regions with QTLs detected consistently for multiple year-location combinations were identified for TKW, KL and KW.

*Identification of molecular markers closely linked to stem rust resistance genes:* The incorporation of multiple rust resistance genes in commercial cultivars is of global importance and is vital to provide durable resistance against the emergence of new rust pathotypes, which can acquire virulence for previously effective resistance genes. The objective of this research is to develop closely linked molecular markers that will assist wheat breeders in pyramiding race-specific and durable stem rust resistance genes. A bulked segregant analysis approach was used to identify simple sequence repeat (SSR) markers linked to stem rust resistance genes *Sr36* and *Sr9e* in the population Yarralinka x Schomburgk, which consists of 150 F<sub>2</sub>

recombinant inbred lines. *Sr36*, located on the short arm of chromosome 2B, was flanked by the SSR markers *barc45* and *gwm4167*, 10.1 and 2.5 cM, respectively. While, *Sr9e*, located on the long arm of chromosome 2B, was co-located with *wmc627* and flanked either side by *wmc175* and *wmc332*, 4.9 and 14.4 cM, respectively. In a second population, Diamondbird x Janz, consisting of 189 doubled-haploid lines, a QTL mapping approach is being employed to identify and validate molecular markers closely linked to major and minor stem rust resistance genes. The population was screened for response to stem rust pathotypes in multiple environment trials conducted in Australia, India and Kenya. Preliminary analysis of these trials together with a genetic linkage map constructed using 401 Diversity Array Technology (DArT) and SSR markers has revealed several chromosome regions of interest associated with stem rust resistance. Additional SSR markers continue to be mapped in this population to increase the overall genome coverage and to target the specific chromosomes of interest.

**Mango flavour biogenesis**

The study deals with the biochemical changes that occur during the development and ripening of the Alphonso mango. Among the sampled Alphonso fruit tissues, the highest concentration of volatiles was detected in 5DAP (15665 µg/g) and the lowest in 2DAH (62 µg/g); ripe fruits (15DAH) (966 µg/g) had more than ten folds higher content of volatile 138 odourants than the raw fruits (90DAP) (94 µg/g). Monoterpene hydrocarbons quantitatively dominated the volatile blend of all Alphonso tissues; except that in 90DAP (79%), 2DAH (53%) and 20DAH (81%) fruits, in all other tissues, these compounds comprised more than 90% of the aroma. This analysis revealed that the monoterpenes remain quantitatively dominant components throughout the fruit life. Based on the volatile profiles, fruit setting and early development were predicted to be vibrant whereas the stages near maturity were thought to be calm. Ripeness was found to be attained on the fifteenth day after harvesting where the levels of most of the flavourants were elevated. It was characterized by the strong presence of lactones, fureneol and mesifuran in addition to the terpenes. Floral blend was found to be dominated by the C6 GLV and monoterpene alcohols suggesting the spatially differential role of aroma volatiles. Overall, the results suggested that





the flavour of the Alphonso is a combination of freshening sap scent and the ripening induced fruity odor.

### Fatty acid pathway analysis in linseed

Flax/linseed (*Linum usitatissimum L.*) is an important oil seed crop having high nutritional as well as industrial value. We have planned to understand and characterize the pathway of Omega 3 fatty acid synthesis in flax. Polyunsaturated fatty acids are derived from saturated fatty acids by sequential action of fatty acid desaturases. Stearic acid is converted into oleic acid, oleic acid into linoleic acid and linoleic acid into Alpha linolenic acid by  $\Delta 9$ ,  $\Delta 12$  and  $\Delta 15$  desaturases, respectively. Hence, expression analysis of the desaturase genes ( $\Delta 9$ ,  $\Delta 12$  and  $\Delta 15$ ) during seed development in variable ALA containing linseed varieties has been initiated. Levels of various fatty acids, namely, Palmitic acid, Stearic acid, Oleic acid etc. have been analyzed in these varieties (Fig. 1). The gene expression profiles of these varieties will be compared with their fatty acid profiles for the same tissue, to reveal variety specific as well as temporal expression pattern of these genes during seed development. Additionally, to study the desaturase genes at genomic level in representative linseed cultivars.  $\Delta 15$  and  $\Delta 12$  gene amplicons have been cloned into *E. coli* by using pGEM-T Easy vector system and positive clones have been sequenced to get full-length genomic gene. This study will help in revealing the molecular features of this gene.

### DNA barcoding of Dalbergia species

DNA barcoding is emerging as an important tool for both identifying existing species and discovering new species. It is well established in animals, but there is no universally accepted barcode for plants yet. For one of the mega-diverse countries such as India, it is critically important that we establish our own national open access repository for barcode data. In case of *Dalbergia*, there is confusion about species identification and many species have been identified by more than one name. The DNA barcoding technology can be proposed to understand and analyze such discrepancies in plants. Six *Dalbergia* species were collected from Pune and other locations. Standardization of DNA extraction from fresh leaf tissue as well as herbaria samples has been performed. A total of 37 primers from chloroplast and nuclear genomes have been attempted, of which eight primers could give good PCR profiles and DNA sequences. Sequencing of some of the above genes has been

completed and based on preliminary analysis, the resolution of species identification using rpoC and matK genes individually was 66.66%. The data are being analyzed to determine suitability of these sequences, either singly, or in combination of 2-3 gene sequences to establish DNA barcodes.

### Regulation of FecB gene expression in Garole sheep breed

The mean ovulation rate (5.7) and litter size (2.6) of the Australian Booroola sheep are quite high as compared to the Indian Garole sheep breed, though the same mutation is present in both these breeds. These differences may be due to environmental variation (for example, plane of nutrition) or a breed effect or the presence of other genetic factors such as modifier genes or novel mutations within the BMPR-IB gene that individually or together dampen the expression of the FecB trait in the Garole sheep. Studies of genetic variation at whole genome scale as well as at FecB gene locus within Garole breed with varying expression of the FecB trait, under similar environmental conditions might help to through light on this issue. Presently, we have concentrated our efforts at and around the Fec B gene. Sixteen samples of pure Garole sheep having low and high EBVs are being used for this analysis.

To study the mutation within BMPR-IB region, eight primer pairs spanning the whole cDNA sequence of the gene using Primer Premier 3 software were designed and synthesized. and will enable to detect mutation other than the Fec B mutation which may be responsible for variation in expression. These 8 primers were subjected to PCR. Primer pairs 1,2,3 and 4 showed no amplification. This could probably be due to introns of unamplifiable size, present in between the primer pairs. The BMPR-IB cDNA sequence of sheep was compared with the BMPR-IB cDNA sequence of humans to find the possible introns present in between the primer pairs (1- 4). Such large size introns have been reported in human Fec B gene towards 5' end. The primer pairs 5-8 form the 3' UTR region of the BMPR-IB gene and they showed appropriate amplifications. The sizes of the amplified products were 450bp, 550bp, 450bp and 400bp, respectively. No size variation was observed between low EBV and high EBV animals. Therefore, direct PCR product sequencing was carried out to check the sequence variation using the primer pairs 5,6,7 and 8. The analysis of the sequence data is in progress. Primer pair for 5' UTR region has been designed which will also be used for this analysis.

Alternatively, dampening of FecB expression may be due to the variation in the flanking region of the FecB locus. Hence, four microsatellite markers (JL 26, JL 2, JL 36 and JP27) closely linked to Fec B locus were synthesized and used to check variation in this region using 16 Garole samples with high and low EBVs. However, except JP 27, all other three primers exhibited monomorphic pattern. Although JP 27 marker showed polymorphic pattern, no specific alleles related to high and low EBVs animals were observed. We need to further verify the results using more markers around 12-15 cM away from the Fec B locus.

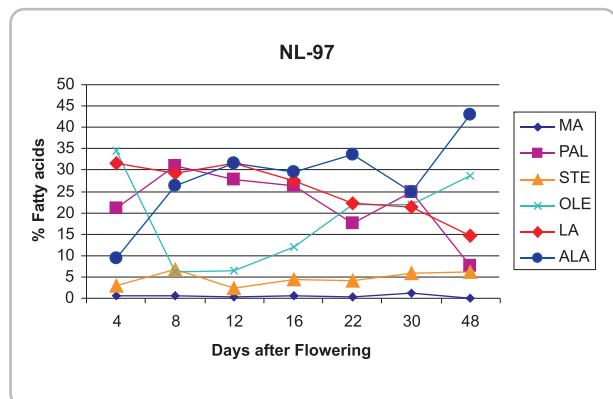


Fig. 1: The levels of various fatty acids in linseed during 4 to 48 days after flowering



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Biotechnological approaches to saffron production

The objectives of this study are: (i) to induce flowering/ proliferate floral primordia *in vitro*, (ii) to induce microcorms *in vitro*, and (iii) to standardize parameters for greenhouse cultivation of saffron in Pune/ elsewhere in Maharashtra (Mahabaleshwar/ Panchgani).

**In vitro induction of microcorms**

Effects of (i) sucrose concentration, (ii) corm size (medium, small), and (iii) incubation temperature on *in vitro* induction of microcorms in saffron were studied. There was microcorm production at all concentrations (2%, 4%, 6% and 8%) of sucrose when incubated at lower temperature ( $10 \pm 2^\circ\text{C}$ ). Incubation temperature was observed to have significant effect on microcorm production. A lower incubation temperature may be simulating the environment in its natural habitat. The size of the microcorms produced was dependent on sucrose concentration and the size of corm used as explant.

**Table1. Effect of sucrose concentration on the number and weight of microcorms produced Greenhouse cultivation**

Sr. No.	Sucrose concentration	Average No. of microcorms	Average weight of microcorms
1	2%	5.000 ± 1.968	0.673±0.31
2	4%	4.125 ± 2.027	0.807±0.28
3	6%	5.375 ± 1.586	0.902±0.20
4	8%	3.125 ± 1.452	1.040±0.00

Effects of (i) season of corms lifting, (ii) size of corms, and (iii) type of planting medium on greenhouse cultivation of saffron in Pune were studied.

Only bigger corms (2-3 cm dia., 10-15 gm weight) were used for greenhouse experiments. On two occasions (July and September), corms were obtained from Pampore, Kashmir. Corms were planted in different planting media. Watering was done once a week. In the last week of October and first week of November, there was flowering in plants raised from corms lifted in September, and grown in 1:1 and 1:2, sand: soil mixture. In the remaining combinations there was no flowering. The flower buds emerged in the morning and developed very rapidly and bloomed. Most of the flowers showed 3 stigmas as in natural habitats. However, some flowers showed only 2 stigmas.

The average fresh weight of saffron (stigmas) harvested from plants grown in the NCL greenhouse was  $21.66 \pm 3.78$  mg, and the dry weight was  $4.0 \pm 1.00$  mg. The average dry weight of saffron obtained from the field in Pampore from where the corms were procured was  $4.9 \pm 1.52$  mg.



Figure 1: Microcorms produced in: 2%, 4%, 6%, and 8% sucrose containing media at  $10 \pm 2^\circ\text{C}$

When saffron harvested from the NCL greenhouse grown plants was compared with that obtained from the field in Pampore, Kashmir, from where the corms were obtained (by HPLC) following points were observed:

- The peaks observed in sample procured from Kashmir were observed also in the NCL sample, indicating the presence of stigma metabolites (crocin, picrocrocin, and safranal) in the NCL sample.
- Some other impurities were observed only in the NCL sample. (Identification is in progress).
- Quantity of metabolites appears to be less in NCL sample. (This work is in progress).



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Chickpea improvement through biotechnological approaches

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**Background / objectives**

*Chickpea (Cicer arietinum L.)* is a cool season grain legume with high nutritive value, cultivated in the arid and semi-arid areas around the world. Fusarium wilt is a widespread and serious chickpea disease caused by the soil borne fungus *Fusarium oxysporum* f.sp. *ciceri* (Foc). Considering these, we undertook mapping of QTLs affecting seven agronomic and yield traits, as well as, mapped three *Fusarium* wilt resistance genes in chickpea. Additionally, we are analyzing the transcriptome of chickpea-*Fusarium* interaction, to understand the differentially regulated genes, as well as, developing race specific markers for the Foc races.

**Work done and discussion**  
**Mapping of agronomic and yield related traits**

A total of 106 significant quantitative trait loci (QTLs) associated with seven agronomic and yield traits in two RILs populations of chickpea (JG and VI) were identified. Single locus QTL analysis was performed using composite interval mapping (CIM) for individual traits, and multi-trait composite interval mapping (MCIM) for correlated yield traits to detect the pleiotropic QTLs. Two-locus analysis was conducted to detect the main effect QTLs (M-QTLs), epistatic QTLs (E-QTLs) and QTL x environment interactions (QE and QQE) (Fig 1). Through CIM analysis, 41 and 65 significant QTLs were identified for the seven traits in JV and VI populations, respectively. One QTL each for plant height and days to maturity were common in both the populations. Six pleiotropic QTLs that were also consistent over the environments were identified. These QTLs could be utilized effectively for marker-assisted selection (MAS). MAS for stable QTLs will permit significant improvement in phenotypic traits across different environments.

**Mapping of Fusarium wilt resistance genes**

An F<sub>9</sub> RIL population of chickpea (JG 62 x Vijay) was evaluated for resistance to three Foc races (1, 2 and 3) in pot culture experiments. Flanking and tightly linked DNA markers were identified on LG2 of the chickpea map for resistance genes corresponding to the three races. The SSR markers H3A12 and TA110 flanked the *Foc1* locus at 3.9 cM and 2.1 cM, respectively, while the *Foc2* locus was mapped 0.2 cM from TA96 and 2.7 cM from H3A12, whereas the H1B06y and TA194 markers flanked the *Foc3* locus at 0.2 cM and 0.7 cM, respectively. These markers were also validated using 16 diverse chickpea

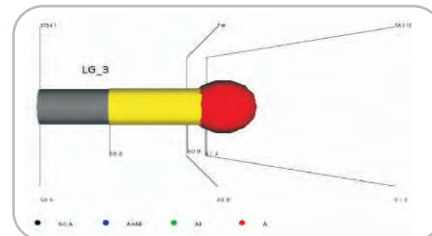


Fig 1: (a) Epistatic Plant height QTL with individual effect

genotypes. Thirteen of these genotypes were resistant to all the three Foc races and also carried the corresponding resistance genes.

**Molecular analysis of chickpea-Fusarium interactions using SAGE**

Serial Analysis of Gene Expression (SAGE) technique was used to perform a large-scale analysis of the chickpea-*Fusarium* interaction and to identify the wilt resistance genes. Two chickpea genotypes (DigVijay, resistant to *Fusarium* wilt; and JG62, susceptible) were selected, and artificially inoculated with three races of Foc (Foc1, Foc2 and Foc4) separately in pot culture experiments conducted in greenhouse conditions. Root and shoot tissues were collected at eleven time points and RNA was extracted. The RNA samples were normalized using Actin gene primers and were pooled in a single sample for each treatment / genotype. Further work to make the SAGE libraries is in progress.

**(d) Identification of Indian pathogenic races of *Fusarium oxysporum* f.sp. *ciceri***

A complex interaction between plant and its fungal pathogen is an outcome of expression of both, plant defense genes as well as fungal pathogenesis related genes. Multiple events are involved in bringing about successful plant defence during pathogen attack. Further, these defence mechanisms are governed by diverse genes, which either singly or synergistically bring about the resistance in plants. In this study, semiquantitative RT-PCR analysis of defence related genes was performed using gene targeted primers in wilt-resistant (Digvijay) and wilt-susceptible (JG62) chickpea varieties. The differential response of these varieties upon exposure to Foc races 1, 2 and 4 at 2, 6, 9, 13 and 16 days after infection was explored. In addition, expression analysis of fungal pathogenesis related genes and their race specific response was determined throughout the course of chickpea-Foc interaction. Some of the genes, which were previously not reported to be involved in chickpea defence against *Fusarium* wilt, have been unveiled in this study.

**Selected publications:**

- ✦ *Molecular Breeding*, 2009, 24, 177
- ✦ *Mycologia*, 2009, 101, 484



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Engineering disease resistance in economically important crops

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The main objective of the project is the development of novel methodology to confer disease resistance in ginger and onion. Ginger and onion are the major crops widely consumed world over owing to their flavor and medicinal properties. However, major crop losses have been reported in these crops due to various bacterial and fungal diseases. Since ginger is a vegetatively propagated crop the spread of disease is multifold. Moreover, due to poor flowering and seed set it is difficult to confer disease resistance through conventional breeding. In onion limitations of resistance genes within usable gene pools is a major concern for conventional breeding.

Therefore to address these problems designing novel antimicrobial peptides (AMPs) and incorporating them in plants is an exceptional approach to ladder of success. These probiotic enhanced crops would lead to increased yield and reduce losses.

The AMPs are a class of natural antibodies found widely in nature in mammals, insects, amphibian, fungi, bacteria and plants. Among them cationic peptides are the most widespread. Besides these natural antimicrobial peptides, the synthetic peptides have been developed. These are unique candidate target peptides (probiotics), which are often half the size of natural counterparts (10-20 Amino Acids) and are active at low concentrations without toxicity to host tissues. In many cases, synthetic analogs of natural antimicrobial peptides offer even more target specificity, increased efficacy at lower concentration, and reduced degradation by plant proteases than their natural counterparts.

The AMPs act either by lysing the microbial cell or by interfering with the cell wall synthesis. Because the primary target of AMPs is cell membrane and not specific receptors or substrates, these peptides confer their activity against a broad spectrum of pathogenic microorganisms and there is less probability of resistance arising by variation of its metabolic pathways.

In this context studies were carried out on isolation and identification of disease causing organisms of Ginger and Onion using biochemical tests and 16srRNA gene analysis. Studies revealed that in ginger bacterial contaminants were *Pseudomonas* spp, *Bacillus* spp, *Staphylococcus* spp and *Xanthomonas* spp. Two fungal contaminants were *Aspergillus niger* and *Rhizopus stolonifer*. The most prevalent bacterial infection was found to be caused by *Pseudomonas* spp and *Xanthomonas* spp. *Rhizopus stolonifer* was the most common fungal contaminant. *Pseudomonas* spp and *Xanthomonas* spp were subjected to molecular analysis using 16S rRNA gene sequence. The bacterial DNA was successfully isolated and the rRNA gene amplified using universal primers. This PCR product was sequenced and similarity search using BLAST tool concluded it to be *Pseudomonas* A5AGN strain and *Xanthomonas* spp BJQ-H4 respectively.

In onion the bacterial contaminants were *Pseudomonas* spp, *Bacillus* spp, *Staphylococcus* spp and *E.coli*. Fungal contaminants were *Aspergillus niger* and *Rhizopus stolonifer*. The most prevalent bacterial infection was found to be caused by *Pseudomonas* spp and *staphylococcus* spp. *Aspergillus niger* was the most common fungal contaminant in Onion. Molecular analysis using 16S rRNA gene sequence identified the organism as *Pseudomonas* spp A5AGN strain and *Staphylococcus aureus* strain PRSR-4.

These organisms were subjected to sensitivity assay towards synthetic antimicrobial peptide D4E1 (17 amino acids peptide). The minimum inhibitory concentration of AMP D4E1 was found to be between 20 -25  $\mu$ M for *Aspergillus* sp, *Rhizopus stolonifer* and *Fusarium Solani* (standard strain). The Minimum inhibitory concentration of D4E1 for *Staphylococcus* sp, *Bacillus* sp, *Pseudomonas* sp, *E.coli* & standard *Pseudomonas syringae* (standard strain) was between 4-6  $\mu$ M concentrations. Thus peptide was found to be broad spectrum in activity.

Simultaneously studies conducted on development of regeneration protocol in ginger and onions have resulted in regeneration of shoots from callii in onion and shoot tip regeneration in ginger.

Further studies are being continued on screening large number of peptides for their potency to inhibit growth of target pathogens and will be used for conferring disease resistance through genetic transformation using gene constructs for the selected peptides.



Fig 1: Growth of *Aspergillus niger* at 11 $\mu$ M concentration of D4E1



Fig 2 : Partial Growth inhibition of *Aspergillus niger* at 19 $\mu$ M D4E1 concentration

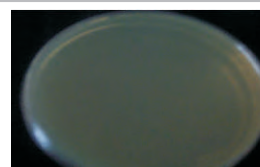


Fig 3: Total Growth inhibition of *Aspergillus niger* at 25 $\mu$ M concentration of D4E1



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Insect-plant interactions

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#### Background / objectives

Our research efforts are focused on studies on insect-plant interactions and multitrophic interactions. The overall objective is to search for, identify and understand how semiochemicals are able to evoke insect behaviours as well as to apply this knowledge for use in agriculture. We employ an interdisciplinary approach that integrates neuroanatomy, neuroethology, electrophysiology and behaviour within a comparative context. As insects show differential sensitivities depending on the chemical image of the host plant, we find that the large majority of species are specialists.

**Chemoreception:** The aim of this study is to identify and characterize sensilla involved in the feeding behavior of the larvae of *S.litura* and *H.armigera* specifically for phagostimulants (including sugars, amino acids and salts), deterrents, lectins and protease inhibitors. Knowledge of the mode of action of compounds affecting larval feeding behaviour could potentially lead to the design of more effective and specific control agents besides possibly providing a structural template for gustatory chemoreception in these two species.

#### Role of induced plant defences:

Undamaged plants release a blend of volatiles that are characteristic for a species based on the individual ratios of C<sub>6</sub> alcohols, aldehydes and their corresponding acetates. Upon feeding by insects, the blend of volatiles released are different, an evolutionary adaptation whereby they serve to attract parasitoids and predators.

#### Volatiles (particularly from human sweat) mediating host selection in mosquitoes:

We are studying the role of human skin emanations in the host seeking behaviour of the malaria vector, *Anopheles stephensi* and how these odours are perceived by the olfactory system. The major objective is to characterize behaviourally relevant chemosensory stimuli and elucidate how these stimuli are detected and integrated in the chemosensory system.

#### Work done and discussion

Electrophysiological characterization of the medial, and lateral sensilla styloconica reveal that they are sensitive to a wide group of chemical compounds including sugars and sugar alcohols, amino acids, salts, deterrents and plant saps. Sugars are universal feeding stimulants and sugar alcohols have been demonstrated to enhance palatability of foods. Of all the sugars tested, only sucrose and inositol evoked significant spike activity by sensilla on the galea and maxillary palpi of *H.armigera* and *S.litura*. Among the two galeal sensilla, sucrose sensitive cells were present on the lateral sensilla styloconica while inositol sensitive cells were present on the medial sensilla. In addition, the response of the inositol sensitive cell in the medial sensillum of *S.litura* to castor leaf sap suggests a 'labeled line' patterning of response

Both *H.armigera* and *S.litura* are able to perceive deterrent compounds including salicin, nicotine and caffeine. Interestingly, the same cell responded to two plant based proteins, namely, lectins and protease inhibitors. These proteins evoke responses characteristic for a deterrent; (a) single cell responses of equal amplitude; (b) inhibit the responses of two known stimulants – sucrose and inositol and (c) evoke additive responses when mixed with other deterrents. Also, the occurrence of two excitatory transduction pathways and diet induced plasticity were observed in the deterrent cell of *H.armigera*

#### Selected publication:

- ✦ *J. Biosciences*, 2007, 33, 339

Microbial technology



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Selected publications:

- ✦ *J. Non-Crystalline Solids*, 2008, 354, 3433
- ✦ *FEBS Letters*, 2008, 582, 3595
- ✦ *J. Nanoscience Nanotech.*, 2008, 8, 3909
- ✦ *J. Microbiology Biotech.*, 2009, 19, 1342

Biotechnology of endophytic fungi: nanomaterials, secondary metabolites and lectins

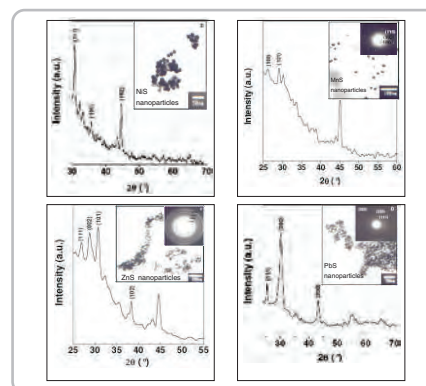
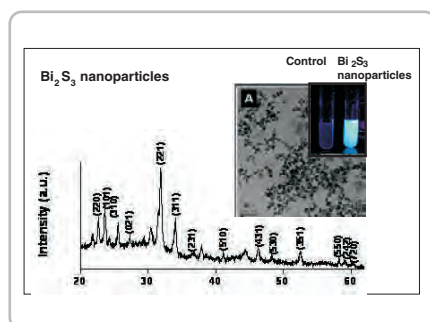
Our research focuses on

- Fungus, actinomycete and plant extract based nanoparticle synthesis and their complete characterization
- Plant based drugs extraction from endophytic fungi and their complete characterization
- Conjugation of nanoparticles to the drug for delivery applications

Nanomaterials

Extracellular biosynthesis of metal sulfide nanoparticles using the fungus *Fusarium oxysporum*

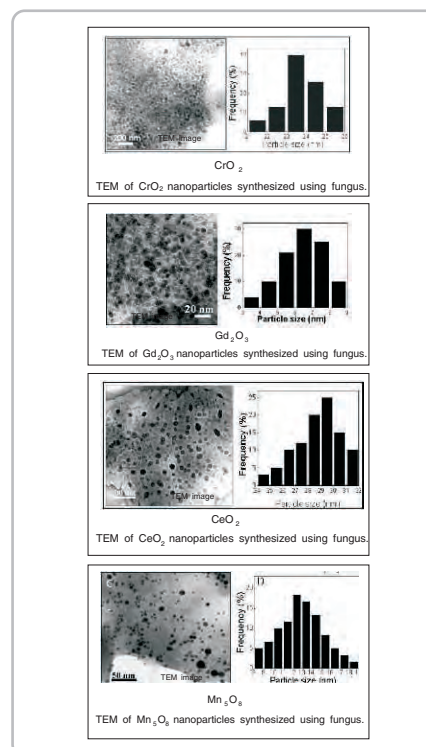
The development of reliable, eco-friendly processes for the synthesis of nanomaterials is an important aspect of nanotechnology. One approach that shows immense potential is based on the biosynthesis of nanoparticles using microorganisms such as bacteria. In this report, we demonstrate the extracellular biosynthesis of metal sulfide (PbS, ZnS, MnS and NiS) nanoparticles using fungus, *Fusarium oxysporum*. We observed that the exposure of aqueous solution of 1 mM metal sulfate to fungus *F. oxysporum* resulted in the formation of highly stable technologically important metal sulfide semiconductor nanoparticles. We have also synthesized highly stable Bi<sub>2</sub>S<sub>3</sub> nanoparticles extracellularly by challenging the fungus to an aqueous solution of bismuth nitrate and Na<sub>2</sub>SO<sub>3</sub>. *F. oxysporum* synthesizes lead sulfide and zinc sulfide nanoparticles of fractal type structure whereas manganese sulfide, nickel sulfide and Bi<sub>2</sub>S<sub>3</sub> nanoparticles are of variable polydispersed morphology. The variable morphology may be due to the dissimilar interaction of metal sulfide nanoparticles with capping proteins secreted by the fungus in solution. The nanoparticles solution is found to be extremely stable with little evidence of aggregation even after a month of storage. The long term stability of the nanoparticles is due to the proteins secreted by fungus in the nanoparticle solution which binds to the surface of the nanoparticle and thus prevents aggregation.



TEM/XRD/SAED of nanoparticles ( Bi<sub>2</sub>S<sub>3</sub>, NiS, MnS, ZnSand PbS ) synthesized using fungus

Fungus-mediated biosynthesis of oxide nanoparticles

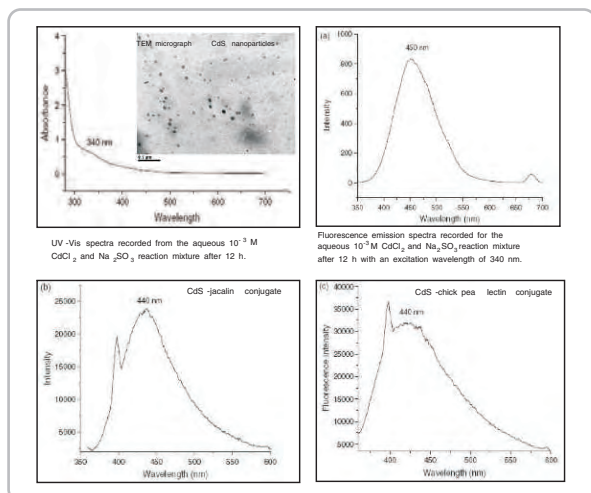
Chemical methods for synthesis of oxide nanomaterials are energy intensive and employ toxic chemicals. On the other hand, the synthesis of inorganic materials (oxides) by biological systems is characterized by processes that occur at close to ambient temperatures, pressures and neutral pH. We have synthesized highly stable CrO<sub>2</sub> nanoparticles extracellularly by challenging the fungus to an aqueous solution of K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>. The Gd<sub>2</sub>O<sub>3</sub>, CeO<sub>2</sub> and Mn<sub>2</sub>O<sub>3</sub> nanoparticles were also synthesized extracellularly by challenging the fungus to an aqueous solution of GdCl<sub>3</sub>, Cerium (III) nitrate hexahydrate and manganese(II) acetate tetrahydrate, respectively.





**CdS quantum dots: Enzyme mediated in vitro synthesis, characterization and conjugation with plant lectins**

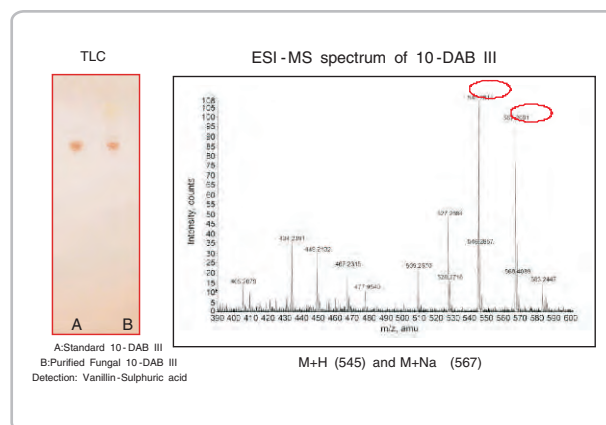
*In vitro* synthesis of CdS quantum dot nanoparticles using sulphite reductase and capping peptide in the presence of a co-factor  $\alpha$ -NADPH, their characterization and conjugation with plant lectins, Jacalin and Chick pea lectin were carried out. Incubation of sulphite reductase with aqueous  $CdCl_2$ ,  $Na_2SO_3$ , and capping peptide in the presence of  $\alpha$ -NADPH, which acts as a co-factor, resulted in the formation of CdS nanoparticles of dimensions 5-20 nm. These CdS nanoparticles were conjugated with plant lectins by EDAC mediated coupling. These observations are of significance, as it will help in the development of eco-friendly process for the formation of CdS nanoparticles and their application as fluorescent biolabels. Moreover the above studies will also help in designing a rational enzymatic strategy for the synthesis of nanomaterials of different chemical composition, shapes and sizes as well as their separation.



**Secondary metabolites from endophytic fungus: Production, purification and characterization of 10-deacetyl baccatin III**

We have isolated endophytic fungi from Indian Yew tree, *Taxus baccata* and then screened for 10-deacetyl baccatin III (10-DAB III) production. Out of the forty fungal cultures screened, one fungus *Gliocladium* sp. was found to produce 10-DAB III. 10-DAB III was purified by TLC and characterized by ESI-MS.

One liter of *Gliocladium* sp. culture yielded 65  $\mu$ g of 10-DAB III.



**Lectin from endophytic fungus: Steady state and time resolved fluorescence quenching and chemical modification studies**

The solute quenching studies of a lectin from endophytic fungus *Fusarium solani* were carried out using different quenchers such as acrylamide, succinimide, potassium iodide and cesium chloride. The lectin showed emission maximum at 348 nm indicating relative exposure of tryptophan. The quenchable fraction of the fluorophore was 100% with acrylamide, whereas it was only 50% with succinimide. The ionic quenchers iodide and cesium showed opposite effects at different pH. In the case of cesium, raising the pH resulted in increased quenching and accessibility of tryptophan residue, while the iodide showed just opposite effect. These studies showed that the single tryptophan residue of the lectin (per monomer) is relatively exposed and might be in the vicinity of positively charged amino acid residues. Various amino acids of the *F. solani* lectin were modified using different reagents to obtain information about the hemagglutinating site. The chemical modification studies suggested tyrosine residues can be modified using N-acetylimidazole, which results in complete loss of hemagglutination activity of the lectin. Kinetics of chemical modification suggested involvement of only 2 tyrosine residues. Modification of arginine, cysteine, histidine, lysine, aspartate, glutamate and tryptophan did not result in loss of hemagglutinating activity of the lectin.

Microbial technology



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Fungal biotechnology

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**Selected publications:**

- ✦ *J. Mycol. Plant Pathol.*,  
2009, 39, 118
- ✦ *Bioorg. Med. Chem.*, 2009  
17, 2433
- ✦ *Biocontrol Sci. Technol.*,  
2009, 18, 809, 337
- ✦ *Tetrahedron*, 2008, 64,  
10214

**Transferring mycoinsecticide technology to the private sector**

Under the Indo-Swiss Collaboration in Biotechnology (ISCB) studies were undertaken to develop a mycoinsecticide for the control of *Helicoverpa armigera* on pulses, in April, 2000. The first phase of proof of concept was concluded in 2004. The project was supported in the second phase to carry out studies for bioefficacy, demonstration and for trans-sectoral issues (2004-08). The project is being continued with the participation of industry to compete the studies for transferring technology to the private sector.

The project started with the isolation of different entomopathogenic fungi, mainly belonging to genera; *Metarhizium*, *Beauveria* and *Nomuraea* which were tested for their effectiveness against *H. armigera* under laboratory conditions. With a view to the introduction of the mycoinsecticide in to the market, in the second project phase large scale field trials (on hector scale), in pulses with *M. anisopliae* formulations were carried out. Significant variation in appressorium formation and cuticle-degrading enzyme production such as chitinase, chitin deacetylase, chitosanase and protease during subsequent sub-culturing and passage through *H. armigera* was observed. The virulence of entomopathogen in the fungus-host interaction is important in its success as a biocontrol agent. In the II phase, though microsatellite markers from non-coding region were developed, they were not useful to discriminate virulent and avirulent strains. Therefore the work on the markers from the coding regions with special reference to the virulence of *M. anisopliae* M34412 was initiated. Nevertheless, ITS and RAPD markers were used for the identification of *M. anisopliae* M34412 *Metarhizium* isolates (63) for cuticle degrading enzymes and their correlation with the virulence against *H. armigera* were studied. These studies will be useful to develop a knowledge-based project for the commercial venture. Experiments were carried out to investigate the potential loss of virulence of biocontrol strain *M. anisopliae* M34412 after subsequent *in vitro* subculturing on artificial media this phenomenon is well known for other fungal biocontrol organisms and demands a strategy for the provision of back-up strains. Three strains (M34311, M81123, M91629) with properties close to those of strain M34412 were identified as back up strains.

**Polyamines, dimorphism in *Y. lipolytica* and the petroleum oil degradation in marine environment**  
*Y. lipolytica* is a nonpathogenic

ascomycetous fungus studied to understand its dimorphic behaviour. The polyamines putrescine, spermidine and spermine are ubiquitous aliphatic polycations required for cell growth and differentiation. Ornithine decarboxylase (ODC) is the key regulatory enzyme involved in the biosynthesis of polyamines. It has been reported that yeast cells of *Y. lipolytica* degraded aliphatic fraction of crude oil when supported with nitrogen and phosphorus at a temperature optimum of 30°C under aerobic conditions. The ability of the strain to degrade oil, both in sea water and fresh water makes, it a, suitable candidate for bioaugmentation trials both in marine and fresh water environments.

**Dimorphism in *B. poitrasii*: A model phenomenon**

Flocculation of dimorphic yeast *B. poitrasii* is altered by modulation of NAD-glutamate dehydrogenase. A strategy to control flocculation is investigated using dimorphic yeast, *B. poitrasii* as a model. Parent form of this yeast (Y) exhibited faster flocculation (11.1 min) than the monomorphic yeast mutant Y-5 (12.6 min). Atomic force microscopy revealed higher surface roughness of Y (439.34 rms) than Y-5 (52 rms). Also, the former had a zeta potential of  $-65.97 \pm 3.45$  as against  $-50.21 \pm 2.49$  for the latter. Flocculation of both Y and Y-5 could be altered by supplementing either substrates or inhibitor of NAD-glutamate dehydrogenase (NAD-GDH) in the growth media. The rate of flocculation was promoted by  $\alpha$ -ketoglutarate or isophthalic acid and decelerated by glutamate with a statistically significant inverse correlation to corresponding NAD-GDH levels. These interesting findings open up new possibilities of using NAD-GDH modulating agents to control flocculation in fermentations for easier downstream processing.

**A model for the development of novel antifungal agents**

A saprophytic zygomycete *B. poitrasii* has been identified to understand the role of NADP- dependent glutamate dehydrogenases in the morphological (unicellular yeast to hypha) transition, its taxonomical relatedness with human or plant pathogens, if any, and to design antifungal strategies. Chitin synthase inhibition study of different organic compounds was carried out to develop antifungal strategy using morphological transitions as a model system.

**Natural yeast flora of different varieties of grapes used for wine making in India**

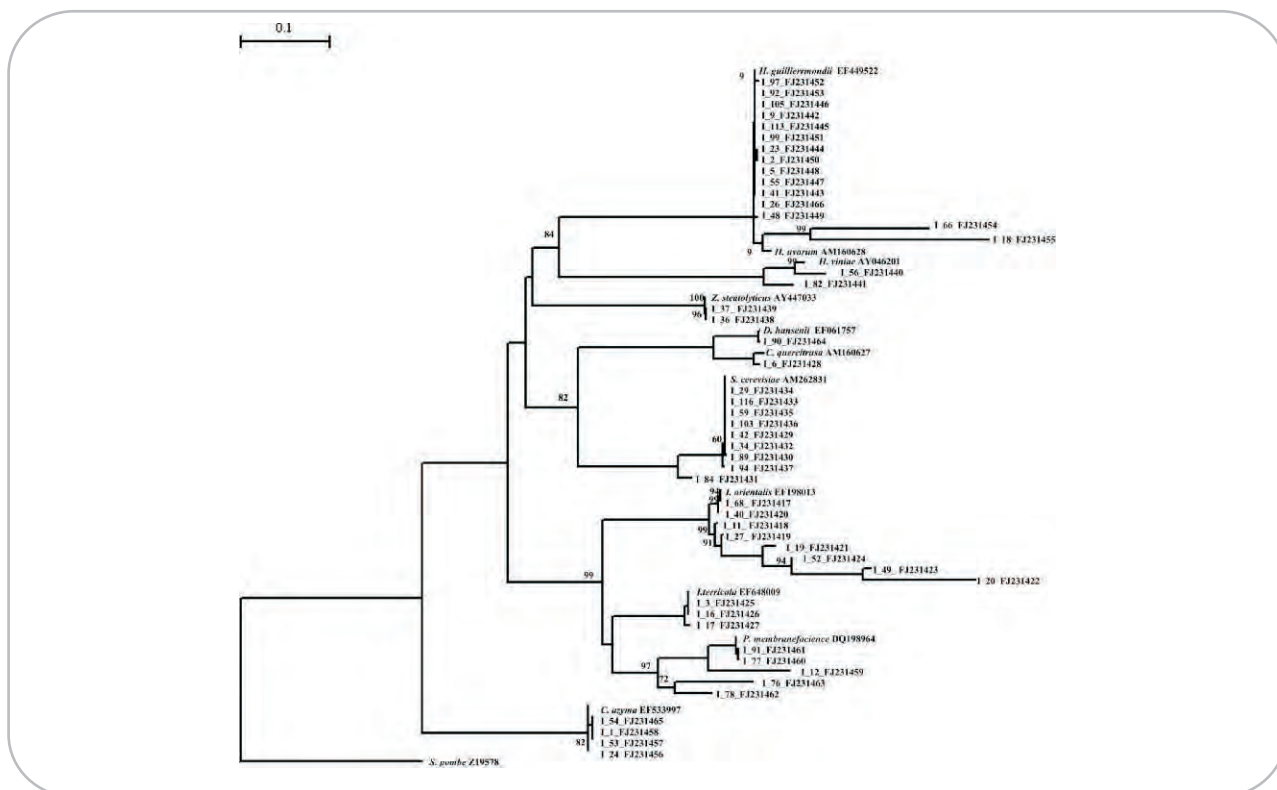
The natural *Saccharomyces* and non-





*Saccharomyces* yeast flora present on the grape berries significantly affect wine production. Six grape varieties, Bangalore blue, Zinfandel, Cabernet, Chenin Blanc, Sauvignon Blanc and Shiraz are being used in India for wine making. The yeast diversity was studied on the basis of morphological, colony, physiological characteristics and 5.8S-ITS sequencing of rDNA of the isolates. Eleven different species belonging to seven genera identified as: *Candida azyma*, *Candida quercitrusa*, *Debaryomyces hansenii*, *Hanseniaspora guilliermondii*, *Hanseniaspora viniae*, *Hanseniaspora uvarum*, *Issatchenkia orientalis*, *Issatchenkia terricola*, *Pichia membranifaciens*, *Saccharomyces cerevisiae* and

*Zygoascus steatolyticus*. *H. guilliermondii* were the predominant species while *S. cerevisiae* was observed occasionally in the six vine varieties. For the first time, *C. azyma* was isolated from Bangalore blue and Cabernet varieties grown in different localities. This association may be attributed to the change in cropping pattern from sugarcane to viticulture in the vine growing regions and the known association of *C. azyma* with sugarcane phylloplane. Further analysis of the indigenous strains and the qualitative and quantitative changes in the flora during fermentation will be useful to understand wine quality and to design preservation strategies to control wine spoilage.



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**Selected publications:**

- ✦ *I. J. Biological Macromol.*, 2008, 43, 373
- ✦ *Peptides*, 2009, 30, 2118
- ✦ *J. fluoresce*, 2009, 19, 967

**Microbial technology**

Hydrolytic enzymes and inhibitors



**Scale-up and techno economics of alkali stable cellulase from alkalothermophilic *Thermomonospora* sp**

Due to increasing environmental concerns and constraints being imposed on textile industry, application of cellulases to cotton fabrics is an eco-friendly process for improving their property. Denim washing with cellulases is a technique providing an environmentally friendly process to achieve a desirable appearance and soft handle to fabrics. In textile industry, there is a need for novel cellulases that are active at neutral and alkaline pH values having short reacting time, good denim finishing properties and low backstaining. An alkalothermophilic *Thermomonospora* sp has been isolated in our laboratory, secreting maximally endoglucanases and xylanases, active and stable in alkaline conditions with negligible exoglucanase activity.

The production of alkali stable cellulase was scaled up from shake flask to a 400 l fermentor in collaboration with an industry unit, Sci molecules Pvt Ltd, Pune. The enzyme activity obtained in shake flask was even achieved at 400 l Level. The trails on biofinishing of denim fabrics using the alkali stable cellulase at Arvind mills Pvt Ltd, Ahmedabad were conducted successfully and the performance was comparable to commercial enzyme with no back staining. The techno economics of the enzyme production was evaluated. The project was funded by DST-TIFAC.

**Aspartic protease inhibitor**

The specific inhibitors of proteases have proved valuable in a number of applications ranging from mechanistic studies to possible therapeutic uses. Elucidation of this paradox is the basis for the extensive research on the structure-function relationship of inhibitors of proteases. Aspartic proteases are found in a wide range of organisms, ranging from viruses, bacteria, fungi, and parasites to plants and animals. They are not only involved in many physiological processes but can also mediate the initial invasion steps of infective organisms. Recently they have received enormous interest because of their significant roles in human diseases; the best-known examples are the involvement of renin in hypertension, cathepsin D in metastasis of breast cancer, and the protease of human immunodeficiency virus (HIV) in acquired immune deficiency syndrome (AIDS).

The purification and biochemical characterization of an aspartic protease inhibitor from the seeds of *Vigna radiata* is

reported. Seeds of different varieties of *V. radiata* were screened for the presence of the inhibitor. The results indicate that the varietal difference could be due to the result of breeding. The low molecular weight inhibitor was purified by RP-HPLC. The inhibitor was a linear, hydrophobic, pH stable and thermostable peptide with molecular weight of 1660 Da. The purified inhibitor showed a pI of 4.36 with the sequence as AEIYN KDG NK LDLYG. The inhibitor was found to be stable in a broad range of pH from 2 to 10 with an optimum of 3.0. The half-life of VrAPI at 100°C was 30 min whereas the maximum activity was observed at 37°C. The initial kinetic analysis of the inhibitor against the endogenous protease showed an IC<sub>50</sub> value of 11 nM while the value of the inhibition rate constant Ki was 34 x 10<sup>9</sup> M.

## Microbial technology



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## Biotransformation

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**Biosynthesis of novel sophorolipids**

We are reporting sophorolipid (SL) production using pure Linolenic acid (18:3) as the lipophilic substrate. We have shown that this fatty acid gets incorporated into the SL structure with unaltered three double bonds in fatty-acid chain. We confirmed this by converting the natural SL mixture obtained from batch fermentation into the single homogenous product. This was followed by esterification reaction, which was carried out by refluxing natural SL mixture with Na metal in methanol solution for 3 hours. After purification by silica gel column chromatography product was isolated and confirmed by Mass spectrometry, <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. We have tested the obtained Sophorolipid methyl ester product for its antimicrobial properties against both gram positive and gram negative bacteria such as *Bacillus subtilis*, *E. coli*, and *Pseudomonas aeruginosa*. This product showed good antimicrobial activity against *B.subtilis* at concentrations 5, 10 and 15 mg/ml, respectively.

**Biosynthesis of sophorolipids and investigation of their ability to induce cell differentiation**

We studied the effects of crude as well as purified sophorolipids against the cancerous cell lines of neuronal origin. As a result, we could see elongation of cells and formation of threadlike extensions from the ends of the cells. Further we checked for the expression of specific marker proteins associated with differentiation.

**Surface functionalisation of nanoparticles and their biological applications**

We report *in situ* synthesis and functionalisation of gold nanoparticles (AuNPs) using  $\beta$ -lactam antibiotics such as cephalixin, cefaclor and ampicillin. The process involves a facile, one-pot reaction method at room temperature, without involving any harsh chemicals. With the onslaught of drug resistant and extremely drug resistant bacteria, we need better warfare; the antibiotics capped nanoparticles could serve as a new tool in combating this upsurge. In addition, the process provides a good system to capture AuNPs during its synthesis by the cephalixin using optical methods such as Dynamic Light Scattering (DLS), Surface Plasmon Resonance (SPR) using UV-Vis light spectroscopy and Transmission Electron Microscopy (TEM). Unique bimodal distribution is observed at different temperatures (15°C, 25°C and

35°C) using DLS. This study also provides a good comparison between the different techniques used.

Surface functionalisation of iron oxide nanoparticles is done by enzyme Penicillin G acylase, in an effort to study the activity of enzyme towards potential immobilization use; use of magnetic nanoparticles serves in the ease of separation for re-use. Good enzymatic activity is observed. Functionalisation of AuNPs using curcumin, the wonder molecule from turmeric, acting both as reducing and stabilizing agent is carried out. These nanoparticles show anti-oxidant activity, which can be used in biomedicine.

**Biotransformation of non-edible oil into biofuels**

In the present study whole cells of lipase producing microorganisms have been used for bioesterification. Screening high lipase producing fungi and yeast is achieved; attempts for whole cell utilization for bioesterification are in progress.

We have isolated a thermophile producing bile salt hydrolase intracellularly. The thermophilic bacterium was identified to be *Brevibacillus borstelensis* by 16S rDNA sequencing. This is the first report of bile salt hydrolase from a thermophilic source.

We studied the characteristics of BSH immobilized on amino-functionalized mesoporous silica. Amino-functionalization using the compound amino propyltriethoxy silane facilitated the immobilization reaction by forming covalent bonds between carboxyl groups of protein and amino groups of mesoporous silica. Physicochemical characterization of the immobilized enzyme indicated that the structure of the support material is stable after immobilization.

In application studies, we screened different probiotic strains for BSH activity and *L. buchneri* was found to have maximum production of bile salt hydrolase, among the tested microorganisms. We observed about 50% reduction in serum cholesterol and 15% reduction in triglycerides in wistar rats when fed with 10U/kg dose of immobilized bile salt hydrolase and 58% reduction in serum cholesterol and 45% reduction in triglycerides in wistar rats when fed with 20U/kg dose of immobilized bile salt hydrolase.

## Selected publication:

- ✦ *J. Physical Chem. C*, 2009, 113, 3478

Microbial technology



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Penicillin acylases and related Ntn hydrolases

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Penicillin acylases (Penicillin amidohydrolases, EC 3.5.1.11) are the group of enzymes that hydrolyze the acyl side chain of penicillin to yield 6-aminopenicillanic acid (6-APA) and the corresponding organic acid. 6-APA is the starting compound in the manufacture of semi-synthetic penicillins such as ampicillin, amoxicillin etc. Penicillin acylases selectively hydrolyse the amide bond at the side chain of the penicillin moiety keeping the beta lactam amide bond intact.

Various microorganisms were screened for penicillin V acylase (PVA) production, extracellular as well as intracellular; as a result of which *R. aurantiaca* (NCIM 3425), *E. aorideae* (DSMZ 30186) and a bacterial isolate were found to be the good producer of intracellular PVA. The enzyme from *Rhodotorula aurantiaca* (*Ra*-PVA) has been purified and characterized comprehensively. It has been found to be the smallest active monomeric PVA. Microenvironment of the tryptophan residues in active and denatured *Ra*-PVA was studied using various quenchers and fluorescence spectrophotometry. It was found that tryptophan residues of *Ra*-PVA are largely buried in hydrophobic core of the protein matrix and surface tryptophan residues were found to have predominantly more electro-positively charged amino acids around them, however differentially accessible for ionic quenchers.

The newly isolated bacterial culture was the novel source of PVA. Identification of

isolated culture was done by polyphasic analysis and the culture identified as *Bacillus cereus*. This was the first report of *Bacillus cereus* producing PVA.

*Erwinia aroideae* (DSMZ 30186) is a potential microbial producer of intracellular penicillin V acylase (PVA). Cell bound PVA activity was improved by permeabilization with various organic solvents. Whole cell PVA activity showed an eight fold increase upon treatment with chloroform for 10 min and diethyl ether for 45 min. Hexane, toluene, ethyl acetate and dichloromethane enhanced the enzyme activity up to two, six, four and two fold, respectively; whereas, PVA activity declined drastically on permeabilization with acetone, pyridine and alcohols. The physicochemical properties of the organic solvents used for permeabilization were correlated with the change in activity. It was found that solvents with high hydrophobicity ( $\log P > 0.68$ ) and lower dielectric constant ( $< 9$ ) were relatively more effective in increasing PVA activity. These results allow systematic selection of suitable solvent for best performance.

Synthesis of crystalline ferromagnetic nanoparticles has been achieved at room temperature and in aqueous medium by a metal tolerant marine bacterium isolated from the coast of Arabian Sea. Energetically unfavourable change in the oxidation state of cobalt atoms from +2 to +3 during synthesis by bacterial strain is reported.

Selected publications:

- ✦ *Process Biochem*, 2008, 43, 961
- ✦ *Chem. Mater.*, 2008, 20, 1484
- ✦ *Res. J. Biotech.*, 2008, 3(2), 26
- ✦ *Appl Biochem Biotechnol*, 2009, 157, 463

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**Selected publications:**

- ✦ *Planta Medica*, 2008, 74, 780
- ✦ *Acta Hort.*, 2008, 785, 147
- ✦ *J. Appl. Hort.*, 2008,10(1), 44

**Plant biotechnology**



T-DNA activation tagging induced insertional mutagenesis in taxol producing fungus

Taxol (*paclitaxel*), isolated from the bark of the yew trees has been found to be very effective in cancer chemotherapy and a wide range of tumours. However, the supply of taxol has been limited and cost of the drug remains an important issue. Endophytic fungi are source of a large variety of useful secondary metabolites including taxol. Recently, Dr. Absar Ahmad's group at NCL has isolated an endophytic fungus (AAT-TS-3) from *Taxus baccata*. This fungus produces taxol and a precursor, 10 deacetyl baccatin-III (10-DAB-III). Yields of taxol and 10-DAB-III are 10 and 65 µg/l, respectively. We aim to generate transformed colonies of this fungus by insertional mutagenesis using *Agrobacterium tumefaciens* strain carrying an Activation Tagging binary vector. This technique utilizes a T-DNA sequence that contains 4 tandem copies of the cauliflower mosaic virus (CaMV) 35S enhancer sequence. This element enhances the expression of neighbouring genes on either side of the randomly integrated T-DNA tag, resulting in gain-of-function mutants. These mutants are screened for cell lines producing higher quantities of compounds.

The work involves construction of a new plasmid vector containing a CaMV 35S tetrameric enhancer sequence, the *gfp* and *gus* reporter genes and the gene encoding for hygromycin phosphotransferase which

confers hygromycin B resistance. This was done by inserting a fragment containing CaMV 35S tetrameric enhancer sequence obtained from the Addgene plasmid into the T-DNA region of the pCAMBIA vector plasmids containing the reporter genes by restriction digestion and ligation of the insert and vector DNA. Also a comparative study of two types of minimal media used during *Agrobacterium tumefaciens* mediated transformation and the effect of presence and absence of acetosyringone during co-cultivation of *Agrobacterium* and the target fungus was done. The results obtained show a positive effect of acetosyringone on fungal transformation by the *Agrobacterium*.

The activation tagging sequence can be transferred into the target fungus by carrying out further experiments by optimizing the ATMT parameters. By further analysis and rigorous selection, fungal transformants showing an enhanced production of taxol or taxol pathway intermediates can be isolated. For this, a robust HPLC or GC system is employed to screen product biosynthesis. Then, these transformants are cultured on a large scale to obtain higher yields of taxol and/or its precursors. Further studies are underway to locate genes coding for products involved in the taxol biosynthetic pathway.

Plant biotechnology



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Metabolic engineering

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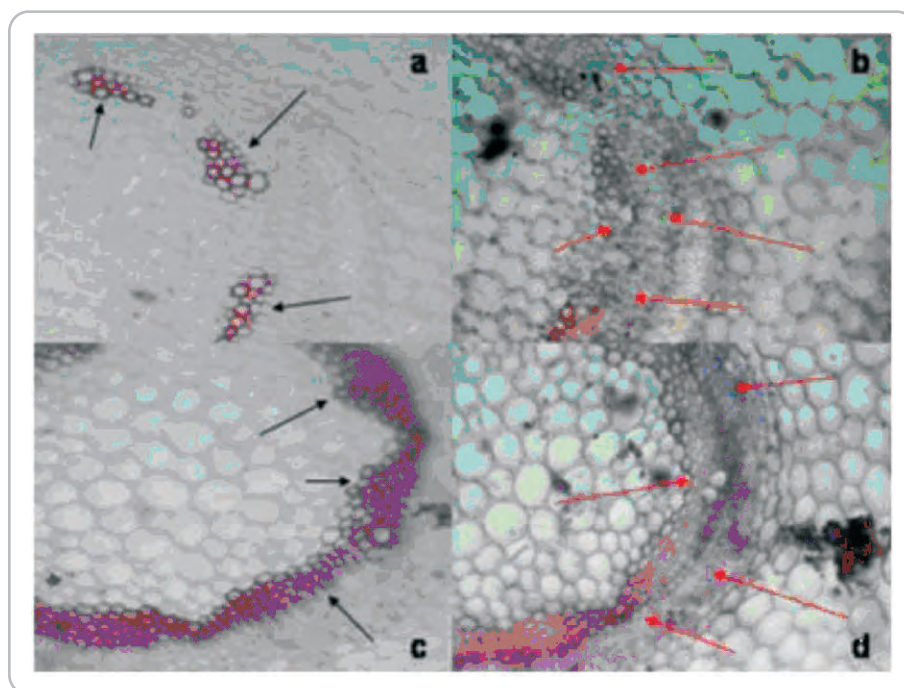
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Metabolic engineering of the phenylpropanoid metabolic pathway of plants has the potential to modify the content and the composition of the plant lignins. A change in the S/G ratio of the plant lignins, for example, would make lignin removal from lingo-cellulose materials easy and environmentally less hazardous. Regulated expression of the caffeoyl CoA 3-O-methyltransferase (CCoAOMT), cinamyl alcohol dehydrogenase (CAD), cinamoyl CoA reductase (CCR), coumaryl CoA ligase (4-CL), coniferin-β glucosidase (CBG) and the coniferyl aldehyde 5 hydroxylase (Cald5H) genes, individually or in various combinations, by antisense, co-suppression or RNA interference technologies is a possibility. It necessitates isolation of the genes and then their use in various constructs to develop and recover transgenics with either reduced lignin content or altered lignin composition.

Cinnamate-4-hydroxylase (C4H) gene (cDNA clone) from *Leucaena leucocephala* has been cloned and characterized. A partial fragment of C4H gene has been cloned in anti-sense orientation in plant transformation vectors pCAMBIA1300 and 1301 and mobilized into *A. tumefaciens* pGV2206 and LBA4404.

*Leucaena leucocephala* is being transformed with anti-sense C4H using embryo axis regeneration system and particle bombardment and *Agrobacterium* mediated transformation.

A 508 bp partial CCoAOMT promoter sequence was obtained using reverse gene specific primer of CCoAOMT gene in tertiary TAIL-PCR reaction, which was, cloned, sequenced and named LISumCMT1. The sequence was analyzed using Matinspector 2.2 software and shows 29 promoter regulatory elements on the sense strand. The above fragment was directionally cloned in p1381Z vector of promoter less pCAMBIA series. The above construct was then transformed to competent *Agrobacterium* strain, GV2260, for carrying out *Agrobacterium*-mediated transformation studies in *Nicotiana tabaccum*. A full length Myb cDNA clone has been isolated, cloned and sequenced. It showed significant similarity to the other Myb sequences. The transgenic plants developed earlier with anti-sense constructs of CCoAOMT, CAD, CCR and 4CL and established in green house are being characterized for gene expression, protein levels and wood characteristics. Initial observations indicate down regulation of the targeted genes, reduction in lignin content in the range of 5% to 12% in various transgenic events.



Immuno-cytolocalization of LI-CCR protein in growing seedling of *L. leucocephala*: Panel a and c are sections of phloroglucinol stained 15 d old stem and root section of *L. leucocephala*. Panel b and d is immunocytochemical 15 d old stem and root sections respectively. Black arrow denotes lignified xylem tissue and red arrow denotes immuno-cytolocalized CCR protein in stem and root section of *L. leucocephala*

Selected publication:

- ✦ *J. Mol. Modelling*, 2009, 15, 203

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**Plant biotechnology**

Tissue culture studies in oil producing plants



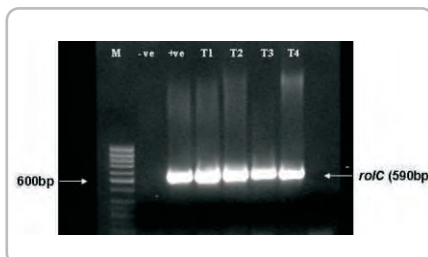
Our objectives are to develop tissue culture protocols for rapid propagation using seedling / mature explants and standardization of protocols for *de novo* organogenesis / embryogenesis.

**Peanut**

The *Agrobacterium rhizogenes* induced peanut hairy root showed a rapid growth on subculture and formed a root bunch within two weeks. Further confirmation of transgenic tissue was done by the PCR amplification of the DNA isolated from the hairy roots using forward and reverse primers of *rol* genes (*rolA*, *rolB* and *rolC*).



Bunch of hairy root developed from single explant



PCR amplification of a 590 bp fragment of the *rolC* gene. Lane 1 = molecular weight marker (100bp ladder); lane 2 = DNA from non-transformed roots (negative control), lane 3 = *A. rhizogenes* DNA (positive control), lane 4 = sample 1, lane 5 = sample 2, lane 6= sample 3, lane 7= sample 4. Sample 1-3 were DNA of transformed root obtained after infection with strain ATCC15834, LBA9402 and A4, respectively, and sample 4 was DNA of transformed Embryogenic mass obtained after infection with strain ATCC15834

**Jatropha**

Hairy roots were induced from different explants of *Jatropha* seedlings using the *A. rhizogenes* mediated transformation approach. However, the induced roots did not continue to grow further and need some more experimentation.

**Semecarpus anacardium**

The work carried out includes:

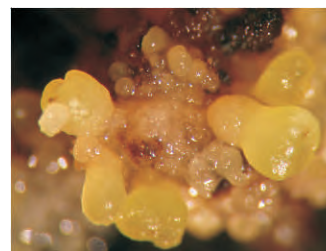
- Induction of somatic embryogenesis from cotyledon explant and cotyledon derived callus.
- *Agrobacterium rhizogenes* mediated transformation was conducted using



Induction of hairy root from leaf and petiole explants of *Jatropha* seedlings

different explants like leaves, stem and shoots to establish hairy root cultures.

- DNA was isolated from cluster of roots induced in various explants and confirmed the presence of *rolA*, *rolB* and *rolC* genes in the roots.
- Oil in seeds of different trees from various locations were extracted and quantified. Variation in the oil content of seeds of different trees was observed.
- DNA isolation was standardized from leaves collected from different locations. Molecular characterization using ISSR markers is in progress.



Induction of somatic embryos from cotyledon derived callus of *Semecarpus*



Induction of hairy roots from leaf explant of *Semecarpus*

**Selected publications:**

- ✦ *Analytical Bioanalytical Chem.*, 2008, 391, 2227
- ✦ *Seed Science Biotech.*, 2008, 2 (2), 70
- ✦ *Int. J. Pl. Dev. Biol.*, 2008, 2, 118

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Plant biotechnology

Medicinal plant biotechnology



Objectives of our study are:

- Assessment of biodiversity, chemodiversity and molecular characterization
- Chemotaxonomic analysis and Identification of chemical elite to generate protocols for *in vitro* propagation of female plants
- Identification of new natural compounds with biological activity
- Development of *A.rhizogene* transformation protocols
- Diversity analysis using ISSR markers

From chemodiversity studies elite plants/populations of *Calophyllum* spp and *Garcinia* have been identified. The correlation between elites with distribution and molecular characterization has been established.

Callus cultures were established for *C. inophyllum* for Secondary metabolites production. The suspension cultures and callus cultures showed expression of dipyrano coumarins.

The callus cultures were subjected to biotic and abiotic elicitation for enhanced production of anti HIV compounds wherein hyperproduction has been observed.

Under NMPB project entitled 'Development of *in vitro* propagation technology for large scale production of female plants of *Garcinia indica* Choiss' protocol has been developed to produce female plants of *Garcinia indica* using *in vitro* techniques.

*Agrobacterium rhizogene* mediated transformation studies were initiated in four species of *Garcinia*, namely, *G.indica*, *G.talbotti*, *G. spicata*, *G.xanthochymus*. Chemical analysis of the leaves and twigs of all the four species have been carried out and a pure compound has been isolated recently which has been confirmed by NMR as the mixture of bioflavonoid.

Genetic diversity studies using ISSR markers have been initiated in *Pinus roxburghii* and the work is under progress.



Initiation of the multiplication



Elongation of shoots



In vitro rooting of shoots

Fig 1 : *Garcinia indica* (Choiss) *In vitro* female to female plants Explant – Apical and axillary buds

**Selected publications:**

- ✦ *Ind. J. Exp. Biol.*, 2008, 46, 482
- ✦ *J. Biotechnol.*, 2007, 130 346



## NMITLI



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Process development of polymer grade lactic acid–down stream processing

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### Background

The production of highly purified monomeric lactic acid is required for various applications such as medical, food etc. Therefore, in recent years, production of lactic acid from renewable biomass and its transformation through fermentation to L-lactic acid has been shown great importance. Purification of dilute lactic acid obtained from bacterial fermentation is difficult due to its low vapour pressure, tendency to undergo self-esterification, and the presence of troublesome impurities. In the literature of this theme several strategies such as adsorption, solvent extraction, electrodialysis, reactive distillation etc have been studied for the recovery of lactic acid from the fermentation broth. However, the reactive distillation has been widely accepted as highly efficient technique for the recovery of lactic acid with high purity and high yield from the fermentation broth.

### Objectives

- Fermentation of sugar cane juice with new strain.
- Development of a cost effective commercially viable process for manufacturing of highly pure lactic acid.
- Scale-up and demonstration of lactic acid synthesis process at 1 kg/hr.
- New application of highly pure lactic acid for preparation of polymer.

### Work done and discussion

- A new lactobacillus based strain has been developed for production of calcium lactate which gives high productivity and can utilize low cost nitrogen source.
- A novel autocatalytic, cost effective, eco-friendly and promising process for the recovery of high quality lactic acid has been developed.
- Further there is no need for separation and regeneration of a catalyst.
- The purity of lactic acid obtained in the pilot plant is more than 99.95%.
- Highly pure lactic acid was successfully used for various applications such as food additives, film and fiber (as a packing material for biodegradable and non-toxic applications).



Continuous production of lactic acid process at pilot plant scale in NCL

### Outcome of the project

- A generic continuous process for synthesis of lactic acid has been developed.
- A continuous process (pilot plant level) for the production of lactic acid has been developed at the NCL and demonstrated to M/s Godavari Sugar Mills.
- M/s Godavari Sugar Mills have started erection of commercial plant for production of lactic acid based on NCL technology.

## NMITLI



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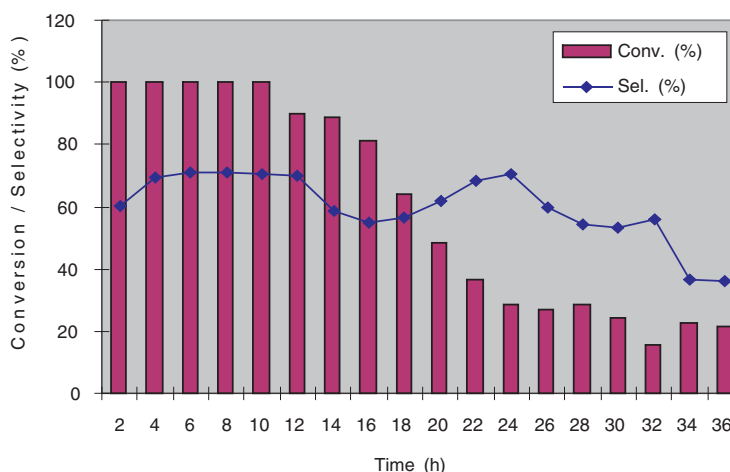
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## Dehydration of glycerol to acrolein

Glycerol is obtained as a by-product of bio-diesel synthesis, hydrolysis of fat and soap manufacture. There is a need to develop economically viable routes to value added chemicals starting from glycerol. The main objective of the work was to develop a catalyst for dehydration of glycerol to acrolein with high activity and selectivity.

Detailed investigations on the effect of reaction conditions on the conversion of glycerol and selectivity to acrolein have been carried out using the catalyst based on silica supported triphenylphosphine trisulphonic acid (20% TPPTS/SiO<sub>2</sub>). Various supports were used for the TPPTS catalyst and SiO<sub>2</sub> was found to be the best support for dehydration of glycerol. The yield of acrolein decreased considerably with increase in nitrogen flow and higher flow of glycerol (50%). Lower selectivity at higher nitrogen

flow can be due to vapour losses of acrolein during the reaction. Selectivity to acrolein was not affected by a change in glycerol (20% aq.) flow rate in a range of 3 ml/h to 9 ml/h. In order to minimize vapour losses, an additional trap was fixed after the sample collector, and was cooled to -7°C. With this trap 4-5% increase in selectivity was observed for the standard reaction and selectivity was found to increase from 65% to 70%. Stability of the catalyst was tested at 325°C (see Figure below) and it was observed that the activity of the catalyst was good for 12 h reaction time (98.3% conversion with 80.5% selectivity to acrolein). Performance of the catalyst decreased with increase in reaction time and 23.3% conversion of glycerol with 60.2% selectivity was observed at the end of 36 h reaction time. However, the catalyst deactivated and could not be reused after 36 h reaction time.



Dehydration of glycerol to acrolein: stability of catalyst at 325°C

Reaction Conditions: catalyst loading: 1 g, glycerol in water:20% (w/w), glycerol flow: 3 ml/h, nitrogen flow: 7 ml/min

NMITLI



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Conversion of cellulose and hemicellulose into sugars and ethanol-  
Part B: Enzymatic hydrolysis and ethanol production

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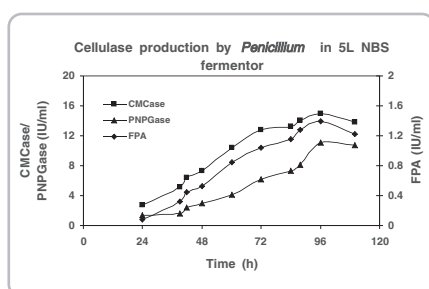
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Energy crunch arising due to the rapid exhaustion of fossil fuels coupled with ever increasing demand has necessitated the search for alternate energy sources all over the world. Ethanol has the capacity to match the features of petroleum and is recognized an alternative biofuel which can be produced from renewable sources such as lignocelluloses. India has vast natural renewable resources available that can be exploited in converting cellulose and hemicellulose to sugars and ethanol. Ethanol production from lignocellulosic materials includes hydrolysis of cellulosic and hemicellulosic fractions into fermentable sugars by powerful cellulases and hemicellulase, and their subsequent fermentation to ethanol by yeasts.

The NCL *Penicillium* strain secretes complete cellulase with all the components, namely, FPase, CMCcase, xylanase and  $\beta$ -glucosidase having cellobiase (PNPGase) activities in 5-6 days and the crude preparation results in hydrolysis of cellulose predominantly yielding glucose as the end product and does not require external addition of  $\beta$ -glucosidase which is highly desirable for its fermentation to ethanol.

**Scale-up of production in fermenter**

Scale-up of cellulase production by *Penicillium sp.* in 7.5L New Brunswick fermenter with 5L working volume were carried out at NCL, Pune. The pattern of growth and the yields were similar and maximum activities of 1.6-1.8 IU/ml of FPase and 15-16 IU/ml of CMCcase activities were reached in 96-108h. A typical fermentation profile is presented in figure below.



**Cellulase production by solid state fermentation**

Cellulase production by solid state fermentation has also been initiated. Among the various support systems for solid state fermentation that were investigated, wheat bran was found to be the best. Addition of cellulose powder and steam exploded bagasse to wheat bran increased the yields compared to those of wheat bran alone. Further optimization studies are in progress.

**Selected publication:**

- ✦ *Bioresource Technology*, 2009, 100, 6679

**Ethanol production from the steam exploded bagasse hydrolysates**

Hydrolysis of steam exploded bagasse at 5%SBC and 20FPU/g yielded around 2% sugar which was converted into ethanol with 93% efficiency in 3h but the ethanol concentration was less than 1 %. Hence hydrolysis at 10% SBC and fermentation were carried out which gave 4.79% sugar with 89.4% conversion efficiencies.

**Effect of substrate concentration on ethanol production by *S. cerevisiae***

	5% SBC Hydrolysate	10%SBC Hydrolysate
Reducing sugar (%)	2.07	4.79
Ethanol (w/v) (%)	0.88	2.184
Efficiency (%)	93.33	89.40
Time(h) to reach maxm	3	6

**Scale-up of enzymatic hydrolysis of steam exploded bagasse and ethanol production**

Based on the earlier experiments, hydrolysis of steam exploded bagasse (SEB), hydrolysis was scaled up to 50g level. The enzyme concentration was increased to 2 fold (40 FPU/g of the substrate) for the complete hydrolysis of available cellulose and hemicellulose in the steam exploded bagasse. A maximum conversion of 63.9% with a reducing sugar of 7.1% was obtained. This was converted to ethanol (27g/L) with 75% efficiency.

**Ethanol production from enzymatic hydrolysate of steam exploded bagasse (50g)**

Hydrolysis Parameters	10%SBC; 40 FPU/g, 50C, 36h
Fermentation Parameters	<i>S.cerevisiae</i> ; 10% cell loading; 40C, 4h
Hydrolysis (%)	63
Reducing sugar (%)	7.1
Ethanol (w/v) %	2.74
Conversion efficiency(%)	75

As per the recommendations of the Steering Committee, a mini workshop was conducted at NCL during January 6-8, 2009 to demonstrate IUPAC assay protocols for cellulases to be followed by the partners for uniformity in expressing the activities of cellulase complex.

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Conversion of bioglycerol to 1,3 / 1,2-propanediol

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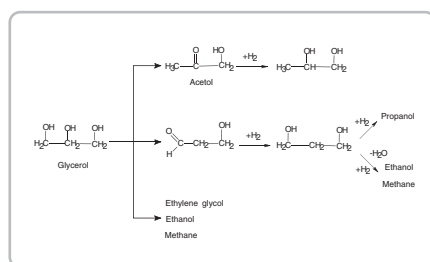
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## Hydrogenolysis of bioglycerol

As glycerol is obtained as a byproduct in the manufacture of biodiesel, its valorization into value added products having sustained market demand is highly essential. Catalytic hydrogenolysis of glycerol to glycols represents feasible, low cost, and green route to 1,2 propylene glycol which is one of the major commodity chemical and is often used in the production of antifreeze functional fluids, paints, humectants, and polyester resins. Hydrogenolysis of glycerol involves several parallel and consecutive reactions giving variety of products (Scheme 1). Hence, developing a suitable catalyst and a process to give the highest selectivity to 1,2 PDO is a great challenge from both point of view, fundamental as well as process.



Scheme 1: Catalytic hydrogenolysis of glycerol

At the NCL, our group has been working on development of catalyst and a bench scale process for selective hydrogenolysis of glycerol to 1,2 propanediol. The highlights of our achievements are giving below.

## Hydrogenolysis of glycerol in a batch reactor

Non-chromium nano structured Cu based catalysts were developed for glycerol hydrogenolysis in a high pressure batch reactor using water and 2-propanol solvents. These catalysts showed very good water tolerance with 38% glycerol conversion with 92% 1,2-PG selectivity at 220°C, H<sub>2</sub> pressure 1000 psi and reaction time 5 h.

The effect of reaction conditions on the glycerol conversion and 1,2 PG selectivity showed that glycerol conversion increased from 29% to 76% with increase in temperature from 200°C to 240°C. Maximum conversion of 76% was obtained at 240°C; however, selectivity to 1,2 PG decreased marginally from 93% to 89%, correspondingly increasing the selectivity to ethylene glycol from 6% to 10%, indicating that the higher temperature favoured degradation products due to C-C bond cleavage. Glycerol conversion increased from 23% to 38% as the hydrogen pressure increased from 35 to 70 bar H<sub>2</sub> pressure.

Conversion of glycerol increased from 38% to 45% with increase in glycerol concentration up to 60% (w/w) beyond which it decreased drastically to 23%.

## Dehydration and hydrogenolysis of glycerol in a continuous reactor

Continuous dehydration of glycerol was carried out in an inert atmosphere, using 20% (w/w) glycerol in 2-propanol, at 220°C, 2.5 inch catalyst bed, with initial feed flow rate of 18 ml/h which was increased to 54 ml/h. Dehydration of glycerol was carried continuously for 50 h. The results are shown in Table 1.

Table 1 Continuous dehydration of glycerol to acetol

Liquid flow rate (ml/h)	%Conversion	% Selectivity		
		Acetol	1,2-PG	Others
18	61	63	8	29
54	43	45	14	41

After the dehydration run, the same catalyst was reactivated *in situ* by passing H<sub>2</sub> for 12h and further used for glycerol hydrogenolysis reaction.

Glycerol hydrogenolysis reactions were performed using 20% (w/w) glycerol in 2-propanol, at 220°C temperature, 300 psi H<sub>2</sub> pressure, 6.25cm catalyst bed, 30 mL/min feed flow rate, H<sub>2</sub> flow rate, 10 NL/h, for 61h. The results are shown in Table 2.

Table 2. Continuous hydrogenolysis of glycerol to 1, 2-PG

Feed	% Conversion	% Selectivity		
		1,2-PG	Acetol	Others
Pure glycerol	54	61	15	24
Crude recycled glycerol	76	55	14	31

After initial hydrogenolysis run of 26 h, the crude reaction mixture was used as a feed to give glycerol conversion in a range of 85% - 90% with 60% selectivity to 1,2-PG, which was continued for 48 h.

## NMITLI



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Biotechnology of leather : Towards cleaner processing - Phase-II

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Leather industry is highly polluting and leads to water and soil pollution. The major source of pollution is dehairing amounting to 70% of pollution load. Development of eco-friendly and cleaner technologies by use of enzymes such as alkaline proteases in place of currently used chemical technologies is highly desirable. Dehairing of skins and hides by totally enzymatic methods as an alternative to the conventional methods is very attractive as well as challenging. The present study aims in developing enzyme cocktails for total enzymatic dehairing.

Two leads enzymes from the Phase 1 of the project, namely, NCL Protease 1 and Protease 3 were selected for process development based on dehairing performance of skins and hides.

Scale up of production and down stream processing of NCL-Protease-1 was carried out at CLRI fermentation facility at Chennai, and dehairing trials were conducted in tanneries. In all, eight 5L, two 50L and one 500L production batches were carried out. Scale up of production of NCL Protease 1 up to 500L and its down stream processing was successfully validated at CLRI fermentation facility with activities around 1500-1700 g Tyr/ml/min on cheap and inexpensive media. These activities are similar to those obtained in 400L fermentor batches carried out at Pune. Down stream processing of protease by ammonium sulphate precipitation and spray drying in presence of maltodextrins was carried out at Pilot Plant facility of CLRI with 99% and 70% recoveries, respectively. De-hairing trials and scale up of NCL Protease -1 are in progress.

Stability of spray dried Protease 1 was studied at 4°C, 28°C and 37°C. The enzyme is stable with no loss of activity at all the three temperatures with 90-95% activity being retained even after 120 days (Fig 1).

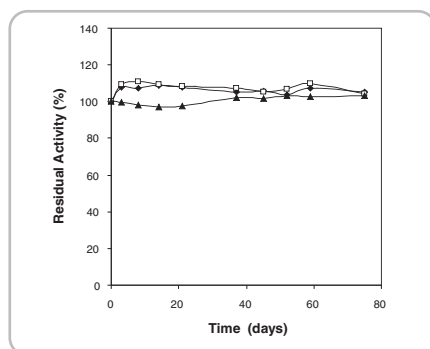


Fig 1 : Stability of spray dried Protease 1

Stability of Protease 3 in presence of detergents and organic solvents was

studied. The protease was stable in the presence of all detergents tested and retained 75%-100% activity at 40°C even after 1 h depending on the detergent.

### Stability of Protease 3 in presence of detergents

Detergent	Residual activity after 1 h (%)
Nil	82.54
Aerial	100.64
Fena	88.03
Rin	79.47
Surf excel	78.64

Stability of protease in presence of organic solvents was tested at 28°C. Protease was stable in presence of ethanol, isopropanol, methanol, butanol and dimethylsulphoxide even after 24h and retained more than 80% activity.

### Stability of Protease 3 in presence of organic solvents at 28°C

Solvent	Residual activity after 24 h(%)
None	26.66
Ethanol	81.60
Isopropanol	84.18
Methanol	91.10
Butanol	82.73
DMSO	93.11

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Conversion of cellulose and hemicellulose into sugars and ethanol-  
Part A: Pretreatment of bagasse and acid hydrolysis

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Sugarcane is one of the important cash crops of India. It generates millions of tones of bagasse, and there is great need to value-add to this important national resource. The greatest impediment to its successful use is the intractability of the biomass structure, which can be overcome by pretreatments. Inexpensive pre-treatment of the bagasse to produce an "open-structure" which can facilitate a large area for bacterial and enzyme interaction would then be a logical way to go about utilizing this biomass resource for producing fuels like ethanol, which are currently made from petroleum resources. One aspect that bears investigation is the minimization or neutralization of inhibitors that are invariably produced by various known pre-treatments. Acid hydrolysis of this pretreated bagasse will make available large amounts of fermentable sugars, and will obviate the necessity of developing new enzyme technologies and their production.

Ethanol is produced by fermentation of molasses (India), corn glucose (America) or sucrose (Brazil). The agronomic residues such as corn stover, wheat or rice straw, forestry and paper mill discards, collectively known as "biomass" can be converted to ethanol. Although new technologies have been developed to produce bioethanol from such biomass, there are still challenges requiring further investigations to develop cost effective processes. India is one of the largest countries producing approximately 200 million tons of sugarcane.

Currently, in spite of extensive research on fuel ethanol production, not a single plant on the industrial scale capable of producing ethanol from cellulosic feed stock through biological processes had been put in operation anywhere.

In our laboratory we are working on issue of converting the biomass, which is highly inaccessible to microbial enzymes, into a form that improves the accessibility of the residual polysaccharides to the microbial enzymes for optimal and economic fermentation to products. Sugarcane bagasse derived cellulose made at NCL gave much higher yield of hydrolysis than Avicel, an expensive microcrystalline cellulose grade. Our work on acid hydrolysis has shown that the pretreated bagasse undergoes hydrolysis to sugars, and the economics of this process are being worked out.

### At NCL, the following work was done:

- Produced pretreated bagasse samples for use by various investigators (project participants from different institutions in India)
- Characterized composition made by steam explosion and acid treatments.
- Prepared bagasse hemicellulose
- Produced fully hydrolyzed hemicellulose
- Characterized hemicellulose solution.
- Detoxification studies of substrates were carried out
- Working with project partners to solve problems with substrates and also during scale-up to pilot plant level.
- Hydrolysis of substrates

Several pretreated samples of bagasse for studies on fermentation to ethanol was prepared and samples given to biochemistry/microbiology colleagues in different institutions of India such as Delhi University, IICB Kolkata, NCL Pune, RRL / NIIST (Thiruvananthapuram) and IMT Chandigarh for evaluation for enzymatic hydrolysis to sugars. Starting bagasse sample along with one sample prepared by steam explosion at 200°C, and one sample by partial delignification and partial removal of hemicellulose, having porous structure was prepared and sent for evaluations. The partially delignified bagasse having a kappa number of about 21 was found to be a promising candidate for exploration. The steam exploded bagasse sample also seems to have promise. Similarly, we prepared bagasse hemicellulose sample for studies on fermentation to ethanol.

## NMITLI



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Development of polymer electrolyte membrane fuel cell stacks of stationary applications

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### Objectives

- Primary objective of this project is to develop 1 KW PEM fuel cell stack in collaboration with CECRI and NPL
- Development of injection moldable bipolar plates that are electrically and thermally conducting, mechanically strong and manufactured in a single step
- Synthesis and evaluation of PBI membranes having better proton conductivity and durability.
- Implementation of the facilities and process standardization for making smaller and larger sized MEAs out of Nafion membranes
- Optimization of Decal process of MEA fabrication with PBI membranes
- Reduction of Pt loading on electrode while maintaining the cell performance
- Single cell durability analysis

### Work done and discussion

Several technological barriers preventing the fabrication of various components of PEMFC have been overcome by concerted efforts of different groups at NCL in conjunction with complementary groups at CECRI and NPL. A summary of NCL activities focused on membranes, bipolar materials and electrocatalyst is given below.

Fuel cells have highly acidic environment which prohibits the use of metallic bipolar plates. Polymer based bipolar plates with sufficient electrical and thermal conductivity can be used instead. They have the added advantage of being light in weight and could be easily processed in fewer steps. PP-graphite based composites were prepared as materials for bipolar plates in low temperature fuel cell applications. Carbon black was added to various extents. Formulations were prepared by melt blending both in small scale (50g) and a large scale (20 kg). The electrical resistance and solid state mechanical properties of the formulations were measured. Accordingly, Fig.1 shows some of this data along with a systematic variation with respect to compositional changes. The melt viscosities of the formulations were measured to assess their moldability.

S.No	1	2	3	4	5	6	7	8	9	10	11	12	13	14
PP	55	50	45	40	40	45	50	50	45	40	35	35	40	45
Graphite	40	45	50	55	50	45	40	40	45	50	55	50	45	40
Carbon Black	5	5	5	5	10	10	5	5	5	5	10	10	10	10
PPMA	5	5	5	5	5	5	5	5	5	5	5	5	5	5
Total	100	100	100	100	100	100	100	100	100	100	100	100	100	100

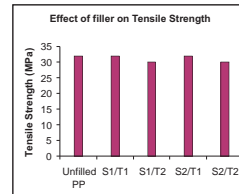
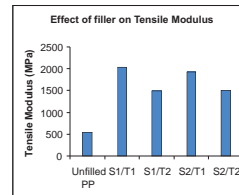
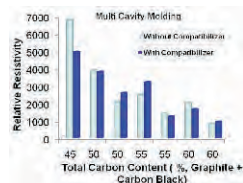


Figure 1: Table (top) shows formulations of PP-graphite-carbon composites. The three plots (bottom) show the relative electrical resistivity and mechanical properties in the solid state of the formulations.

Compression molded bipolar plates (200 x 150 x 4 mm) were made for trial purposes. Fig. 2 shows these plates along with their main design features.

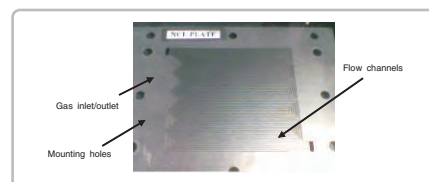


Figure 2 : Bipolar plate of NCL's 3 kV stationary fuel cell

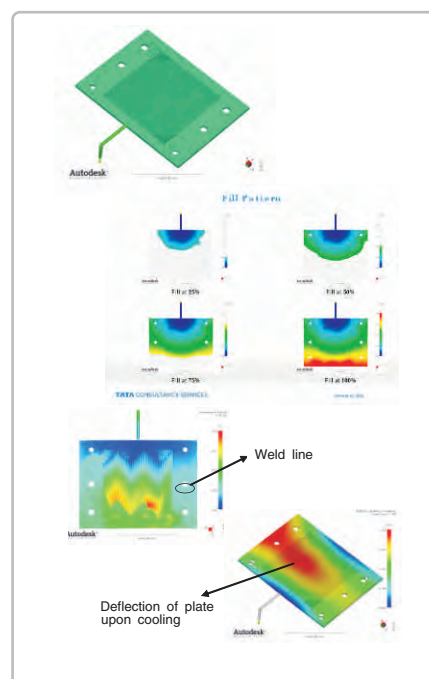


Figure 3: MoldFlow analysis of a single-gated bipolar plate (top left), fill pattern during molding (top right), prediction of weld-line positions



## Development of polymer electrolyte membrane fuel cell stacks of stationary applications

Mold flow simulations were performed on an equivalent PP composite to design the number of gates, weld line positions, fill time and shrinkage analysis. This data is shown in Fig. 3.

Regarding the membrane activities, three reactions of PBI synthesis with 100 g scale were performed. PBI-I synthesis, purification, membrane casting and doping with  $H_3PO_4$  took almost 50 days. If PBI reaction mixture could be used directly for casting membrane, this time could be reduced considerably to 3-5 days. Initial efforts in this direction offered delicate membranes, indicating the necessity of separate reaction parameters than the established ones. Also, synthesis of low molecular weight PBI-Bul by changing DAB: Acid and DAB: PPA ratio was carried out in order to incorporate PBI solution instead of Nafion in the slurry used in decal process. Some of the data has been displayed below in Table 1 and 2.

Table 1. Reaction details for synthesis of PBI with low viscosity

Reaction code	Memb. No.	Coupon No.	Thickness ( $\mu\text{m}$ )	Acid uptake (mol/RU gravimetry)
I 33	M1	C1	121	15.3
	M1	C2	135	15.2
I 38	M1	C1	225	19.7
	M1	C2	236	18.6

Table 2. Details of membranes prepared by direct casting method

Reaction code	Scale of reaction (g)	DAB: Acid ratio(g)	DAB: PPA ratio(g)	% Yield	Inherent viscosity (g/dl)
Bul <sub>3</sub>	10	1 : 0.5	1 : 30	50.2	0.89
Bul <sub>4</sub>	10	1 : 1.1	1 : 30	98.3	0.83
Bul <sub>5</sub>	10	1 : 1.1	1 : 50	80.3	0.52
Bul <sub>9</sub>	25	1 : 1.1	1 : 30	98.9	0.95
Bul <sub>10</sub>	25	1 : 1.1	1 : 50	84.7	0.66

Since membrane thickness has an important role to play in the performance of PEMFC's, membranes of varying thickness have been prepared. Also, the synthesis of PBI having different chemical compositions is under process.

The Decal process of Electrode/ MEA fabrication is a well established procedure amenable for large area fabrication. It holds certain advantages over the brushing method which include prevention of Pt deposition into the pores of carbon

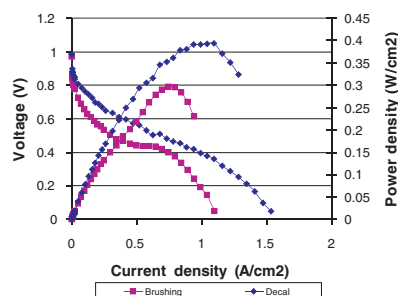


Fig. 4: Comparison of Decal with brushing method (N1135, Pt loading  $\sim 0.2 \text{ mgPt/cm}^2$  in both cases)

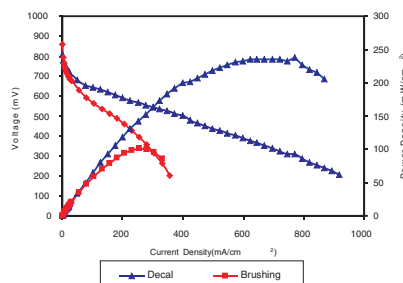


Fig. 5: Comparison of Decal with brushing method (PBI, Pt loading  $\sim 0.15 \text{ mgPt/cm}^2$  in both cases)

paper or diffusion layer, high reliability, uniform Pt loading and high Pt utilization. This process has been successfully implemented with Nafion membrane by hot pressing the membrane with electrodes at a certain temperature and pressure ( $130^\circ\text{C}$ , 1 ton, 1.5 minutes). Single cell polarization studies clearly reflect the predominance of decal process over the brushing method (Fig.4).

It was also found that Nafion 212 gave a better performance ( $700 \text{ mW/cm}^2$ ) as compared to Nafion 1135 ( $400 \text{ mW/cm}^2$ ), both having a Pt loading of  $0.2 \text{ mgPt/cm}^2$ . In the case of PBI, catalyst transfer by decal process was difficult due to the presence of surface phosphoric acid. In order to overcome this issue, a modified procedure was adopted. The wet membrane was hot pressed first to remove surface phosphoric acid followed by hot pressing with electrodes. Here also, decal process scored over brushing method (Fig.5). The barriers we have faced during the MEA fabrication with PBI by decal process are membrane distortion during hot pressing and puncturing of MEA during the Polarization analysis at the temperature above  $100^\circ\text{C}$  which might be solved by optimizing the conditions of MEA fabrication.

Now the focus is on vacuum dried PBI membranes, which is comparatively more stable and easier to handle. Complete transfer of catalyst on these membranes via Decal process has been achieved. Experiments have been oriented to prepare larger sized MEAs using both Nafion and PBI membranes. Also, to solve compatibility issues, PBI as a binder is to be incorporated in the catalyst layer while making MEAs by decal process.

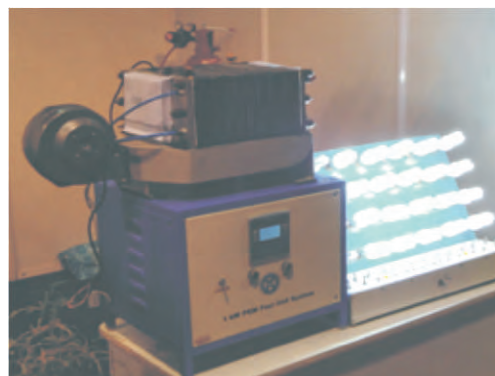


Fig. 6: 1 kW PEMFC (Nafion) stack





### Demonstration of PEM Fuel cell stacks

The CSIR Team (NCL, NPL and CECRI) successfully demonstrated three PEM Fuel cell stacks. Two stacks employing Nafion as membrane were put on display amongst which one was a 30 cell stack giving a total power of 1kW, using H<sub>2</sub>-air. The other was a 10 cell DMFC stack which had a total power capacity of 20 W.



Fig. 7: 20 W DMFC (Nafion) stack

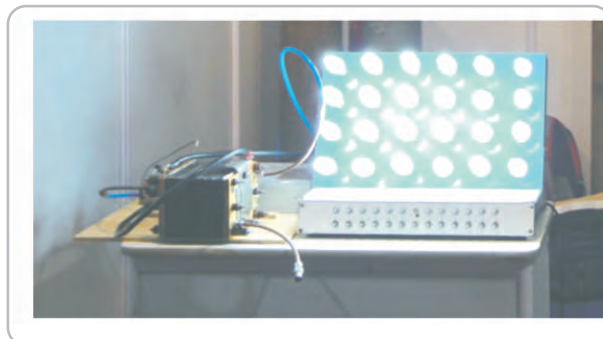


Fig. 8: 350 W PBI based PEMFC

The most attractive part of the demonstration was a 350 W PBI Fuel cell stack which was completely made of indigenous components. Durability measurements of the stack are being carried out at CECRI.



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## NCL - IGIB

Institute of Genomics and Integrative Biology (IGIB) and NCL, two of the premier CSIR laboratories, recognizing the importance of both chemistry and biology and with an objective of benefiting from synergies of these two disciplines as well as from the complementary areas of expertise existing at both the laboratories, created a 'Joint Research Initiative' (JRI) to undertake activities in the cutting edge of Interdisciplinary technologies of biology and chemistry.

The main objectives of this initiative are to nurture, promote and encourage research at the interface of chemistry and biology and to undertake collaborative research at the interface of chemistry-biology, including:

- Development of peptide scaffolds. Identification, chemistry and biological applications.

- Development of chemchips for protein inhibitors and aptamers for diagnostics.
- Re-engineering the discontinued drug molecules for use in new appropriate applications. The theme of this project is that finding the alternative suitable and important targets for the drugs that were found to be safe in Phase I & II trials but withdrawn after Phase III due to side effects.
- Nanomaterials for biology: structure-function studies New biomolecule - synthetic molecule nano composites will be looked into for potential applications in targeted delivery of therapeutics.

Screening and utilization of biocatalysts for the useful transformation to produce biologically important molecules or to produce chiral intermediates

The diversity of microorganisms and their catalysts is immense. The recognition of biocatalysts as important manufacturing tool has increased within chemical and pharmaceutical industries in recent years due to shortage/limited source of petroleum products. Biocatalysts can simplify, or in some instances even enable the production process of the complex chemicals and drug intermediates with highly stereo- and regio-specific manner. Exploration of biocatalysts (Microbes as well as isolated enzymes) in carrying out transformations of natural products has been an important and fascinating method in the synthetic organic chemistry. Biocatalysts offer the opportunity to effect selective transformations - a feature of great utility in organic syntheses, that otherwise would be difficult to carry out by conventional methods. With their unerring stereoselectivity, regioselectivity, and high catalytic efficiency, nature's catalysts (microbes or enzymes) have been a stimulus and counterpoint. Biocatalysts are capable of accepting a wide array of complex molecules as substrates, and exquisitely selective, catalyzing reactions with unparalleled chiral and positional selectivities. As a result, biocatalysts can be used in both simple and

complex transformations without the need for the tedious blocking and deblocking steps that are common in enantio- and regioselective organic synthesis. Such high selectivity also affords efficient reactions with few by-products, thereby making microorganisms/enzymes an environmentally friendly alternative to conventional chemical catalysts.

In the proposed project the microorganisms (isolated as well as from culture collections) will be screened for efficient and useful transformation with oxido-reductase in particular cytochrome P450 system and nitrile hydrolases such as nitrilase and nitrile hydratase activities. Efforts will be made towards the isolation and biochemical characterization of microorganisms which can efficiently convert the nitriles into corresponding primary amines.

We have screened biocatalysts for the oxido-reductase and nitrilase activities. We have found several microorganisms were able to carryout efficient hydroxylation and reduction of nitrile group. Work is progressing towards the characterization of metabolites and standardization of process.

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#### Selected publication:

- ✦ Protein J., 2008, 27, 7

## NCL - IGIB

Re-engineering discontinued drug molecules for use in novel applications and understanding drug toxicity by proteomic approaches



During drug development programs, several lead molecules, after optimization, are taken to the stage of development where they are rigorously studied for pharmacokinetic properties. This gives vital information on drug bio-distribution, rates and sites of distribution etc. Molecules satisfying the desired conditions are evaluated simultaneously for their toxicity effects in cell and animal models. After a strenuous and systematic evaluation of drug activity and other properties, several winning candidates may have to be dropped for their unsatisfactory performance in toxicity studies. When toxicity is unacceptable at the levels of administered dosage, the molecules are not carried forward for further studies in spite of their good activity, bio-distribution and PKD properties. This results in a great loss of time and resources on molecules, which are good drugs, but cannot be pursued further. In many other cases, the toxicity effects are seen long after the drugs have been approved and are in use, forcing the regulatory agencies to withdraw the drug from market. For example, Pfizer's Viagra and Rogaine both originally failed as antihypertensives, but patients in clinical trials reported side effects that signaled the drug's potential in other indications.

Lilly's cancer drug Gemzar was first developed as an antiviral. And thalidomide, a sleep aid that was never approved in the U.S. because it was found to cause serious birth defects, is now on the market to treat leprosy and could gain approval later this year as a treatment for multiple myeloma, a type of blood cancer. The main aim of this proposal is to revisit such important cases and reorient their structure or biological activity for a different application of their structural scaffold and reduce toxicity effects. The project on re-engineering discontinued drug molecules, if successful, would introduce a new dimension for the present drug discovery paradigm. It takes care of all the existing causes for drug failure to build new concepts in drug discovery and resuscitate the presently discarded drug molecules on safer grounds. The concept itself has IPR value in addition to the fall outs which may introduce existing molecules and their analogues for new activities. It will also considerably bring down the cost of new drug discovery process.

#### Broad objectives

- To identify novel uses for drugs
- To understand the molecular mechanism of drug toxicity by proteomic approaches

#### Approaches to accomplish the above objectives

- Chemical proteomic approach to identify drug binding proteins
- Disease specific screening of drugs

#### Understanding the molecular mechanism of gatifloxacin toxicity by proteomic approach

Gatifloxacin is an antibiotic of the fourth-generation fluoroquinolone family, inhibits the bacterial enzymes DNA gyrase and topoisomerase IV. The drug was withdrawn in 2006 because of its life threatening side effects and also causes acute hypoglycemia and chronic hyperglycemia. Our study aims to identify the molecular mechanism by which it causes acute hypoglycemia and chronic hyperglycemia. Proteomic studies involving two dimensional electrophoresis and mass spectrometry suggest that gatifloxacin affects the glucose metabolism. Perhaps, this could be way by which it causes deregulation of glucose levels in human beings.

#### Discovery of rifampicin as a novel antiglycating molecules using insulin glycation assay

Non-enzymatic glycation is a complex series of reactions between reducing sugars and amino groups of proteins leading to browning, fluorescence, and cross linking of proteins. Glycation and advanced glycation end products (AGEs) have been implicated in diabetic complications such as nephropathy, neuropathy, retinopathy and atherosclerosis. Inhibiting glycation and AGE accumulation has been considered to be one of the intervention strategy to prevent glycation mediated diabetic complications. Known glycation inhibitors such as aminoguanidine, N-phenacyl thiazolium bromide etc are not yet FDA approved and show severe side effects. FDA approved drugs such as metformin, aspirin, diclofenac show antiglycating activity, however they are not very efficient inhibitors of glycation. Therefore, it is important to find new molecules with better antiglycation activity. Here we report a MALDI-TOF-MS based insulin glycation assay for screening molecules that inhibit the glycation reaction. In this assay insulin and glucose were allowed to react in vitro leading to formation of glycated insulin. Glycation inhibition of insulin is monitored in presence or absence of glycation inhibitor using MALDI-TOF-MS.

In this study, we describe a high throughput MALDI-TOF-MS based in vitro insulin



glycation assay for screening glycation inhibitors. The glycation reaction was monitored by measuring the intensity of the glycated insulin peak using MALDI-TOF-MS. The mass of unglycated insulin is 5808 Da (Figure 1A), while the mass of glycated insulin is 5970 Da (Figure 1B). The glycated insulin peaks shows an increase in mass of (162 Da) with a relative intensity ranging from 30-50% compared to unglycated insulin peak. The intensity of glycated peak decreases in presence of aminoguanidine (Figure 1C). This assay was used to screen molecules for antiglycation activity. The antituberculosis drug rifampicin showed higher glycation inhibition than aminoguanidine (Figure 1D). It was observed that rifampicin shows higher antiglycation activity even at concentration as low as 0.5mM when compared to other known antiglycating compounds. The results of MALDI based insulin glycation assay were compared with BSA-glucose fluorescence assay. Further, the  $IC_{50}$  of aminoguanidine and rifampicin was determined by MALDI based insulin glycation assay. The  $IC_{50}$  of aminoguanidine and rifampicin was found to be 11.83 mM (1.31 mg/ml) and 0.12 mM (0.09 mg/ml) respectively, suggesting that rifampicin is strong glycation inhibitor. For the first time, we report that rifampicin has a strong antiglycation activity at a very low concentration. Rifampicin has been shown to inhibit the retinal neovascularization in vitro and in vivo suggesting a role in anti angiogenesis. The anti-angiogenic property of rifampicin could be due to inhibition of glycation. In vivo studies using experimental animal models are necessary to elucidate the exact mechanism of rifampicin mediated glycation inhibition. The finding of an additional therapeutic property of rifampicin as a glycation inhibitor is very significant considering the fact that rifampicin is already FDA approved drug for the treatment of tuberculosis. And therefore, this drug can be repositioned as a potent antiglycating molecule for the treatment of diabetic complications, aging, and Alzheimer's diseases.

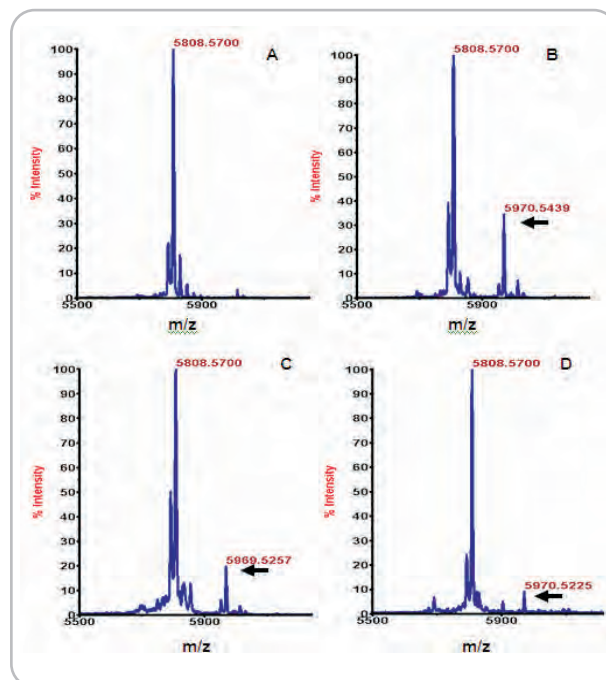


Figure 1. Insulin glycation assay by MALDI-TOF-MS, A control insulin; B, glycated insulin without inhibitor; C, glycated insulin in presence of 10mM aminoguanidine; D, glycated insulin in presence of 1mM rifampicin

## NCL - IGIB



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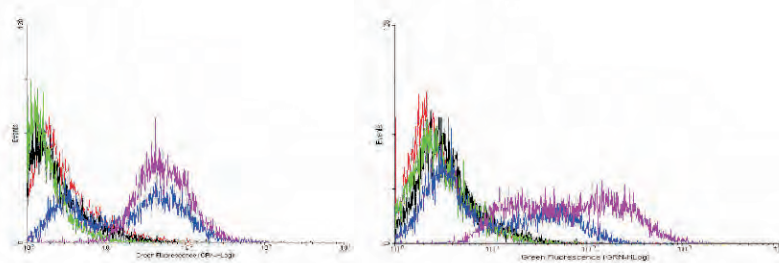
Novel cationic conformationally constrained peptides: Applications in gene delivery

**Background / objectives**

Synthetic oligopeptides are finding large application as delivery systems of biologically relevant cargo. The positively charged oligolysine and oligoarginine peptides have shown their utility to penetrate across the cell membrane. The important hurdle of these cell penetrating peptides as delivery systems is that the cargo gets trapped in the endosomes after uptake and the active material remains unavailable to be biologically relevant. To overcome the obstacle of endosomal-release several synthetic oligopeptides are being developed using strategies such as inclusion of non- $\alpha$ -peptide spacers to separate positive charges. This project is directed towards inducing conformational constraints on the positively charged peptide backbone, thereby structuring them towards better uptake and endosomal release properties. The synthesis of constrained, chiral lysine, arginine and aminohexanoic acid monomers, synthesis of oligomers using these novel amino acids and study of their biological relevance is aimed in this projects.

**Work done and discussion**

The positively charged oligopeptides exhibit cell penetrating properties. This property of natural oligoarginine and oligolysine peptides is further improved by introducing neutral, hydrophobic non- $\alpha$ -amino acids such as aminohexanoic acid. The interaction of such peptides with cell surface is through the array of arrangement of positive charges and flexibility of the backbone. Introducing chirality and constrained flexibility in these backbones will help to attain a peptide conformation with optimum properties for efficient cellular uptake and release from the endosomes. We synthesized several conformationally constrained, chiral analogues of lysine and arginine and hexanoic acid (Figure 1) for relevant constrained oligopeptides were synthesized and characterized. The results of the cell uptake studies that were carried out in IGIB were quite interesting and have given way for the synthesis of several new modified peptides that are currently being studied as delivery agents for nucleic acids.



Peptide 1. CF-(AAEP)<sub>7</sub>-NH<sub>2</sub>

Peptide 3. CF-(Aaep)<sub>7</sub>-NH<sub>2</sub>

Peptide 5. CF-(AAEP<sup>9</sup>)<sub>7</sub>-NH<sub>2</sub>

Peptide 7. CF-(Aaep<sup>9</sup>)<sub>7</sub>-NH<sub>2</sub>

Peptide 9. CF-Arg<sub>7</sub>-NH<sub>2</sub>

Peptide 2. CF-(AAEP-Ahx)<sub>6</sub>-AAEP-NH<sub>2</sub>

Peptide 4. CF-(Aaep-Ahx)<sub>6</sub>-Aaep-NH<sub>2</sub>

Peptide 6. CF-(AAEP<sup>9</sup>-Ahx)<sub>6</sub>-AAEP<sup>9</sup>-NH<sub>2</sub>

Peptide 8. CF-(Aaep<sup>9</sup>-Ahx)<sub>6</sub>-Aaep<sup>9</sup>-NH<sub>2</sub>

Peptide 10. CF-(Arg-Ahx)<sub>6</sub>-Arg-NH<sub>2</sub>

Figure 1: The synthesis of peptides with non-natural amino acids and their cell uptake studied by fluorescence techniques

## NCL - IGCAR



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NCL-IGCAR Joint Research Programs in Chemical and Engineering Sciences

NCL has joined with IGCAR Kalpakkam to offer its competencies in chemistry and chemical engineering sciences by undertaking research programmes in the areas of Chemistry, Chemical Engineering and Material Sciences, relevant to the fast breeder reactor (FBR) programme. The efforts are expected to provide basic science understanding to the complex technology challenges associated with the DAE's FBR programme.

IGCAR is a premier research institution of Department of Atomic Energy (DAE), with broad-based multidisciplinary competencies in the science, technology and advanced engineering directed towards the development of technologies for FBR with associated Fuel Cycle (FR&FC). NCL will bring its competencies in the areas of computational science, polymer science, thermodynamics, organic chemical process design and engineering, as well as chemical engineering and separation science to bear on problems of relevance to IGCAR's efforts in the area of FBR technology.

One of the key focuses of the joint programme is to train high quality PhDs and post-doctoral students at NCL on such joint research problems linked to the nations' programme on FR&FC. The students will have an opportunity to work at IGCAR labs for extended periods on joint research programmes, thus, enriching their learning experience. This effort will contribute to development of human capital that will address some of the S&T challenges associated with critical technology needs of the nation. Research projects based upon this collaboration will serve as valuable input to FR & FC programme running at IGCAR, Kalpakkam. Key research problems proposed to be addressed relate to design and synthesis of solvents and resins, large-scale production of solvents for separation of actinides and lanthanides, ab initio design of extractant system, modeling-directed synthesis of ionic liquids, ion exchange separation, thermodynamics and CFD modeling.

### Non-ideal behaviour of aqueous ionic species in nuclear solvent extraction systems

The project aims at establishing comprehensive modeling ability for non-ideal aqueous ionic systems of high ionic strength, which is an integral part of nuclear solvent extraction. The research work on volumetric properties and related ion-ion interactions would be beneficial for putting a thermodynamic basis of the density equation of state for electrolytic solutes as well as of calculation of important parameters like osmotic coefficients, which could be utilized in the estimation of thermodynamic activities

of the ions of the interest. In this work, the basic data, generated at Reprocessing Research and Development Division (RR&DD) of IGCAR for the identified solutes, were used for modeling of thermodynamic parameters like ion-ion interactions, osmotic coefficient and possibly the solvent and solute activities. The developed model and related information are valuable addition to the existing knowledge base available at RR&DD for modeling and simulation of nuclear solvent extraction.



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CFD modeling of primary controller and vortex diode

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#### Collaborator:

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Indira Gandhi Center for Atomic Research (IGCAR) had experimentally studied the performance of a few fluidic devices that are used in the nuclear waste processing plants. A capability of making 'a priori' predictions of performance will be very useful for interpreting the experimental data, for selecting appropriate sizes and for steering designs to more promising configurations. The present project aims at developing design guidelines for two important fluidic devices used in the nuclear waste processing plants. These devices are primary controller and the vortex diode. In both the devices, i.e., a primary controller and a vortex diode, CFD models provide wealth of information about the relevant fluid dynamics. Some of the insights gained via analyzing the predicted results are discussed and recommendations leading to design guidelines are submitted to IGCAR. The ideas explored to achieve enhancement in diodicity will be experimentally verified. Following are the major accomplishments of the project.

#### Primary controller

Primary controller is used to control the air flow rate and thereby operate the fluid suction and delivery of the fluids from one storage unit to another in the radiation zone. CFD simulations of primary controller were shown to predict the experimental data from

IGCAR for throat diameters and diverging angle with good agreement. The marginal variation can be due to the small variations in the experimental data. The pressure profiles along the axis of the geometry showed the choking effect to occur in the throat region and the extent of choking was seen to increase with inlet pressure. The pressure recovery was seen to decrease with increasing inlet pressure values for given geometry. Thus, the required pressure recovery can be achieved with specific geometrical design parameters. The information from all the simulations of the primary controller was assimilated and compared in terms of the % leakage through the radial port.

The % leakage and the extent of pressure recovery are inter related and are largely governed by the design of the throat and the diffuser sections. The effect of various design parameters (Diffuser area ratio, Diffuser angle, Inlet Pressure and the recovery pressure, Throat diameter, Length of diffuser, Radius of curvature on the converging as well as diverging sections of throat, Radius of curvature on the converging sections of throat, etc.) on the performance of the primary controller unit was studied and the observations have been analyzed to get the design guidelines. Design recommendations are submitted to IGCAR for further experimental validation.

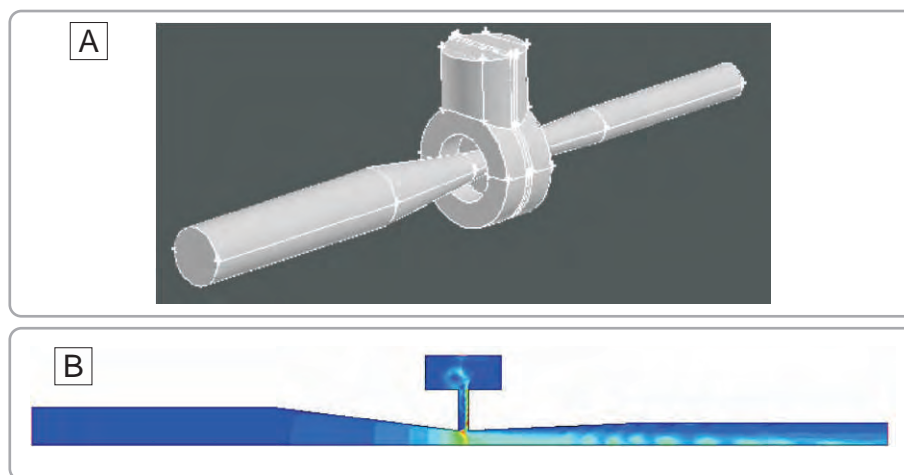


Figure 1: A) Geometry of primary controller given from IGCAR, (B) Contour plot of Mach number in the primary controller ( $D_n = 6$  mm,  $\theta = 7$ ) at inlet pressure value of 3.4 Gauge Pressure (kg/cm<sup>2</sup>). (Blue: Ma = 0, Red: Ma = 2.03)

#### Vortex diode

Vortex diodes are used as leaky non-return valves in many applications, especially in nuclear industry. As a part of the first project on the design and development of vortex diodes that can deliver high diodicity performance, IGCAR had experimentally

studied performance of vortex diodes over a wide range of sizes. In the previous project, NCL team had shown the capability and usefulness of the CFD based models to predict the diode performance accurately. Considering that as the basis and with the knowledge developed from that work, it was



proposed to develop new designs for the vortex diode that would yield higher diodicity than the designs used so far. The new designs and their enhanced performance will help to use these devices with confidence. CFD simulations of vortex diodes were carried out. Based on the systematic numerical experiments that were carried out in the first phase of this project to understand influence of numerical issues and turbulence models, here we simulated the diode with internal design modifications. The results from the developed designs were compared with the experimental data provided by IGCAR (for 150 mm diode). Some experiments were also carried out at NCL to obtain possible error bars on experimental data (for 150

mm diode). This report discusses these results. The flow pattern inside the diode was obtained experimentally by measuring the instantaneous velocity profiles in the diode using an Ultrasound Velocity Profiler. The details on the methodology to analyze the data is reported in the literature with a few representative results. More analysis on the transient variation of diodicity for different flow rates during an operation will be studied in detail as the diodicity when analyzed dynamically was seen to change continuously over a range. Fourier analysis of such data has been seen to yield the information about the prominent features in the vortex dynamics.

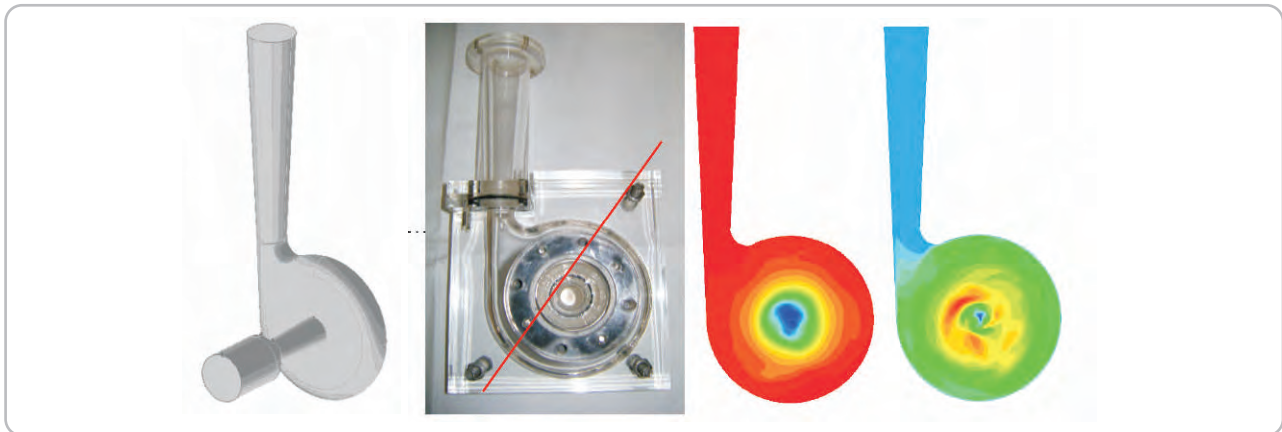


Figure 2: (Left to right) Isometric view of a vortex diode, photograph of diode, contours of static pressure and tangential velocity for the reverse flow entry at  $Q = 2600\text{L/hr}$ ,  $\phi = 150\text{ mm}$



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NCL - IGCAR

Development of high temperature proton conducting solid polymer electrolyte based hydrogen sensor



**Objectives**

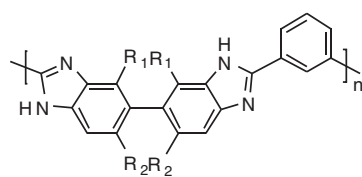
To explore in identifying and developing new routes for synthesizing novel substituted monomers for synthesis of polymers such as modified polybenzimidazoles, polyimides and polytriazoles, whose polymeric films are used for hydrogen sensing in nuclear reactor applications.

**Work done**

In this project, our initial role involves the synthesis of new monomers of modified benzimidazoles and triazoles. Subsequently, modified polymers were subjected to polymerization to get the respective PBI and polytriazoles. Several, polymeric membranes were cast into films from these polymers (PBI, PT) and supplied them to IGCAR for evaluation studies for proton conductivity measurements.

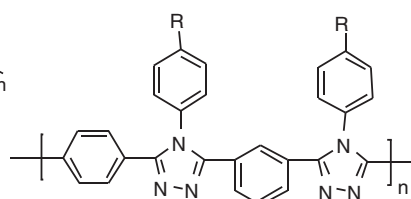
**Future work plan**

- We propose to make polymeric films with modified polybenzimidazole using 5-sulfo-1,3-isophthalic acid (modified PBI) and supply the same to IGCAR for conductivity measurement.
- Preparation of 1,2,3-polytriazole (PT) is to be further studied in detail so as to get higher viscous polymer. We also propose to synthesize polytriazole from 1,2,4-triazole monomer.



$R_1 = R_2 = CH_3$   
 $R_1 = R_2 = H$

Polybenzimidazole (PBI)



$R = H, CH_3$

Polytriazoles (PT)



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## Functional organic materials for energy efficient devices

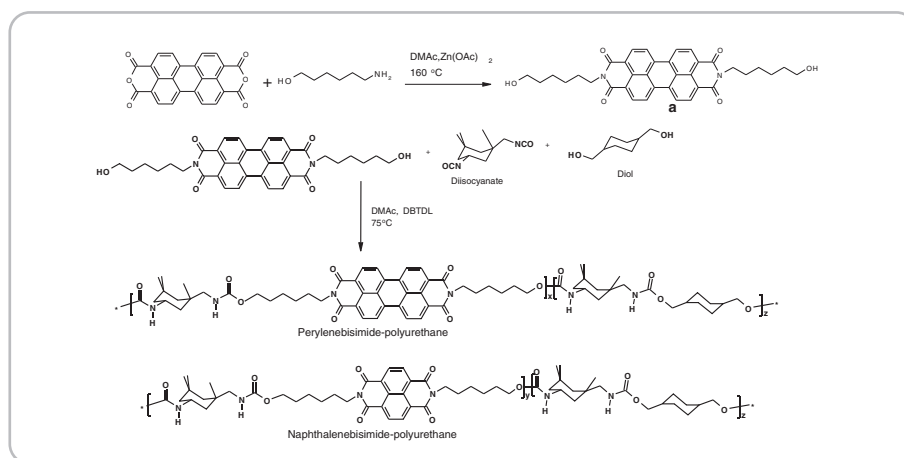
### Background / objectives

Aromatic polyimides are a class of high-performance polymers that have gained considerable attention in microelectronics, aerospace and photoelectronics because of their excellent thermal stability, mechanical strength and electrical property. For many applications of these polymers, processability and film formation is a prerequisite. Polyimides having perylene and naphthalene moieties in the main chain are an important class of polymers due to their favourable

photochemical behaviour, excellent thermal and photo stabilities, electron acceptor and photo-conductive properties and application as laser dyes.

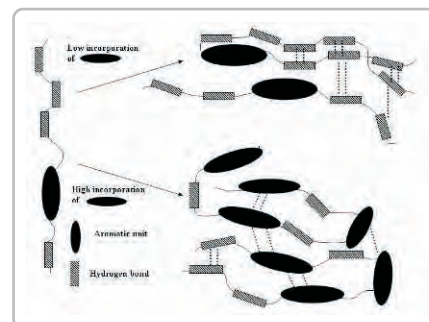
### Work done and discussion

A series of perylene and naphthalene diimide containing random copolyurethanes with different ratios of perylene/naphthalene diimide content was synthesized and characterized.



Scheme -1. Structure of perylene and naphthalene bisimide based copolymers

Copolymerization improved the solubility of these rigid aromatic diimides and the copolymers were soluble in common organic solvents such as chloroform, tetrahydrofuran etc. The absorption spectra of perylene based copolymers showed a red shifted peak at a wavelength of 557 nm corresponding to J-type aggregates. For naphthalene copolymers, the quenching of fluorescence at higher naphthalene incorporation suggested the presence of aggregates due to extensive  $\pi$ - $\pi$  stacking of the aromatic core. FTIR spectroscopic analysis showed that the hydrogen bonding tendency of the polymer decreased with increase in perylene/naphthalene incorporation. The fluorescence spectra of the naphthalene polymers at higher naphthalene incorporation showed a red shifted excimer such as emission peak which was assigned as static excimers based on their excitation spectra. These polymers could exhibit two types of secondary interaction modes, namely, hydrogen bonding (via urethane linkage) and  $\pi$ -stacking (via aromatic perylene or naphthalene units) thus highlighting the importance of polymer design in inducing self-organization at both low and high incorporation of the rigid bisimide moieties.



Scheme-2 Schematic representation of mode of self-organization at low and high incorporation of the rigid aromatic moieties. The copolymer undergoes self-organization via hydrogen bonding interactions of the urethane linkage at low aromatic diimide incorporation and via  $\pi$ - $\pi$ stacking interactions at high diimide incorporation.

### Selected publication:

✱ *J. Polym. Sci. Polym. Chem.*, 2009, 47, 1224



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Development of transgenic crop plants for resistance to insect pests (NWP0003)

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### Background

One of the plants natural defense mechanism relies on causing indigestion in the infesting insects and thus disrupts the nutrient acquisition system in insects. Plant proteinaceous proteinase inhibitors (PIs) are the best example of this type of post-ingestive defense. Wound-inducible Pin-II PIs belonging to serine PI family are of interest because of their large structural and functional diversity mostly in solanaceous plants. In our previous studies we observed that diverse Pin-II PIs from *Capsicum annuum* differentially influence *H. armigera* growth and development. CanPI-7 with more number of IRDs and higher diversity in IRDs was found to show anti-metabolic effect on *H. armigera*. Furthermore, *C. annuum* upon *S. litura* and aphid attack shows strong upregulation of multiple IRD PIs. Different tissues of *C. annuum* have characteristic CanPI expression pattern. For example, in leaves-predominance of 2-IRD, in fruits 3-, 4-IRD and in stem 1- and 2-IRD CanPIs. The plant defense and endogenous significance of CanPI diversity still remains poorly understood. Using proteomics tool, here we attempt to address the question how and to what extent can insect tackle presence of PIs in its diet? We selected different CanPI

genes with 1- to 4-IRD and characterized recombinant PI proteins with specific reference to their (i) processing by *H. armigera* gut proteinases (HGP) (ii) stability in proteolytic environment (iii) inhibitory activity against proteinases and HGP.

Six CanPI genes were selected for functional characterization on the basis of sequence variation, specificity and number of IRDs. Using, intensity fading MALDI mass spectrometry assays (IF-MALDI-TOF), enzyme assays and PI-activity gels interaction of rCanPIs with *H. armigera* gut proteinase were performed. The results provide an insight in to the fate of these PIs in the insect midgut. Since all these studies are based on product of particular PI gene(s), it leads to identification of potential PI(s) or IRD(s) effective against constitutive and induced gut proteinases.

### Results and discussion

Six representative *C. annuum* genes (CanPI-13, -15, -19, -22, -5 and -7) comprising one, two, three or four Inhibitory repeat domains (IRDs), displaying highest amino acid divergence were selected for cloning and recombinant protein expression in *Pichia pastoris* (Figure 1).

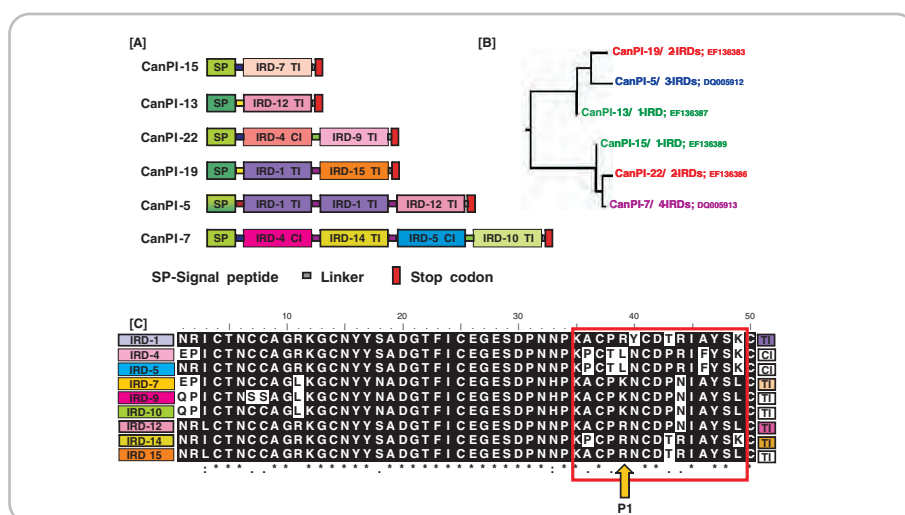


Figure 1: (A) Diagrammatic representation highlighting the gene structure of four types of CanPIs found in *C. annuum*, with their signal peptide sequence (SP), various IRD(s), linker region(s) and the stop codon. The signal peptide, IRDs and linker regions varying in the aa sequence are shown in different colors and indicate their positions. (B) Neighbor-joining tree of CanPIs based on deduced aa sequences of full length genes, number of IRDs and the accession number. (C) Multiple sequence alignment of deduced aa sequences of unique IRDs from the CanPIs selected for the present study. The IRD numbers are according to earlier report (Tamhane et al., 2009). The inhibitory active site in the particular IRD is referred to as TI for trypsin and CI for chymotrypsin inhibition. The reactive site residue P1 is marked by an arrow and the region close to the active site showing major variation is marked by a box.

### Selected publications:

- ✦ *Gene*, 2007, 403, 29; 2009, 442, 88

Electrophoretic visualization and MALDI-TOF-MS of recombinant CanPIs revealed the presence of multiple processed repeats

in the native purified CanPI proteins during *P. pastoris* expression (Figure 2). Recombinant CanPIs inhibited 90% of



Development of transgenic crop plants for resistance to insect pests (NWP0003)

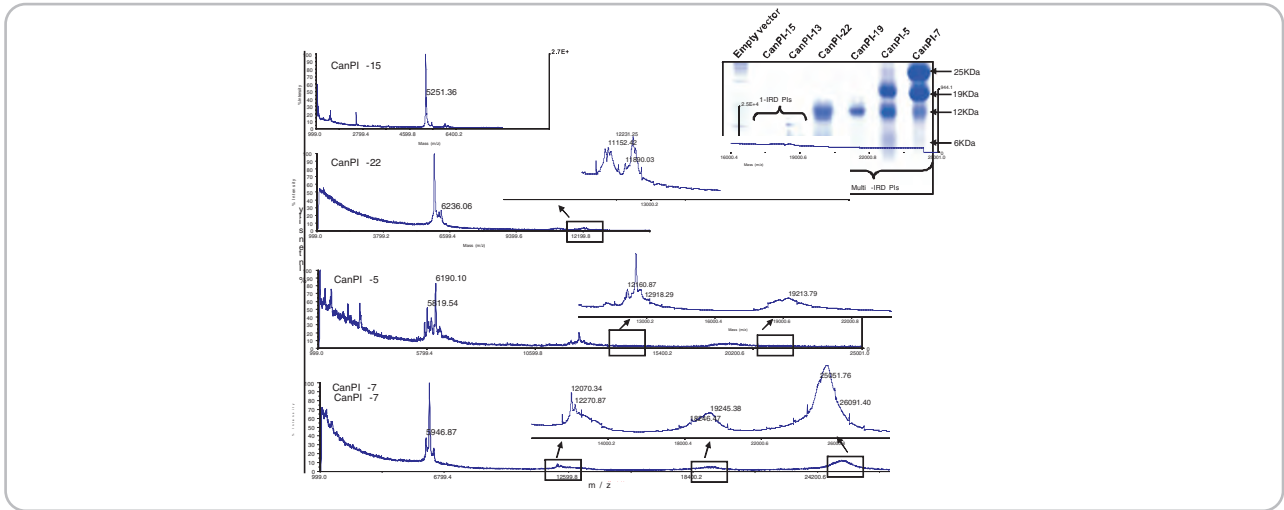


Figure 2: Characterization of rCanPIs having either 1- to 4-IRDs each by SDS-PAGE and MALDI-TOF. Proteins stained with Coomassie Blue and mass peaks of 25KDa (4-IRDs), 19KDa (3-IRDs), 12kDa (2-IRDs) and 6KDa (1-IRD) were detected depending on the number of IRDs present in the rCanPIs. The proteins of increasingly higher molecular weights appear as low intensity peaks in the mass spectras because of the drop-off of the detection efficiency with increasing mass. These peaks are shown in enlarged scale in the insets.

bovine trypsin (TI), varying chymotrypsin inhibition depending on number of CI domains and 60% of total gut proteinase activity of *Helicoverpa armigera* (HGP), besides CanPI-15 which exceptionally showed very low efficiency against all of them. Intensity fading (IF) MALDI MS was used to study the rCanPI-HGP interaction (Figure 3). Processing of multi-IRD forms of rCanPIs in to the active IRD form (6kda) by the action of HGP at the protease sensitive linker regions was suggested by major

variations in the relative intensities of the peaks with time in the MALDI analysis. By in vitro studies, rCanPI-5 and rCanPI-7 showing inhibition of maximum HGP isoforms, were found to be more stable in presence of HGP as compared to other CanPIs.

The in vivo studies, proved the overall reduction in gut proteinase activity and also confirmed the stability of rCanPIs with varied specificity, in presence of proteolytic environment of insect gut (Figure 4).

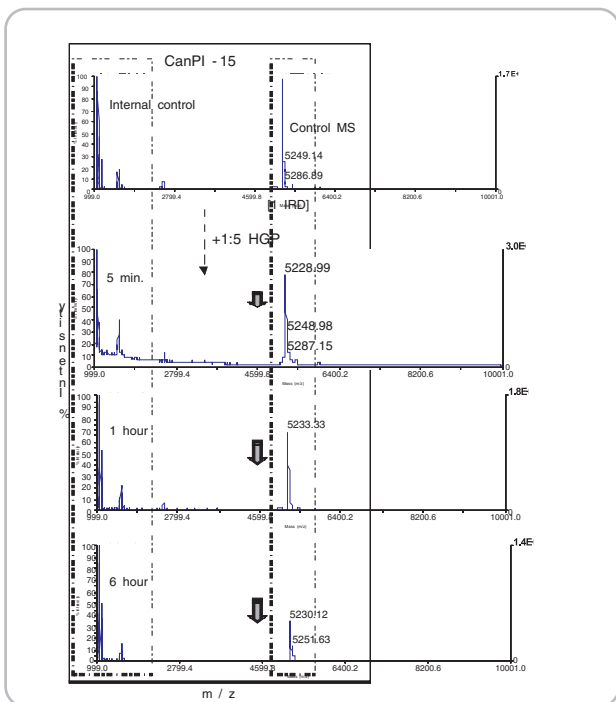


Figure 3: Intensity fading MALDI analysis of rCanPI-15. The decrease in the relative intensity of rCanPI-15 (6KDa) upon addition of target protease, HGP was evident. The internal control (1062 Da) has been used as reference for relative quantification.

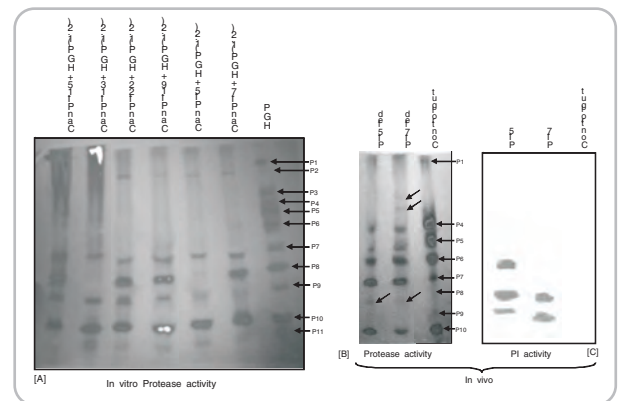


Figure 4: Stability of CanPIs to *H. armigera* gut proteinases. (A) In vitro: Comparative inhibition of HGP isoforms by different rCanPIs. Equal HGPI units of CanPI-15, -13, -22, -19, -5 and -7 were incubated with HGP for 30 min at 24°C. The above reaction mixtures were then resolved on 8% native PAGE. The gels were processed for proteinase activity visualization by GXCT. rCanPI-7 and -5 show inhibition of maximum HGP isoforms. (B) In vivo: Inhibition of HGP isoforms by rCanPIs. Equal amounts of tissues of guts of *H. armigera* fed on rCanPI-5 and -7 containing artificial diet and those fed on control diets were extracted in 1:1 (weight: volume) in 0.2 M Gly-NaOH pH 10.0 buffer. Equal volumes of these gut extracts were resolved on 8% native PAGE. The gel was processed for proteinase activity visualization. CanPI-7 fed *H. armigera* gut extract shows an overall reduced proteinase activity as compared to the controls. Appearance of inhibitor insensitive isoforms is evident from this analysis. (C) In vivo: Stability of rCanPIs in *H. armigera* gut. The rCanPI-5 and -7 fed *H. armigera* gut extracts were analyzed for TI activity visualization by GXCT after deactivation of the proteinases by heat treatment at 70°C for 15 min. TI activity proteins of both CanPI-5 and -7 could be detected in this extracts indicating their in vivo stability even in the gut extract after several days.



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Discovery and pre-clinical studies of new bio-active molecules and traditional preparations

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Novel secondary metabolites isolated from biomaterials viz. plants, bacteria, marine organisms etc. can be used as lead molecules for the development of new drugs, pest control agents etc. New techniques in the field of chromatography, spectroscopy and bioassay have made it possible to identify complex molecules which are available even in small concentrations. Wide range of biomaterials in one of the biodiversity hotspots (Western Ghats), which are available for exploration, is an added advantage for identification of new/novel bioactive lead molecules. Chemical analysis of traditional medicinal plants, can lead to the development of standard herbal / traditional drugs for the treatment of different diseases. Botanical pest control agents can be developed for the control of economically important agricultural pests and vectors which can address problems like pesticidal residue, toxicity to non-target organisms and overall ecosystem protection.

### Development and commercialization of bioactive molecules from plant sources

Under the programme for development and commercialization of bioactive substances from plant sources, extracts prepared from plants collected from Western Ghats, have been evaluated for different biological activities such as anti-malaria, anti-filarial,

anti-bacterial, anti-fungal, against kala azar, tuberculosis, hypertension, diabetes, ulcer, neurological disorders, cancer, immunomodulation and insect control activities against leaf eating caterpillars, fruit borers, mites, termites and stored-grain insects. These studies have yielded lead extracts active as antifungal, anti-malarial, tuberculostatic, anti-dementia and anti-psychotic. Further work on the identification of lead molecules from these extracts and also development of herbal drugs is currently being actively pursued.

### Development of botanical pesticides

One of leads has been found to exhibit control of stored grain pests *Rhizopertha dominica* (lesser grain borer) and *Sitophilus oryzae* (rice weevil). This lead has been processed further for the development of a product. Developed product (NCL0049) has shown control of both *R. dominica* and *S. oryzae* for more than 100 days. This product has been formulated as 5% dust (5D) and is now being evaluated as seed protectant under field conditions at National Seed Corporation (NSC), New Delhi. The field trial with NCL0049 has been initiated with ~750kg seeds. Further larger, multi-centered field trials have been planned.

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Biotransformation of pharmaceutically important compounds using recombinant glycosyl-transferases

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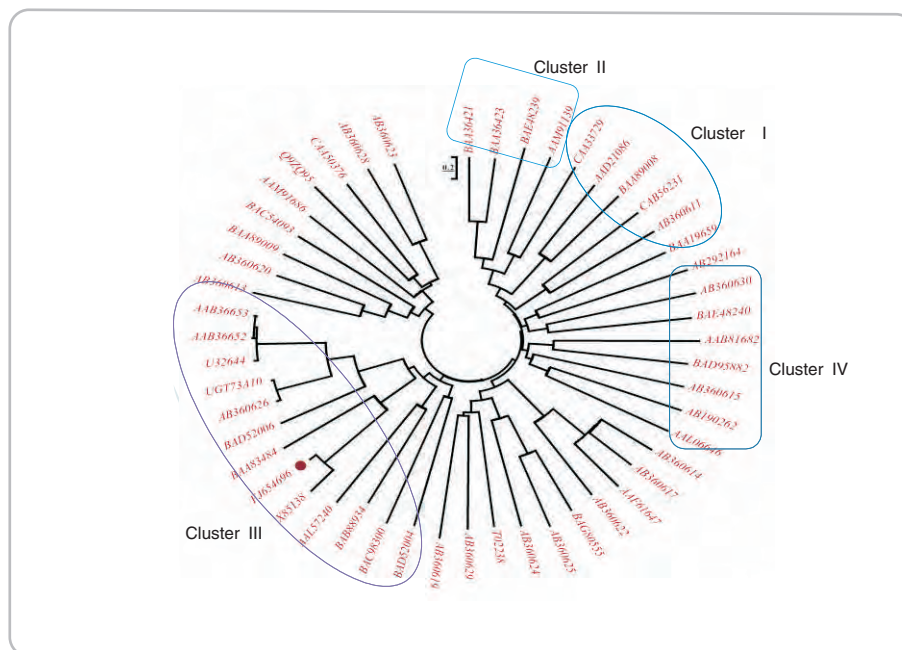
Biotransformation capability of plants has been far little explored so far, as the field of biotransformation has been solely dominated by microbial strains in nativity or their randomly mutated strains. The present state of art in biotechnology has removed barriers of species and allows heterologous expression of selected and characterized catalytic trait in the hosts of choice. Thus, it opens the field of knowledge based 'hybrid biotransformation system' combining novel biocatalytic characteristics of plants and its *in vivo* functionality in suitable microbial or cell culture host. Glycosylation is often the last step in the biosynthesis of natural products in plants and is responsible for improving solubility, bioavailability and efficacy of compounds. In this programme our main aim is to isolate, clone and characterize various GTs from medicinal plants. Heterologous expression of GTs and use them for regiospecific biotransformation of pharmaceutically important compounds.

We have isolated full length GT genes (cDNA) from *Withania somnifera* (4 genes) and *Bacopa monniera* (2 genes). These genes have been expressed in heterologous system (*E. coli*), recombinant enzymes have been purified and being characterized for substrate specificities. One of the GT

from *Withania* has shown activity towards some of the important flavonoids: kaempferol, naringenin, isorhamnetin, apigenin, hesperetin, luteolin, genistein, 3-hydroxy flavone and daidzein. This GT can produce 7-O and 3-O glycosylated compounds. These GTs and some more GTs will be used for regiospecific glycosylation of pharmaceutically important compounds.

These cluster I, II, III, are characterized by flavonoids glycosyltransferases

- Cluster I: Flavonoids-3-o-glycosyltransferases (e.g. BAA19659 and AAD 21086 PSPGs)
- Cluster II: Flavonoids-5-o-glycosyltransferases (e.g. T02238 and BAA89009 PSPGs)
- Cluster III: Flavonoids-7-o-glycosyltransferases (e.g. BAA83484 and X85138 PSPGs)
- Cluster III also contains the glycosyltransferases that are capable of glycosylation at 4' position of flavonoids.
- Cluster IV contains PSPGs that catalyze glucosyl transfer to sugar moieties of anthocyanin glycosides



Phylogenetic tree for withania GT



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Metabolic pathway engineering for production of high-value pharmaceuticals

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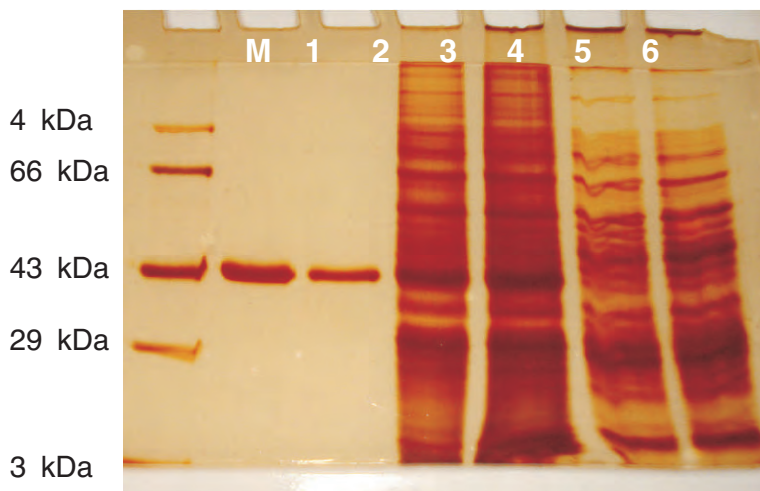
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The high value compounds, artemisinin, withanolides and bacosides are isolated from *Artemisia annua*, *Withania somnifera* and *Bacopa monniera*, respectively. If the genes involved in biosynthesis of artemisinin, withanolides and bacosides can be isolated and expressed in heterologous system such as yeast/bacteria with high biomass, it can be harvested economically. The main objective of this project is isolation, cloning and expression of available pathway genes from *Artemisia annua*, *Withania somnifera* and *Bacopa monniera* in heterologous system and production of pharmaceuticals at an affordable cost.

Full length squalene synthase gene (cDNA clone) from *Withania somnifera* has been isolated using RT-PCR strategy. Nucleotide sequence of the cDNA shows 93% similarity with the squalene synthase reported from *Solanum tuberosum*. The Squalene synthase gene is 1236 bp long encoding a protein of 411 Amino acids. The gene sequence has been submitted to NCBI Gene Bank database with the accession

no. **GU181386**. The full length cDNA has been cloned in pET vector for Heterologous expression of the protein and its characterization.

The full length cDNA clone for the first enzyme of mevalonate pathway, acetyl-CoA C-acetyltransferase from *Bacopa monniera* has been isolated, cloned and sequenced. It shows >95% similarity with *N. tabacum* acetyl-CoA C-acetyltransferase gene at nucleotide level. Sequence has been submitted to NCBI Gene Bank Database with Accession no. **FJ947159**. Heterologous expression was done in *E. coli* and conditions for active protein was optimized (temp.20°C, IPTG Conc. 0.08 mM and 14h duration). Recombinant protein was purified by affinity chromatography using Ni+2-NTA Agarose beads. The activity was confirmed by reverse reaction using Acetoacetyl-CoA as substrate. One of the important genes for mevalonate pathway, HMG-CoA reductase has been also isolated, cloned and sequenced (partial cDNA, 657 bp). Efforts are being made to isolate full length HMG-CoA reductase gene.



Heterologous expression and purification of acetyl-CoA C-acetyltransferase

Lane M- Molecular weight marker  
Lane 1&2-Purified Protein (~44kDa)  
Lane 3&4-Lysate  
Lane 5-Uninduced BL21 with pET Plasmid  
Lane 6-Induced BL21 with pET Plasmid

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Development of hollow fiber membrane technology for water disinfection/purification and waste water reclamation (NWP 0047)



### Objectives

Flat sheet membrane preparation with various additives and their analysis.

### Work done

PAN based UF membranes (17 % dope) were prepared using different additives ( $ZnCl_2$ , CA, TA and MA) in the dope solution. Their effect on crucial membrane properties (water flux, rejection, pore size distribution, SEM, AFM, etc.) was studied.

Water flux and rejection analysis: Water flux of PAN17 membranes containing different additives is shown in Figure 1. For a given membrane, water flux at 1 bar transmembrane pressure by the cross flow mode was higher than that by the dead end mode, as anticipated.

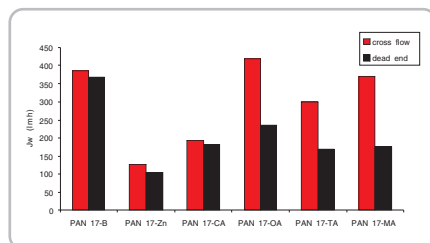


Figure 1. Water flux of membranes with different additives

Table 1. Rejection performance of PAN<sub>17</sub> membranes prepared with different additives

Additive used	R <sub>BSA</sub> (%)	R <sub>ovalbumin</sub> (%)	R <sub>PEG35k</sub> (%)
None	94	75	20
$ZnCl_2$	94	81	17
MA	95	80	20
CA	96	78	19
TA	96	76	21
OA	95	75	22

The highest water flux of the membrane without additive can be attributed to the formation of bigger size pores (supported by its lower bubble point), wherein, control on the pore size is poor. Oxalic acid (OA) based membrane offered highest water flux than membranes prepared with any other acid as an additive. The flux of  $ZnCl_2$  based membrane was lowest. SEM images illustrated more open porosity using OA and CA additive than that with  $ZnCl_2$  as an additive. Rejection performance of these membranes is given in Table 1. All membranes showed > 90% BSA rejection while more than 75% ovalbumin rejection. This depicts that these membrane have molecular weight cut off (MWCO) between 68 - 43 kDa.

### Pore size distribution and AFM analysis

The pore size distribution of PAN17 membranes is given in Figure 2. The mean pore radius of membrane prepared with CA and  $ZnCl_2$  additive was 4.54 and 4.4 nm; while surface porosity was 1.48% and 0.9 % respectively. The AFM image (Figure 3) showed 1.58 nm and 1.14 nm surface roughness for CA and  $ZnCl_2$  additive, respectively.

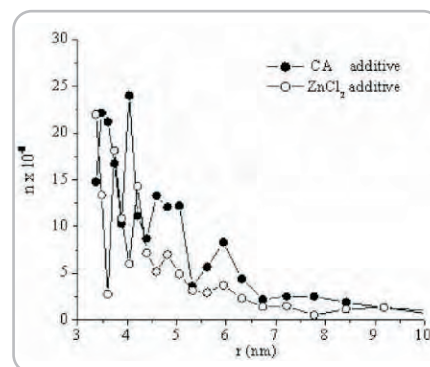


Figure 2. Pore size distribution of PAN17 membranes

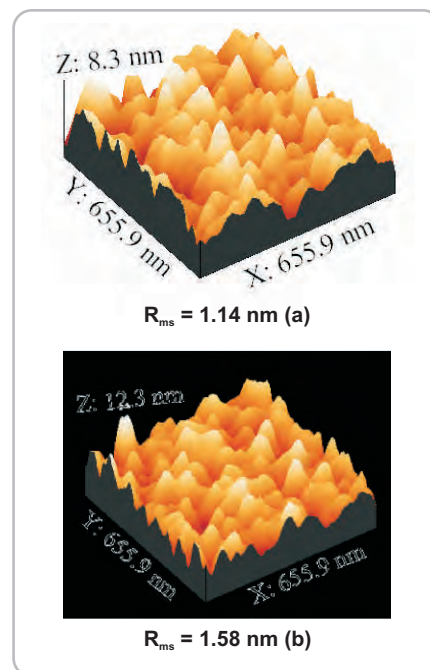


Figure 3. AFM analysis of PAN17 membrane prepared using (a)  $ZnCl_2$  and (b) CA additive in the dope solution





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Identification and characterization of glycated proteins and advanced glycation end products (AGEs) in diabetic complication

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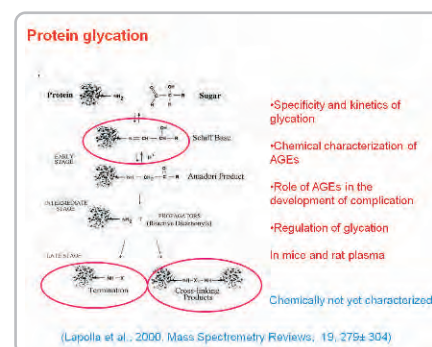
### Background / objectives

Diabetes is characterized by chronic hyperglycemia, if uncontrolled leads to development of microvascular complications like retinopathy, nephropathy, and neuropathy. These complications arise mainly because of a non-enzymatic reaction between glucose and protein called glycation. Glycation triggers a cascade of events leading to formation of advanced glycation end products (AGEs) that results in alteration of protein structure and function of various proteins such as hemoglobin, albumin, IgG, collagen, crystalline, and severe metabolic enzymes. In diabetic patients, the rate of AGE accumulation and extent of protein cross linking is accelerated in plasma due to rise in blood glucose levels. Glycated proteins and AGEs from the plasma are not yet chemically characterized. Identification and characterization of these glycated proteins in vivo is very important to understand the molecular mechanism of glycation mediated development of diabetic complication.

Quantitative and qualitative analysis of glycated proteins and AGEs in the plasma is a technically challenging job. Current advances in proteomics technologies involving protein / peptide separations and mass spectrometry combined with anti body - based methods offer strong prospects of analyzing plasma proteins

### Work done and discussion

- Established protocols for 2DE for separation of plasma proteins
- Standardization of protocol for removal of high abundant proteins is in progress
- Established mice model for studying diabetes and glycation.
- Development of methods to isolate and characterize glycated proteins is in progress
  - Affinity purification- amino phenyl boronate column
  - Using anti-AGE IgGs
  - Autoantibody approach
  - Identified glycated proteins by MALDI-TOF-MS.
- Developed a MALDI based insulin glycation assay to understand the role of albumin in regulating glycation of low abundant proteins.



### Selected publication:

- ✦ *Protein Peptide Lett*, 2008, 15, 663



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## Comparative genomics of non-coding RNA

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### Background / objectives

Majority of the genome is made up of non-coding regions, some in close vicinity and functionally related to protein coding regions, such as the untranslated regions of the mRNA, and others that have apparently no protein products even when they can give rise to RNA transcripts. Conservation in the non-coding region indicates their functional role and recently the widespread regulatory reach of these molecules have come to light following identification of a large number of non-coding RNA molecules which can modulate the expression of protein coding genes. This project aims to explore the functional relevance of these early leads using experimental approaches towards understanding the regulatory potential of these small regulatory RNA molecules.

The main emphasis of the research is to develop strategies for treatment of diseases at the level of genes rather than at the level of proteins. This novel approach, known as antisense therapeutics, uses oligonucleotide analogues (DNA/RNA) as drugs and is applicable to fearsome diseases of viral, genetic or cancerous origins where small molecular therapies remain ineffective. Our work addresses the most important challenges concerning the practical applications of oligomers in this research area such as specific and strong RNA recognition, intracellular stability, cell-delivery, ease of synthesis and safety.

We chose to replace the sugar-phosphate backbone in DNA by electrically neutral, non-canonical peptide backbone as in the case of peptide nucleic acids (PNA). The oligomers with 5-atom thioacetamido backbone replacing 4-atom phosphate linkages in mixed DNA-TANA were found to pair stably with RNA and also were found to have ability to discriminate between DNA and RNA targets.

### Work done and discussion

Application of TANA modified oligonucleotides synthesized at NCL for the relevant miRNA detection of is undertaken at IGIB. The replacement of a dimer block at 3'-terminal region of the 14-mer sequence was undertaken which was further used at IGIB as a PCR primer. The results indicated that the modification is well received by the polymerase enzyme and shows as a good activity as modified single LNA primer. Further work is currently undergoing in NCL to improve the efficacy of the modification. The iso-TANA derivatives were thus synthesized but this proved to be less efficient than the TANA derived oligomers as studied by UV spectroscopy.

Several TANA modified oligomers were synthesized to carry out detailed biophysical work at IGIB.

### Selected publications:

- ✦ *Nucleic Acids Symposium Series* 2008, 52, 145
- ✦ *J. Phys. Chem. B*, 2009, 113, 2944



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## Studies on metal tolerance in plants

The objectives of the project are: Identification, characterization and development of plants useful for eco-restoration, and clean-up of contaminated sites and generate useful products.

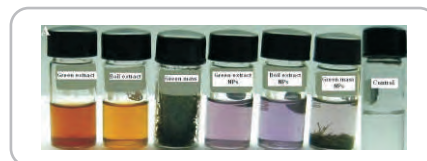
Preliminary assessment of protein profile of metal induced stress in peanuts seedling showed more expression of 20Kd and 100Kd proteins as compared to the control tissues. The difference in the intensities of the electrograph bands in 50 $\mu$ M and 200 $\mu$ M concentration of Cd and Cu indicate that they are more toxic to peanuts as compared to Cr.

Determination of metal tolerance in *Jatropha* and their suitability for different metal contaminated sites using techniques such as tissue culture, atomic absorption spectroscopy, and protein analysis.

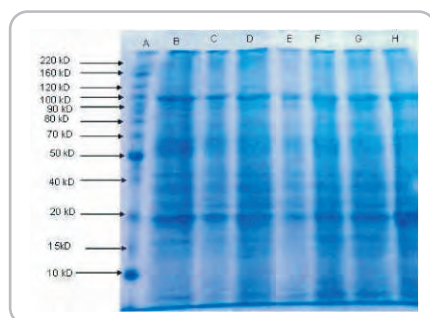
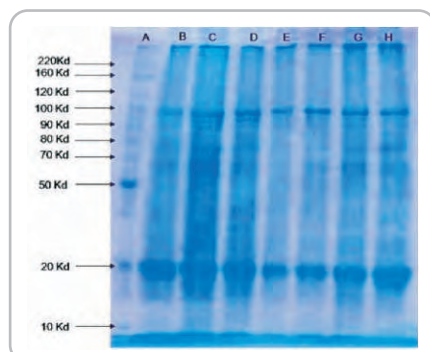
Gold nanoparticle (NP) formation by *Semecarpus anacardium* leaves using boiled extract, green extract and green

biomass. Formation of NPs was more in green extract. Characterization of NPs was carried out by TEM, ESEM, FTIR, XRD and EDAX.

Biosynthesis of intra and extra cellular nanomaterials by peanut seedlings and characterization of NPs by using TEM, HRTEM, ESEM, FTIR, XRD and EDAX is in progress.



Appearances of the green extract, boiled extract and green mass used for reduction of  $10^{-4}$  M  $\text{HAuCl}_4$  and the change in colour after the reaction and formation of gold NPs. No change in colour in control with  $10^{-4}$   $\text{HAuCl}_4$ .



Electrograph of SDS-PAGE of total proteins in root (on Left) and stem (on right) of Peanut seedling. Protein ladder (A), Control (B) and treatments with 50 $\mu$ M Cd (C), 200 $\mu$ M Cd (D), 50 $\mu$ M Cr (E), 200 $\mu$ M Cr (F), 50 $\mu$ M Cu (G), 200 $\mu$ M Cu (H), after 4 weeks of incubation

### Selected publication:

- × *Bioremed. Biodiversity Bioavailability*, 2009, 3 (1), 43

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Conducting polymer paints and coatings for corrosion protection and shielding of concrete structures in strategic areas



**Background / objectives**

Development of radar absorbing material is of utmost importance and related to national security. In the defence sector, radars are largely used for target visualization and detection. Radars send out microwaves and detect the reflected radiation. If we develop ways to make the fighter flights and naval ships detection or visualization difficult that would be beneficial to our national security. Towards this goal, several techniques were developed that provide a reduction of the radio frequency that returns from the target to the radar. One of the methods is to modify the aerodynamic shape of the target. Although, this is well developed, the process is very expensive. Developing a radar absorbing coating would be cost efficient and easy to execute method. It will be an added advantage, if we could develop a coating material that is also a corrosion protector. We have developed methods to prepare polyaniline composites that exhibit good corrosion resistance properties and a potential candidate for being a radar absorber.

**Work done and discussion**

Chemical synthesis of polyaniline is well documented, but synthesis of processable polyaniline that is necessary for the objective of this proposal is not trivial. In order to achieve processable polyaniline, we synthesized the polymer in presence of dodecyl benzene sulfonic acid, which is an anionic surfactant. Polyaniline was synthesized in presence of dodecylbenzene sulfonic acid using aniline as monomer and ammonium persulfate as initiator. We found that the polymerization proceeds well albeit the solution pH is close to neutral. Towards the objective of making corrosion resistant cement and radar absorbing coatings, we synthesized polyaniline in presence of nano-SiO<sub>2</sub>. We attempted to make a film by dip coating the dispersion on mild steel surface. The film was found to be uneven and porous, hence we decided to use a binder that would act as a filler.

While choosing the binder, we must consider the solubility of the binder polymer in the solvent where PANI-nanoSiO<sub>2</sub> is dispersed. Poly(vinyl butyrate) (PVB) have been used as a binder in coating technology for a while and that prompted us to use PVB in our studies. PVB is insoluble in water but soluble in methanol. We did a control experiment to check whether PANI-nanoSiO<sub>2</sub> precipitates

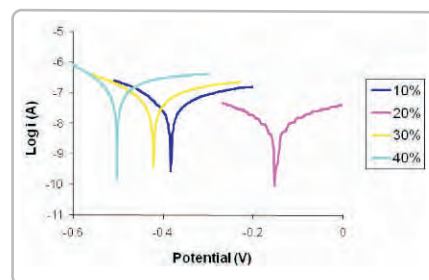


Figure 1. Tafel plot showing the potentials for various compositions of PANI-nanoSiO<sub>2</sub>

upon addition of methanol. We were gratified to note that the PANI-nanoSiO<sub>2</sub> dispersion is stable in a mixture of methanol and water. Therefore, further experiments were carried out using mixture of methanol and water. The dispersions synthesized using PVB-PANI-nanoSiO<sub>2</sub> in methanol-water was utilized to make film on the surface of mild steel. We were pleased to note that the composite of PVB-PANI-nanoSiO<sub>2</sub> forms a good film by dip coating. In order to optimize the ability of film forming and corrosion protection, the composition of PANI-nanoSiO<sub>2</sub> was varied in the composite. The composites synthesized using 10%, 20%, 30% and 40% was found to form a good film. Therefore, the films formed using these compositions were studied for protection of mild steel corrosion. First, we carried out tafel plots of the films formed using the abovementioned compositions. The mild steel corrosion was protected by the following order 40<30<10<20% of PANI-nanoSiO<sub>2</sub>. PANI is known to be a better corrosion resistant material; hence one would expect the corrosion resistance to increase upon increase in PANI-nano-SiO<sub>2</sub> concentration. But, we have found that 20% is the best followed by 10% (Figure 1). Therefore, upon increase the PANI-nanoSiO<sub>2</sub>, the corrosion resistance increases, but it starts decreasing upon further increase in PANI-nano-SiO<sub>2</sub> concentration. This is presumably because of the porous morphology created by the presence of increased concentration of nano-SiO<sub>2</sub>. We indeed observe the same trend, while we measured the corrosion resistance using impedance spectroscopy. Further, we also characterized the corrosion resistance at elevated temperatures. The PVB-PANI-nanoSiO<sub>2</sub> films exhibit better corrosion protection. Now the objective is to study the radar absorbing property of polyaniline and PVB-PANI-nanoSiO<sub>2</sub>.



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Exploration of India's rich microbial diversity

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### Objectives

To explore the microorganisms (isolated as well as from culture collection) and isolated enzymes to catalyze "chemically difficult or impossible" reactions to produce chirally pure bio-active compounds or pharmaceutical intermediates or to modify biologically active natural products.

- To explore cost-effective biotransformation processes including chemo-enzymatic processes for challenging target molecules such as (i) 10-Hydroxy camptothecin, (ii) Hydroxy steroids, and (iii) Anti-HIV drug intermediates

At NCL we will be carrying out

- Construction of an enzymatic tool box that would comprise well characterized biocatalysts (microorganisms or enzymes) which will be useful for different reactions such as asymmetric carbonyl reductions, asymmetric double bond reductions, stereo- and regio-specific hydroxylations, and chiral resolution of esters.

We have screened microorganisms isolated from various environments and found that some of the fungal strains are able to carry out the hydroxylations at non-activated carbon atoms in xenobiotics in stereo- and region-specific manner. We have also found that some of the fungal strains are able to resolve the esters into single enantiomer of corresponding alcohol in efficient way.



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Hydrogen Energy: Overcoming materials challenges for the generation, storage and conversion of hydrogen using fuel cells

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### Selected publications:

- ✦ *Science*, 2008, 319, 939
- ✦ *J. Am. Chem. Soc.*, 2008, 130, 12626
- ✦ *J. Am. Chem. Soc.*, 2009, 131, 3875
- ✦ *Catalysis Today*, 2009, 141, 72
- ✦ *Applied Catalysis B: Environ.*, 2008, 84, 21
- ✦ *J. Phy. Chem. C.*, 2009, 113, 17572
- ✦ *Chem. Mater.*, 2008, 20, 601
- ✦ *Langmuir*, 2008, 24, 3576; 2009, 25, 8299
- ✦ *Angew. Chem.*, 2008, 47, 2653

### Background / objectives

- Generation of ultra pure hydrogen through fossil fuel reforming, biomass utilization, photocatalytic and electrolytic water splitting strategies
- Storage of hydrogen using advanced materials such as carbon nanotube, metal organic framework and similar materials
- Conversion hydrogen to electrical energy by using polymer electrolyte membrane fuel cells, fabricated with innovative nanomaterials as electrodes and electrolyte materials

### Overview

Since hydrogen economy provides an attractive method for ensuring the future energy security of a country like India, a comprehensive R&D activity concerning the generation, storage and conversion of hydrogen using polymer electrolyte membrane fuel cells has been initiated by CSIR. The general aim is to create a linked network of projects concerning the generation of hydrogen through fossil fuel reforming, biomass utilization, and storage using advanced materials followed by conversion using a variety of fuel cell technologies. Hydrogen production is a potential area in this context and at NCL scientific activities are being progressed on aqueous phase and steam reforming of oxygenated hydrocarbons from biomass sources. Development of better catalysts for Water Gas Shift reaction is another ongoing activity. For hydrogen storage, there are two programs targeted to exploit carbon nanotubes and metal organic frame works. Hydrogen utilization is another area where, considerable progress has been accomplished. This includes the development of hybrid electrodes and electrocatalysts for PEMFC, development of low-Pt and Pt-free electrocatalysts for fabricating low cost electrodes, development of micro-patterned electrodes for PEMFC to achieve better reactant distribution and product removal and finally the development of new generation of proton exchange membranes. The main highlights of the project are briefly explained in this report.

### Work done and discussion Hydrogen from biomass through steam reforming and aqueous phase reforming

Commercial H<sub>2</sub> is produced either by steam reforming or autothermal reforming of natural gas. If this hydrogen is utilized as fuel for H<sub>2</sub> based fuel cells, it accomplishes reduction in the CO<sub>2</sub> emissions only to some extent, as a result of higher efficiencies of the fuel cells when compared to traditional power

generation units. However, the full benefits can be obtained if H<sub>2</sub> is produced from renewable sources such as oxygenated hydrocarbons (glycerol, sorbitol, xylose etc), which are derived from biomass.

Steam reforming (SR) of hydrocarbons is carried out at very high temperatures, while reforming of oxygenates need relatively moderate temperatures. However, no commercial process is available for reforming of renewable oxygenated hydrocarbons due to many associated problems. Serious impediments to this process are coking of catalysts as well as poor H<sub>2</sub> selectivity due to the formation of low molecular weight hydrocarbons (methane, ethane etc). To overcome some of these problems the novel idea of reforming these oxygenates in the aqueous phase, called aqueous phase reforming (APR), has been proposed at very low temperatures (~500K) in liquid phase. Though this process in principle is noteworthy for its novel approach, it suffers from poor thermal efficiencies as highly dilute (<5 wt%) aqueous solutions are used as input feed, rather than stoichiometric solutions. We have carried out aqueous phase reforming in a CSTR (continuous stirred tank reactor) mode in presence of excess water, while continuously pumping the feed in stoichiometric ratio. The reformat gas evolved was condensed, cooled and analyzed. This process has resulted in much better thermal efficiency, although it needs highly active catalysts as traditional catalysts coke rapidly.

The hydrogen energy group at NCL has developed novel catalyst formulations to achieve high conversion of oxygenates and greater H<sub>2</sub> selectivity. These nanostructured metal catalysts and their alloys are being tested for suppressing hydrogenation activity of metal catalysts, thus improving H<sub>2</sub> selectivity. Two types of reaction systems (one for APR and another for SR) have been assembled to carry out reforming in steam reforming as well as aqueous phase reforming mode. The later system was optimized by carrying out glycerol reforming using known catalysts such as Raney nickel. Figure 1 shows steam reforming of glycerol on a CeO<sub>2</sub>-ZrO<sub>2</sub> supported catalyst containing 1%Rh and 15% NiO developed at NCL. The results show conversion of glycerol and H<sub>2</sub>, CO, CO<sub>2</sub> and CH<sub>4</sub> selectivity's at different temperatures where conversion of glycerol occur at 550°C. However, the hydrogen content of the reformat reaches maximum only at 600°C perhaps due to the formation of methane at low temperatures. This catalyst was also tested at different liquid gas hourly space velocities.

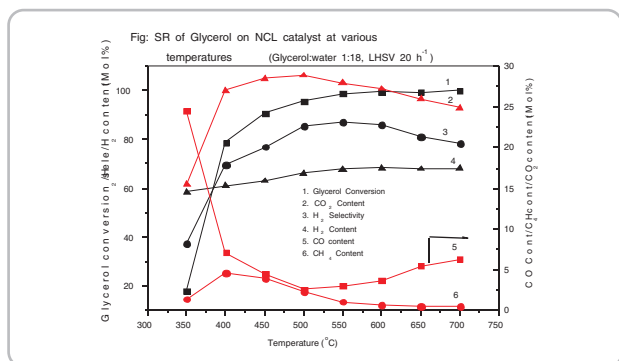


Fig.1. SR of glycerol on NCL catalyst at various temperatures. Glycerol: water 1:18, LHSV 20h<sup>-1</sup>

**Better catalysts for water gas shift reaction: Exploring structured and mesoporous oxides**

Water Gas Shift (WGS) reaction is an important component of fuel processing which not only reduces the concentration of poisonous CO but also enriches the feed with H<sub>2</sub> by using water. Noble metal catalysts are found to be most suitable for WGS in small scale fuel processors, however, agglomeration of active metal particles and subsequent deactivation has been a challenging problem faced by the community. The main aim of this project is to develop oxide based catalysts for Water Gas Shift reaction aiming at low temperature activity and on stream durability. Two aspects specifically focused are (i) increasing the surface area of the ceria and related supports thereby improving the dispersion of the active noble metals by developing novel methods of preparing mesoporous supports with noble metal encapsulation and (ii) Improving the on-stream stability by incorporating the noble metals in lattice points. Perovskites are very stable structures with high tolerance to oxygen vacancies. The oxygen vacancies which can be created by isomorphous substitution will aid in enhancing the WGS activity. The perovskite selected for current study was BaCeO<sub>3</sub> in comparison to the previously developed CeAlO<sub>3</sub> with Ce in 4+ and 3+ oxidation states respectively. The overall mechanism can be envisaged to be different in these different redox systems.

Mesoporosity in oxides has been achieved by using surfactant or polymer micelle templates during synthesis. Cationic surfactants like CTMABr and nonionic polymers like polyethers were successfully employed for synthesising mesoporous silica. Preliminary characterization was carried out by powder X-ray diffraction studies at low as well as wide angles to follow the

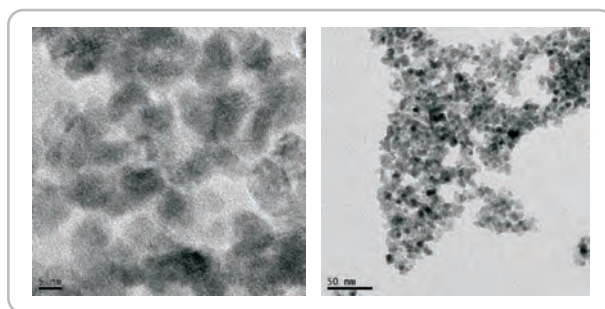
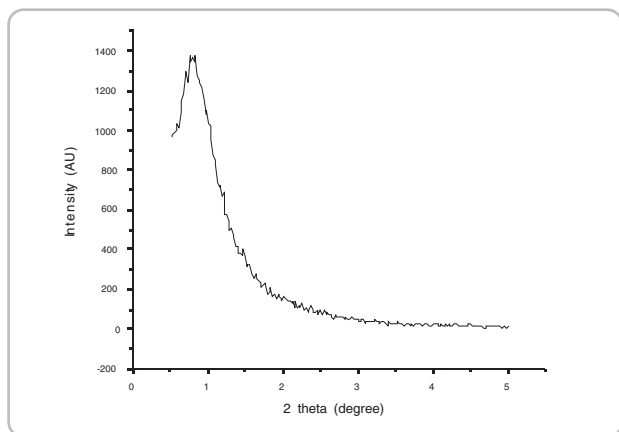


Fig. 2. Low angle XRD of CeO<sub>2</sub> synthesised with P123-CTAB mixed micelle showing mesoporosity (left) and HRTEM images showing ~10 nm particles of CeO<sub>2</sub> (right).

formation of mesoporosity and ceria respectively. We could synthesise monodispersed particles of ~10 nm with good mesoporosity (Fig. 1). BaCeO<sub>3</sub> perovskite could be synthesised without any CeO<sub>2</sub> or Pt impurities. However, presence of BaCO<sub>3</sub> was found to be present persistently. These materials are being investigated for their catalytic activity.

**Preparation of low-Pt and Pt free nanostructured electrocatalysts for oxygen reduction.**

In a recent development in the group, selective decoration of Pt on both inner and outer surface of carbon nanofibre (Fig.3) displayed better oxygen reduction activity compared to Pt in carbon nanotubes and Vulcan XC-72. Functional groups present on the surface of CNF and unsaturated carbon valency along the inner wall originated by the terminal graphene edges helped to utilize both inner and outer surface of CNF for Pt dispersion. Pt on functionalized carbon nano fibre (Pt/FCNF) shows high oxygen reduction reaction and methanol oxidation, as revealed in Fig. 4. From hydrodynamic voltammogram it could be confirmed that the overall performance of the electrocatalyst is significantly high compared to Pt on bare carbon nano fibre (Pt/CNF) and carbon nanotube (Pt/CNT).

Similarly studies on core-shell type materials such as Fe@Pt, Cu@Pt also lead promising results with respect to the oxygen reduction activity and stability under the electrochemical environment, leaving a scope for developing active catalysts with significantly low Pt content. These core shell catalysts show better CO tolerance compared to the commercial platinumized carbon. The stability of some of these materials under electrochemical environment is also promising. In a significant step to develop Pt-free electrocatalysts, we are currently involved in a process of developing a Fe based electrocatalyst by anchoring Fe particles in the available slit pores along the inner wall of a carbon nanofibers substrate.

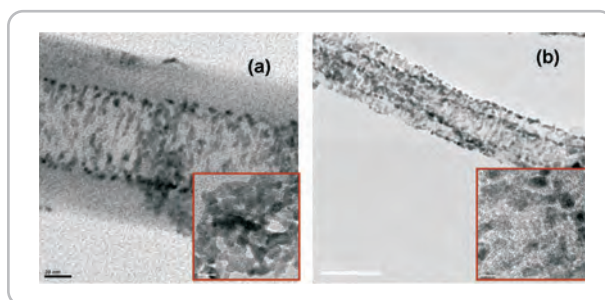


Fig.3. (a) Pt on inner wall of CNF and (b) Pt on inner and outer wall of functionalized CNF

Hydrogen Energy: Overcoming materials challenges for the generation, storage and conversion of hydrogen using fuel cells

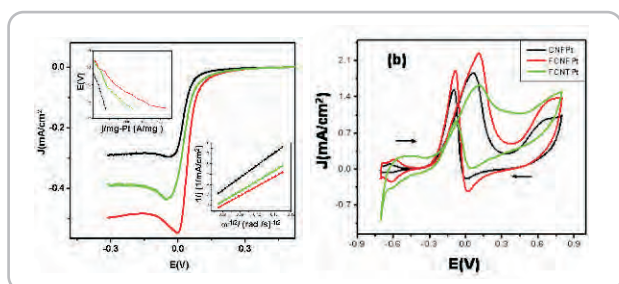


Fig.4. (a) Hydrodynamic Voltammogram and (b) Methanol oxidation reaction of FCNF-Pt, CNF-Pt and CNT-Pt.

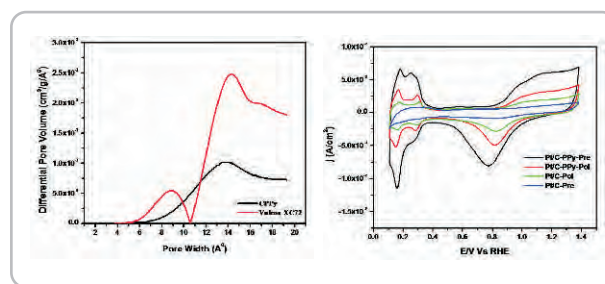


Fig.5. (A) Pore size distribution of Vulcan XC-72 and carbon coated polypyrrole. (B) Cyclic Voltammogram of Pt prepared by different methods on polypyrrole coated carbon

## Inorganic-organic nano-composite electrodes and composite membranes for MEA preparation

PEMFCs represent a credible alternative for environmental friendly energy conversion with  $H_2$ ,  $CH_3OH$  etc as fuels. However, it has a number of practical limitations, including cost of the catalyst and its poisoning, need for humidification during operation, large cross-over and easy puncturing of membrane etc. Maximum catalyst utilization, hence high fuel cell performance can be achieved by modifying the morphology of catalyst support. High fuel cell performance can also accomplish by modifying the polymer electrolyte by adding some organic and inorganic materials, which helps for proton conduction with conventional Nafion and PBI membranes.

As a practical approach to maximize platinum utilization, we attempted to wrap the meso and micropores present on the surface of carbon by a conducting polymer, polypyrrole. This modification helps to block nanopores on the surface up to some extent and thereby to avoid large level deposition of nanoparticle in the pores present on the surface of carbon. Pt nanoparticle in the pores generally do not attain triple phase boundary (TPB) with ionomers due to the size mismatch between the ionomer and pore dimensions. Platinum nanoparticle on the surface of polypyrrole coated carbon (C-PPy) is well dispersed and Pt agglomeration could be prevented by the hetero atom on C-PPy resulting into better TPB formation and higher oxygen reduction activity. Cyclic voltammetry shows that Pt nanoparticles prepared by the pre-precipitation method have higher effective active surface and oxygen reduction capacity compared to those prepared by the conventional polyol process on both Vulcan-XC-72 and C-PPy. These results show that both modifications of the catalyst support and the mode of preparation of the catalyst have great influence in deciding the overall fuel cell performance (Fig.5). We have also demonstrated a novel strategy of deliberate manipulation of hydrophilic domain sizes in Nafion by gradually introducing sulfonic acid functionalized multiwalled carbon nanotubes (s-MWCNT) into the matrix. Proton conductivity of the membrane was increased with increase in s-MWCNT introduction to an optimum value of 0.05%. Along with Nafion, s-MWCNT, another composite electrolyte using PBI-phosphonated multiwalled carbon nanotube membrane is being prepared. This membrane shows good proton conductivity and hence high current density and power density at  $160^\circ C$ .

## Development of micro-patterned electrodes and electrolyte membranes for MEAs: Soft lithography approach

The overflow of excess water produced during fuel cell reaction on cathode will diminish the mass transport which in turn reduces the fuel cell performance. We have attempted to solve

the problem by making patterned electrode using soft lithography techniques. This shows enhanced performance compared to that of flat electrodes. Micro channel present in the electrodes will help to the removal of water from the electrode surface and provide better mass transfer and our preliminary results suggest a bipolar plate-less fuel cell development using these revolutionary approach.

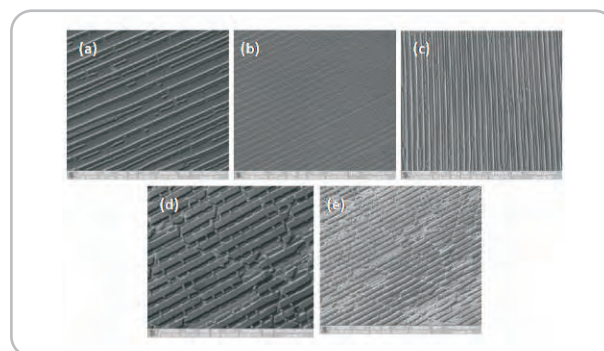


Fig. 6: Micro-patterned electrodes directly formed on Nafion membrane electrolyte enabling a bipolar plate-less MEA

## Host guest type PEM by pore intrusion

Since optimization of PBI needs long time (~20 hrs) and three stages of temperatures control for obtaining polymer with appreciable viscosity, new strategies have been carried out to reduce this time in view of demand for large scale synthesis of PBI, which was performed by two ways. (I) PBI synthesis using catalyst: PBI polycondensation reaction rate was enhanced by using different catalysts ( $SnCl_2$ ,  $PPh_3$ ,  $PO(OPh)_3$  and  $PPh_3$ ). The reaction duration was lowered down up to 7 hrs offering PBI viscosity of 0.57-1.45 dL/g for different catalysts and (II) Lowering PPA : Amine ratio: The second parameter greatly affecting the PBI reaction rate is amount of PPA used for synthesis. This is usually taken as 30 times than the wt of amine. The reduction to this value to 20 lowered reaction time to 8-10 hrs without any need of catalyst.

In order to incorporate PBI in the ink making for MEA preparation, high viscosity solution (high concentration) is required. This was achieved by lowering the viscosity of PBI. Since PBI used for membrane making has an inherent viscosity of ~ 1.1 dL/g we had reduced to ~ 0.8 by using larger amount of PPA in during PBI synthesis (40 / 50 g of PPA per g of amine). Several other PBIs such as those containing aliphatic dicarboxylic acids are being investigated for physical properties that are crucial for their applicability as proton exchange membrane materials.





## Pd-functionalized MWNTs for hydrogen storage

Multi-walled CNTs (MWNTs) were synthesized by thermal decomposition (CVD method) of methane over MgO supported Fe-catalyst. The as-synthesized MWNTs were purified by

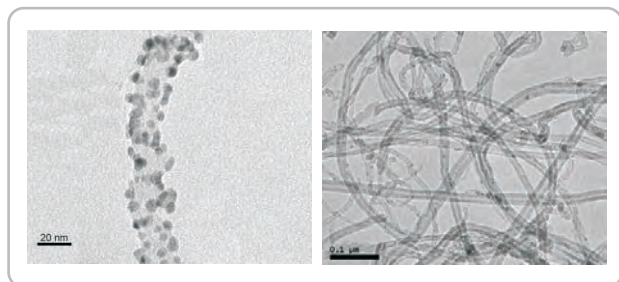


Fig.7. TEM images of (a) purified MWNTs and (b) Pd-MWNTs used for hydrogen adsorption studies

chemical and thermal treatments. The purified MWNTs were treated with a mixture of  $\text{HNO}_3$  and  $\text{H}_2\text{SO}_4$  to form COOH and OH functional groups on the nanotube surface. The COOH-functionalized MWNTs were further treated with acidified  $\text{PdCl}_2$  to produce Pd-functionalized MWNTs. The  $\text{Pd}^{2+}$  ion in the Pd-MWNTs solution was reduced using  $\text{NaBH}_4$ . The samples of MWNTs, COOH-MWNTs and Pd-MWNTs were characterized by SEM, TEM, EDX, Raman and TGA / DTA. The hydrogen adsorptions on Pd-MWNTs were measured by pulse titration at 93 K and ambient pressure. The diameter of MWNTs as seen in the TEM image (Fig.7) of purified MWNTs was in the narrow distribution range of 20-30 nm. The TEM image of Pd-functionalized MWNTs showed numerous Pd nanoparticles anchored onto the external walls of the nanotubes. The Pd loading on the outer walls of MWNTs was estimated to be 4.4%. The Raman analysis of all MWNT samples showed three characteristic peaks: disorder-induced D-band around 1330  $\text{cm}^{-1}$  for graphitic carbon, graphite related G-band around 1580  $\text{cm}^{-1}$  and  $\text{G}'$ -band as first overtone of D-band. The intensity ratio of D-band to G-band (ID/IG) was observed to increase significantly from 0.194 of purified MWNTs to 0.878 of Pd-MWNTs due to the surface modification. The surface area analysis showed a decrease in the surface area of MWNTs by 7.7% after Pd-functionalization. The results of hydrogen sorption studies (Fig.8) indicated much higher hydrogen uptake capacity for the Pd-MWNTs, i.e. 4.6 wt% hydrogen uptake at 25% Pd loading. The temperature dependence of hydrogen uptake obeyed the Langmuir relation.

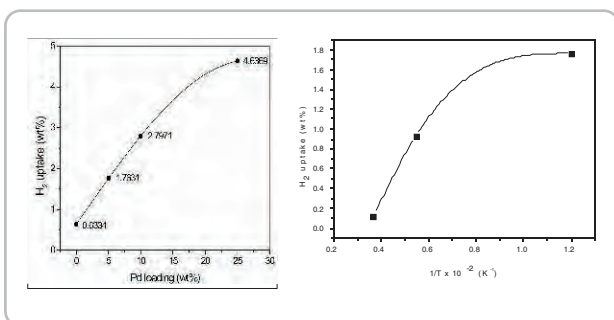


Fig.8. Hydrogen uptake profiles for Pd-MWNTs in liquid nitrogen at atmospheric pressure

## Mesoporous metal organic frame works for hydrogen storage and carbon sequestration

The aim of this project is to design porous metal organic framework materials (MOFs) 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. Our interest in the use of fluorinated links in synthesizing fluorinated metal organic frameworks (F-MOFs) is based on reports of interesting  $\text{H}_2$ -storage properties in materials containing porous surfaces with exposed fluorine atoms. However, there are only a few reports of MOFs containing fluorinated carboxylates as perfluorinated carboxylates are significantly more acidic than non-fluorinated carboxylates, and subsequently less soluble in common organic solvents. Fluorinated acids are also less stable than their non-fluorinated analogues and it has been found that they often decompose at temperatures commonly used to form MOFs of higher dimensionality (125-180°C). We so far have investigated the flexibility of the ligands on the resulting framework (Fig. 9), we synthesized more than 50 F-MOFs with flexible fluorinated dicarboxylate building block and various heterocyclic co-ligands. We attempt to rationalize the influence of the solvent ( $\text{H}_2\text{O}/\text{DMF}$ ) on the formation of the F-MOFs. These F-MOFs have been determined by single crystal X-ray diffraction analyses and further characterized by IR spectra, PXRD, and thermogravimetric analyses. In addition, the luminescent properties of the complexes have also been investigated in the solid state.

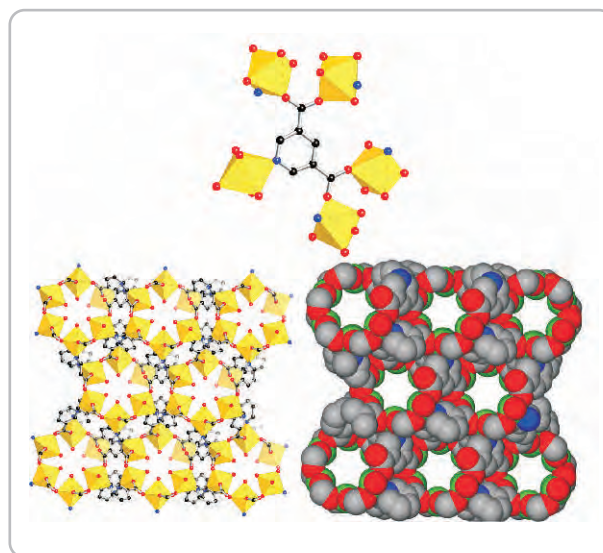


Fig. 9: Porous Mg based metal organic framework. Secondary building unit (SBU) has been shown on the top and the space filling model has been shown on the bottom

## Multi-scale modeling and simulation of polymer electrolyte membranes and molecular transport in fuel cells

Polybenzimidazole (PBI) membranes in presence of phosphoric acid show good proton conductivity at high temperature for fuel cell applications. Understanding the mechanism of proton conductivity in such systems and also for functionalized PBI is useful to design and calibrate such membranes. Therefore we are developing force field parameters for benzimidazole, PBI and functionalized PBI and running molecular dynamics



simulations in atomistic scale to elucidate the proton transport and molecular transport mechanism in these polymer electrolyte membranes (Fig.10).

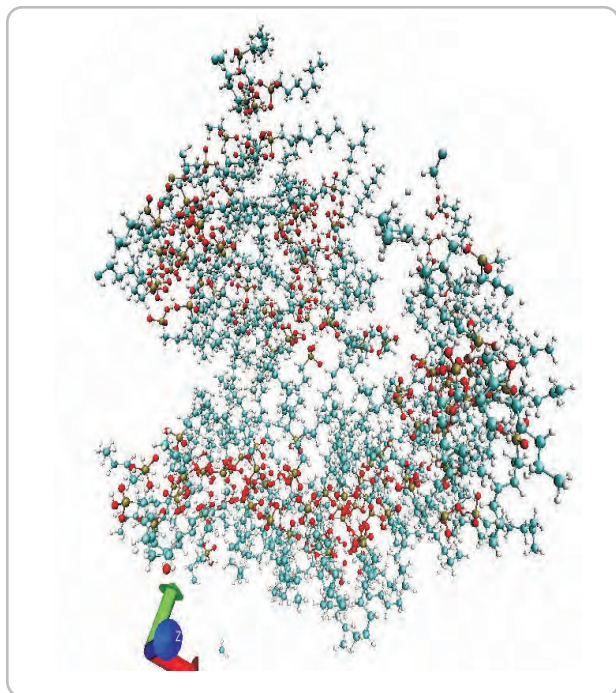


Fig. 10: Formation of network in phosphonic acid based systems

### Conclusions

During 2008- 09, NCL has shown enormous progress in some of the XI five year plan projects in the area of hydrogen production, storage and utilization. For example, Aqueous phase reforming (APR) based reformates have been developed and for steam reforming of glycerol Rh and Ni based bimetallic catalyst have been demonstrated. For reducing the CO poisoning in the  $H_2$  gas by Water Gas Shift reaction at low temperature and for stream durability, better catalysts based on  $BaCeO_3$  have been prepared by different methods. Hydrogen storage using carbon nanotubes (CNTs) and Metal Organic Frame works (MOF) has been initiated to enhance gravimetric storage although much remaining to be accomplished in the coming years. For hydrogen utilization using polymer electrolyte membrane fuel cells, many new materials for components such as catalyst, catalyst support, polymer electrolyte membrane for membrane electrode assembly (MEA) have been developed. Hybrid membrane of Nafion and functionalized multi walled carbon nanotubes shows enhanced proton conduction and good mechanical stability. For maximum platinum utilization, modification in the catalyst support (Vulcan Carbon) by polypyrrole shows enhanced catalytic activity. Platinum decoration in the inner and outer wall of Carbon Nanofiber also shows enhanced catalytic activity. To reduce platinum loading in the electrode core shell type materials (Pt @ Fe, Cu) also tried. To achieve better reactant distribution and product removal in the electrode during fuel cell reaction under high relative humidity could be reduced by making micro pattered electrode by soft lithography.



The Center of Excellence in Scientific Computing has been established in April 2008 to promote scientific computing in different domain areas. Scientific computing is used not just to analyze the experimental results, but also to predict phenomena. Development of modeling techniques and computational tools has helped it achieve an important role in all areas of science. Some of the important programmes carried out under the Center during the year are described below:

### Development and coding of many-body coupled-cluster methods for properties

**PI : Sourav Pal**

**Members :** Arijit Bag, SRF; R. Lalitha, SRF; Subrata Banik, SRF

Lagrangian formulation of energy derivatives based on multi-reference coupled-cluster method has been coded for states, which demand a description of such method. In particular, excited states are important examples of such requirements. First implementation of energy derivatives with respect to external electric field for excited states has been done. Prototype tests of the code has been done for excited state dipole moments and polarizabilities of molecules (a strong example is ozone) [**J. Chem. Phys.**, **200**], **131**, 024102].

The results incorporate extensive use of both non-dynamic and dynamic electron correlation and preserve size-extensivity of the properties calculated.

We have also made first implementation of the above response approach to magnetic properties (dia-magnetic susceptibility) for doublet open-shell radicals using standard Gaussian basis sets [**Int. J Quantum Chem**, **2009**, **109**, 2191].

Vibrational energy of molecule has also been calculated using equation-of-motion based coupled cluster linear response theory in bosonic representation. Excited vibrational states have been calculated for water and formaldehyde molecules using model potential energy surface. [**J. Chem. Phys.** **2008**, **129**, 134111]

### Density functional investigation of relativistic effects on the structure and reactivity of tetrahedral gold clusters

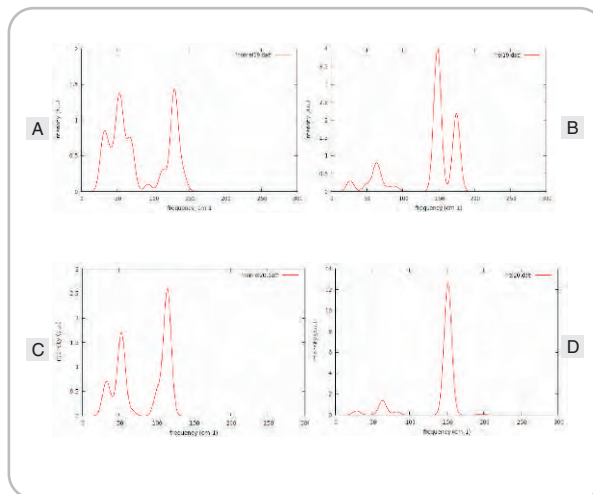
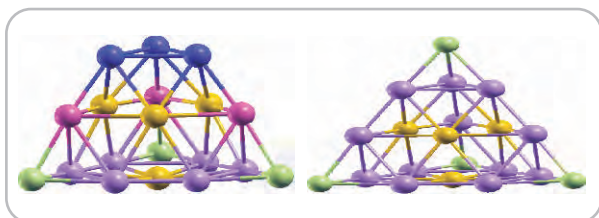
**PI : Sourav Pal**

**Members :** Himadri S. De, SRF

**Collaborator:** Sailaja Krishnamurthy, CECRI, Karaikudi

The influence of relativistic effects on the structure, vibrational modes and reactivity of tetrahedral gold clusters, Au<sub>19</sub> and Au<sub>20</sub> have been investigated using Density functional (DF) methods. The intra-molecular reactivity of the clusters was analyzed using DF-based reactivity descriptors. The following figures depict the structures of the molecules in non-relativistic limit. Effects of relativistic effects have also been studied. These change bond angles and bond lengths by 6-7 % [**J. Phys. Chem**, **2009**, **C 113**, 7101].

The vibrational frequencies of the above molecules have been calculated in both non-relativistic and relativistic limit. The above figures show the frequencies of the two molecules. The reactivities of the atoms for both the molecules are also calculated.



Calculated vibrational frequencies; (a)Au<sub>19</sub> non-relativistic (b) Au<sub>19</sub> relativistic (c) Au<sub>20</sub> non-relativistic (d) Au<sub>20</sub> relativistic. Graphs with scale factor of 1.29 and half width 6 cm<sup>-1</sup>.

The work shows that while the structural properties and vibrational modes are affected by the relativistic effects, the reactivity trends based on Fukui function calculation on various atoms within these clusters remains unaffected by the absence or presence of relativistic effects.

## Scientific Computing

Improving hydrogen storage in MgH<sub>2</sub> by doping

**PI : Sourav Pal**

**Member :** Tuhina Kelkar, SRF

Magnesium hydride has been considered to be an excellent candidate for hydrogen storage. However, while thermodynamics of adsorption of hydrogen has been good, there are concerns about dehydrogenation kinetics. The objective of this work is to dope the Magnesium hydride by Si and Al and study its thermodynamics and kinetics using density functional theoretic calculation for periodic systems. We considered three phases of MgH<sub>2</sub>. Our results indicate

that Si doping consistently decreases  $\Delta H_f$  of all 3 phases more than Al. No particular trend is observed for activation barrier, i.e. Eact. There is need to make trade-offs between thermodynamics and kinetics for  $\alpha$ -MgH<sub>2</sub>. Doping  $\gamma$ -MgH<sub>2</sub> with Si would prove useful. Best results are obtained by using  $\beta$ -MgH<sub>2</sub> in pure form. However, the challenge is to look for material which has hydrogen adsorption between chemi-sorption and physi-sorption [**ChemPhysChem** 2008, 9, 928; **J. Mater. Chem.**, 2009 in Press].

## Artificial Intelligence Systems Group

**PI : S. S. Tambe**

**Member :** Ashish Gangwal, PA-II

**(A)** Artificial Intelligence (AI) Based Modeling and Optimization for Supervisory Control of Thermal Power Plant (Sponsor: National Thermal Power Corporation)

**Work Done:** The project objective has been: (i) to develop artificial neural network (ANN) based models for improving boiler efficiency of NTPC's 500 MW thermal power plant based on the process data supplied by the NTPC, comprising values of the process operating (causal) variables such as temperature, actual load, mill combination, feed water flow, etc., and the corresponding response (output) variables and (ii) the artificial neural network (ANN) based models will be used for optimizing the process performance. The work done under these objectives is described below.

- ✦ Java based Supervisory Control software package has been developed for NTPC's coal-based 500 MW power plant. The software comprises nearly 31,000 lines of Java code.
- ✦ The plant data were supplied by the NTPC.
- ✦ Offline and online modeling of the power plant is conducted using Multi-layer Perceptron (MLP) and Generalized Regression Neural Networks (ANNs).
- ✦ A number of ANN-based models have been developed for predicting boiler performance variables.
- ✦ Genetic Algorithm (GA) based strategies have been designed and developed for optimizing performance of the power plant and generating set-point advisory for plant engineers and operators.
- ✦ The supervisory control software has a facility to perform artificial intelligence based online plant modeling and constrained optimization.
- ✦ The software can be integrated with the Distributed Control System (DCS) of the power plant.

- ✦ Modules performing Gross Error Detection (GED), Data Validation (DV) and Data Reconciliation (DR) have been incorporated into the supervisory control software for assessing integrity of data arriving from the power plant and applying due corrections whenever necessary.
- ✦ The software has Graphical User Interface (GUI) whereby plant operators can monitor several important plant variables online.

**(B)** Synthesis and Optimization of Functionally Absorbing Materials (Sponsor: Proctor & Gamble, USA; Project leader: Dr. S. Ponrathnam).

**Work done:** In this project, an extensive experimental work involving synthesis of Functionally Absorbing Materials (FAM) using monomers, initiator and an inhibitor was conducted by the group headed by Dr. S. Ponrathnam, Polymer Science and Engineering Division. The experimental data comprised results of variations in the concentrations of inhibitor and initiator. Variations in the reaction temperature also were extensively studied. The task of kinetic modeling of synthesis of FAM using the experimental data was conducted by the Artificial Intelligence Systems Group wherein a number of models such as inhibition time model, polymerization rate model and polymerization rate model in terms of initiator and inhibitor concentrations were developed.



**Modeling to understand nonlinear kinetics and regulation mechanisms in biological systems**

**PI : Chetan Gadgil**

Biological processes and pharmaceutical interventions affecting these processes involve nonlinear kinetics and interlinked and intricate regulation mechanisms. The goal of modeling and simulation activities is to help achieve a better understanding of such complex biological systems. To this end, we study such systems at several scales from the intracellular to the pharmacological. Some of the current projects in the lab are:

- ✦ Analysis of autocatalytic biological processes
- ✦ Modeling transcriptional regulation
- ✦ Modeling drug development assays and drug delivery systems
- ✦ Stochastic reaction analysis
- ✦ Analysis of DNA microarray data

Autocatalysis is seen at all length and time scales of biological systems, shows several common features and can be analyzed by a common set of mathematical tools [AICHE Journal, 2009, 55, 556]. For a particular system, autoregulation of TATA Binding Protein production, a mathematical model was developed and analyzed to suggest explanations for experimental observations regarding TBP concentrations in the zygote and the pathological effects of certain TBP variants (collaboration with IGIB).

A theoretical analysis of discrete stochastic reactions resulted in the identification of a class of systems where the long-term behavior is proved to be different from the prediction of the corresponding continuous deterministic model irrespective of the size of the system (Bull Math Biol, 2009). Quantification of the degree of this difference as a function of initial state and reaction rate parameters is underway (DST project).

Model for two assays that measure the efficacy of cyclooxygenase inhibitors was developed. The experimentally observed order-of-magnitude differences in the  $IC_{50}$  concentration predicted by these assays could be explained using the combined model (sponsored project/collaboration with GlaxoSmithKline). Modeling non-oral drug delivery mechanisms is planned for this year.

A model was developed for regulation of transcription by small RNA (miRNA) species. Incorporating this mode of regulation in a model for the cell cycle resulted in a better match between model predictions and experimental observations (collaboration with IGIB).

Analysis of methods for DNA microarray data analysis led to the identification of a robust method for feature identification and classification (Int J Bioinf Res Appl, 2009). Comparison of methods for identification of periodically varying data (collaboration with Mugdha Gadgil, NCL) and application to an experimental system (collaboration with NII) are underway.

**Relativistic coupled cluster method for molecular properties**

**PI : Nayana Vaval**

**Member :** Sumantra Bhattacharya, SRF

This project involves development of coupled cluster based analytic response using relativistic effects for the calculation of molecular properties of heavy atoms and molecules. Relativistic effects are important for the heavy atoms. It is known that electron correlation plays important role in accurate calculation of molecular properties. Thus, in the heavy atoms/molecules the effect of electron correlation and relativistic effects play important role on equal footing. It is challenging to treat them simultaneously on equal footing to obtain accurate molecular properties.

To include the relativistic effects we first need to get the one and two electron integrals in the spin orbit basis. We have successfully obtained the one and two electron integrals in spin-orbit basis. The implementation of this has been done in collaboration with the Indian Institute of Astrophysics. The coupled-cluster code for the calculation of the energies of the heavy atom with the relativistic effects has been developed. The expression for the calculation of properties with the proper spin-orbit factors is under development.

## Scientific Computing


**Protein conformational disorders: Probing the mechanisms and pathways for protein misfolding and aggregation under ambient conditions**

**PI : Neelanjana Sengupta**

**Member :** Deepti A. Mishra, PA-II

The research carried out thus far involved developing an understanding of early seeding events, by studying the structural and dynamical changes taking place in the helical form of the Amyloid  $\beta$  (A- $\beta$ ) peptide. Recent experiments suggesting the role of the helical form in membrane poration and the A- $\beta$  peptide is itself created from a larger, membrane spanning precursor protein. Thus, the pathway from the helical to the amyloidogenic, extended  $\beta$ -sheet form may provide insight into ways of trapping the peptide into non-amyloidogenic conformations.

**Synopsis of simulations:** Molecular dynamics (MD) simulations of the helical form of the amyloid peptide, starting with structural coordinates of the peptide obtained from NMR based studies in apolar solvents (Crescenzi et al., Eur. J. Biochem. 269,5642–5648 (2002), PDB code IYT), have been performed. Two MD trajectories, each about 25 nanoseconds long, were created by solvating the peptide in different quantities of explicit water. The TIP3P

water model was used, and the simulations were performed at room temperature and a pressure of 1 atmosphere. The CHARMM22 force field and the NAMD simulation package were used.

**Trajectory analysis:** A variety of time correlation functions (TCFs) have been constructed at well separated time windows in the MD trajectories. The intra-peptide amide hydrogen bonding TCFs show the time scales of structural decay. A change in structural persistence should be accompanied by changing structural correlation with the surrounding water, which is probed by calculating the peptide-solvent hydrogen bonding TCFs. The persistence length of the peptide has been obtained from the end-to-end distance correlation of the peptide. Also, these TCFs, as well as the radial distribution functions of solvent waters constructed at individual amino acid residues help determine which residues play major roles in structural deformation. The diffusion of water and the mean residence times within the protein solvation layer are other important quantities that help characterize the time evolution of the peptide in the solvent.

**Molecular dynamics simulation of Pleckstrin protein**

**PI : Sudip Roy**

**Member :** Surekha Bansal, project trainee

We have carried out a series of molecular dynamics calculations on Pleckstrin protein solvated in water to elucidate the conformation of the protein. For the simulations we have used NMR geometry and PELDOR distances as a guess for initial structure. We have also parameterized the spin label which was used in the PELDOR experiments by quantum chemical calculations. From the MD simulations we have calculated the distance

histograms between the spin labels which are attached to the cysteins at different positions of the protein. These distance histograms are in good agreement with the experimental observations. In this way combining NMR, PELDOR and MD results we are capable of finding the conformation of this protein which has no crystal structure information because of its complexity. The work is still ongoing for different initial structures to produce the best fit to the experimental distance histograms and NMR local structure, thus able to report the perfect conformation of the protein.

**Density functional studies of organo-metallic catalysis**

**PI : Kumar Vanka**

**Member:** Shantanu Kadam, PA-II

(1) Asymmetric hydroformylation catalysis: The Heck-Breslow mechanism has been investigated with detailed calculations for a real rhodium-based catalyst system: Rh-BINAP. Three complete cycles pertaining to the formation of the three aldehydes - the linear and the two (R and S)

branched aldehydes - have been studied for the styrene substrate. The intriguing result from these calculations is that the results do not match what is observed from experiment, which appears to imply that the generally accepted Heck-Breslow mechanism may not be the primary mechanistic route for the bidentate ligand rhodium catalyst system. Alternate mechanistic pathways are currently being explored.



(2) Ziegler-Natta heterogeneous catalysis: The influence of donors – both internal and external - has been investigated for  $MgCl_2$  based Ziegler-Natta systems. The coordination of donors such as phthalates and alkoxy esters on different  $MgCl_2$  planes has been studied and interesting results have been obtained, which may provide explanations for experimental observations that show that certain internal and external donors do not work well together in providing isotacticity to the polypropylene product.

(3) Nickel-based oligomerization catalysis: Nickel-oxime systems have recently been found to be effective in dimerizing and trimerizing ethylene – leading to formation of butene and hexene respectively. Calculations have been done to study the mechanism and the rate determining steps for this reaction and the results to date indicate that the Cossee-Arlman mechanism is not active in these systems, and that the cyclic mechanism is the dominant oligomerizing mechanism.

### Studies of complex networks in chemical and biological systems

**PI : V. Ravi Kumar**

**Members:** Rahul Y Doiphode, JRF; Ketan D Sarode, JRF

#### Chemical systems

Development of multiscale-multifractal formalisms for identification and characterization of flow structures in chemical process equipment

During the year, the work has been towards developing multiscale methodologies for identification and characterization of flow structures from complex data monitored from reactors (e.g., annular centrifugal contactor, jet loop reactor, ultrasound, reactor channel flow, stirred tank and bubble column reactor). The complex data in the form of velocity measurements was obtained from planned experiments/simulations and recorded using sophisticated techniques, i.e., hot film anemometry, particle image velocimetry, LES simulation and in collaboration with ICT, Mumbai. Using the computational facilities of CoE-SC, the monitored process space-time data has been extensively studied to identify the formation of structural networks, i.e., micro- and macro structures in turbulent flow fields. The advantages of wavelet transforms (WT), as an efficient multiscale mathematical tool to study complex processes and its usefulness for data interpretation has been shown earlier in NCL for applications like filtering noise, characterizing chaotic dynamics, feature identification, pattern recognition, parameter estimation etc. Applying these principles it was found that the micro-macro structures could be studied in a reduced dimensionality and the hydrodynamics classified on the basis of their multifractal properties. Hydrodynamical classification, independent of type of process equipment is now possible and this will be useful for choosing a reactor type, its design and operational strategies [**Chem. Engg. Sci. 2008, 63, 5330**].

In the coming year, it is planned to study the effects of flow structures on heat transfer properties in single and multiphase reactors. The study would analyze the heat

transfer properties at interfaces like solid-liquid (e.g., at reactor walls), vapor-liquid(e.g., at plumes) from data. Inferring the interactions between the flow hydrodynamics and heat transfer behavior at different scales will be useful in characterizing heat transfer mechanisms and to accurately calculate heat transfer coefficients for complex systems than what is available presently.

#### Biological systems

Biological engineering of *C. elegans* locomotion : Modeling and simulation of neuronal circuit based mechanical model

Living organisms have ways to adapt to various conditions and external environments. If we can replicate on the computer the principles followed by these organisms then it may become possible to apply biological and biomimetic principles to the engineering of artificial machines and robots. For this view point, we took up the activity of building a mathematical model and carrying out simulation studies for replicating the snake-like locomotion behavior of the nematode, *C. elegans*. The model is built on the complete information available in literature about its neural circuitry (which is a complex network of touch sensory neurons, chemoaxis neurons, interneurons, and motor neurons) and the way signals are transmitted to the body muscles for locomotion. The communication model between the neuronal architecture and the mechanical body has been carried out for various patterns of locomotion and the parameters tuned by genetic algorithms. This is computationally intensive because the number of parameters to be optimized are large due to size of the biological network.

We now propose to study the stability of the complex network to locomotion properties and damages induced in the neuronal circuit. This would help to bring out inferences on the nature of adaptation in biological systems for changed conditions/environment. Thus, the reflexes of the worm to touch simulation will be interesting situation to study.



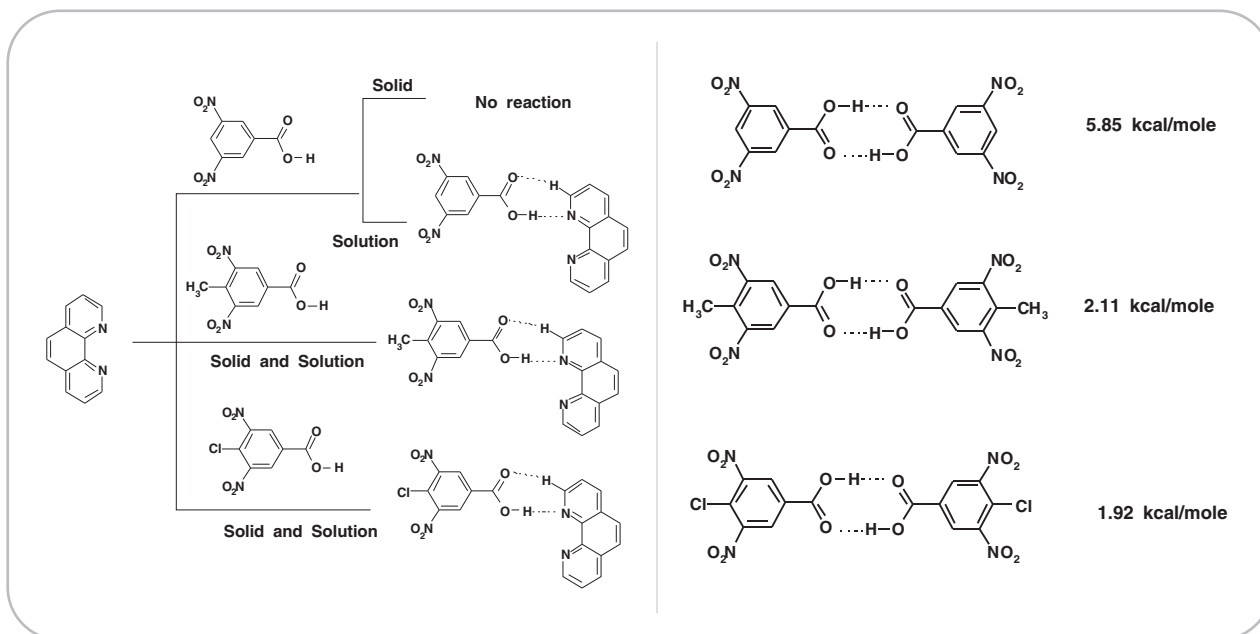
**Hydrogen bond energy directed anomaly in the formation of supramolecular assemblies in solid and solution states**

**PI : V. R. Pedireddi**

In the formation of supramolecular assemblies, although hydrogen bonds play a vital role in the aggregation of molecules, quantitative estimation of the energy of the associated bonds in the formation of specific molecular assembly are not well studied. It was perhaps, mainly due to the fact the assemblies are often being synthesized from solution. In contrast, taking into account the literature reports of formation of supramolecular assemblies in solid state by simple grinding of the substrates in mortar with pestle, we have considered supramolecular reactions of carboxylic acids with aza-donor compounds, to perform both in solid and solution states. In this process, we have found that 3,5-dinitrobenzoic acid and its two analogues 4-chloro and 4-methyl-3,5-dinitrobenzoic acids form complexes with 1,10-phenanthroline in solution state while in the solid state the former did not yield a complex as shown below.

Analysis of the assemblies, obtained from solution, by single crystal x-ray diffraction reveals that in all the three complexes, the respective acid molecules interact with the

phenanthroline through the formation of O-H...N/C-H...O pairwise hydrogen bonds as shown in the above scheme. Since it is a well known fact that -COOH groups generally exist as dimers, such a reaction is possible only if those dimers are dissociated and the isolated acid molecule instantaneously interact with the phenanthroline. However, in solution the dimers formation and dissociation is a continuous process, thus, the formation of the observed products is quite facile. Whereas in the solid state, the dissociation is related to the energy being supplied. Hence, we calculated the hydrogen bond energy of all the three acid molecules and it has been observed that 3,5-dinitrobenzoic acid is associated with ~ 6 kcal/mole, which is nearly double the energy of the dimers in the corresponding 4-chloro and 4-methyl analogues. Since in the solid stage grinding experiments, the energy being supplied is through simple grinding, it can be concluded that the acids with less energy easily dissociated to yield a single acid molecule to form the corresponding complexes, while strongly hydrogen bonded 3,5-dinitrobenzoic acid remain intact, thus, failed to aggregate with phenanthroline. Studies pertain to several other functional groups are in progress.







**In-silico study of the recognition process involving proteins possessing wide binding specificity for small biomolecules and thus to design proteins for specific applications**

**PI : C. G. Suresh and B. M. Khan**

**Members :** Manas Sule, SRF; Prashant Sonawane, JRF; Priyabrata Panigrahi, JRF

One aspect of this project involves studying the recognition of various substrates by three related enzymes showing penicillin acylase and bile salt hydrolase activities. The study involves finding the reason for variation in affinities for a set of substrates by these enzymes and engineer them to bind cephalosporin C. Software available in the public domain are not suitable. Commercial software MOE did not provide decisive results. Preliminary investigations using evaluation copies of softwares supplied by Schrodinger and Accelrys were encouraging. We have also tried to install the biosuite programs but not completely successful due to non-compatibility with 64 bit linux operating systems. Presently the workstations for both computation and connecting to the cluster computer are available. Purchase of a suitable software is awaited for further studies. Lignin is a biopolymer; in abundance is next to cellulose. The seven genes involved in lignin biosynthetic pathway

isolated from *Leucaena leucocephala* have been cloned and sequenced. All the proteins involved have broad substrate specificity. One of them, Cinnamoyl-CoA reductase (CCR1), catalyses the conversion of cinnamoyl-CoAs into their corresponding cinnamaldehydes. This is the first step of the phenylpropanoid pathway specifically dedicated to the monolignol biosynthetic branch. This enzyme has been already studied in maize and rice.

As a first step we have carried out modeling of the three-dimensional structure of CCR1 from *L. leucocephala* using its protein sequence. A search using BLAST in the PDB database detected dihydroflavinol-4-reductase (2c29) to have 40% sequence identity with CCR1. Submitting the sequence to MODWEB modeling server output a model using homology modeling based on the template structure of dihydroflavanol reductase from *Vitis vinifera*. The resultant model was validated using assessment tools of Modeller and checked its quality using PROCHECK. Further substrate binding studies and affinities can be undertaken only using good docking softwares.

**Computational heterogeneous catalysis**

**PI : Kaliaperumal Selvaraj**

**Members :** Reshmi Kurian, PA-II; Geetha Arumugan, PA-II  
**Collaborator:** Prof. B. Viswanathan, IIT, Chennai

The Objectives of this study are:

- ✦ To understand the influence of alkali elements on the pre- nucleation species those exist during the synthesis of silicate / zeolite, and
- ✦ To study the structure-property relations of noble bimetallic nano and sub-nano clusters for Fuel-Cell (DMFC) applications

*Study on the influence of alkali elements on the pre-nucleation species of zeolite synthesis.*

The interactions of the most basic building block of zeolite synthesis, namely, the ortho-silicic acid  $[\text{Si}(\text{OH})_4]$  (also known as  $\text{Q}^0$ ) species with the reaction mixture and within themselves are key factors to drive a zeolite synthesis on a specific route to form different microporous silicate structures. Zeolite based on its structure and pore architecture entitles to be one of the best industrially known catalyst for complex reactions. It is well known that the presence of alkali element in the reaction mixtures brings a substantial difference in the crystallization time. However, its role on the kinetics of the synthesis is not completely

understood as the  $\text{Q}^0$  species are highly challenging to be studied using experimental spectroscopic techniques namely, NMR etc. Quantum mechanics (Density Functional Theory - DFT) based computational studies carried out in our laboratory has brought a significant insight into this crucial problem.

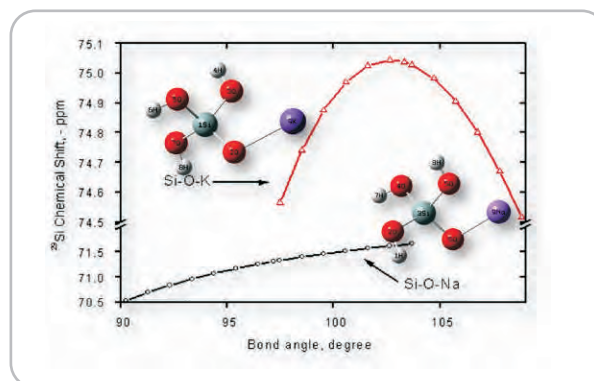


Figure 1. Distinct trends in the  $^{29}\text{Si}$  NMR chemical shifts as a function of changing Si-O-M<sup>+</sup> bond angle of different alkali-Q<sup>0</sup> species.

*Ab initio* theoretical calculations were carried out over a wide range of optimized models of  $\text{Q}^0$  species with different alkali cations such as  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$  etc., at DFT level with the HF self-interaction corrected, hybrid B3LYP functional with split valence basis set along with polarization and

## Scientific Computing

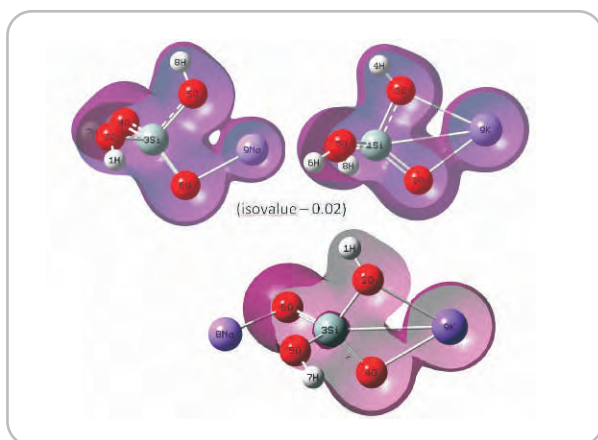


Figure 2. Sliced electron density iso-surfaces for different alkali-Q<sup>0</sup> species shows distinct interaction between the alkali and the non-bonded bridging oxygen.

diffuse parameters namely, 6-311G+(2d,p). Their <sup>29</sup>Si NMR chemical shifts were also calculated using GIAO method. Natural Bonding Orbital (NBO) and Perturbation Theory based energy analysis were used to understand various interactions between different alkali ions with Q<sup>0</sup> species. NMR chemical shift variations as a function of geometrical parameters indicated a possibility of different modes of interactions with different alkali elements with Q<sup>0</sup> species which was also confirmed by the NBO occupancy analysis. The electron density iso-surfaces (Fig. 2) showed that few alkali cations have characteristic non-bonded interactions that significantly modify electron density around the central Si atom which is reflected in the NMR chemical shift values. On the use of more than one alkali elements for example, Na<sup>+</sup> and K<sup>+</sup> in the synthesis, the calculations show that the kinetics of zeolite crystallisation would alter as the polarization of the Q<sup>0</sup>, namely, species changes drastically [**Micropor. Mesopor. Mater.**, 2009, 122, 105].

*Study on the structure-property relations of noble bimetallic nano and sub-nano clusters for Fuel-Cell applications*

'Methanol crossover' is a serious problem that challenges the overall performance of a direct methanol fuel cell (DMFC).

An attempt to solve this by making a methanol resistant cathode material is a key focus globally. Noble bimetallic nano-particles are showing excellent improvements while used on the electrode. However, the effective compositions and interactions between them are not yet completely understood. We have used *deMon2k*, a DFT supporting code to study the structure, stability aspects of various compositions of noble bimetallic subnano-clusters, viz., Au<sub>m</sub>, Pt<sub>n</sub>, and [Au/Pt]<sub>m+n</sub> where m+n = 2-8 and their interactions with oxygen and methanol.

The studies show clear proof for the stabilization effects of one metal on the other and the compositional effects on

gradual alterations in the methanol oxidation capabilities of the clusters. An example of conspicuous evidence for the fine tuning of oxidation capabilities of the bimetallic cluster may be demonstrated using a detailed analysis of CH<sub>3</sub>OH interactions with bimetallic clusters. Figure. 3 provides the structure details of the methanol adsorbed Au, Pt and Au/Pt dimer clusters of the most stable spin state and their energies of methanol adsorption on them. Pure Au cluster known to normally exist in singlet state shows a CH<sub>3</sub>OH adsorption energy of 0.41eV while the Pt dimer shows about 0.17 eV. However, the bimetallic effect drastically brings down to just 0.06 eV. A significant charge transfer from Pt to Au is observed to stabilize the structure and alters the cluster's redox capabilities. These results will be highly useful to predict the effective metal compositions and their redox capabilities that in turn help to selectively coat the cathode with preferred bimetallic pairs of noble metals and their ratios (**J. Phys. Chem A. 2009; accepted**).

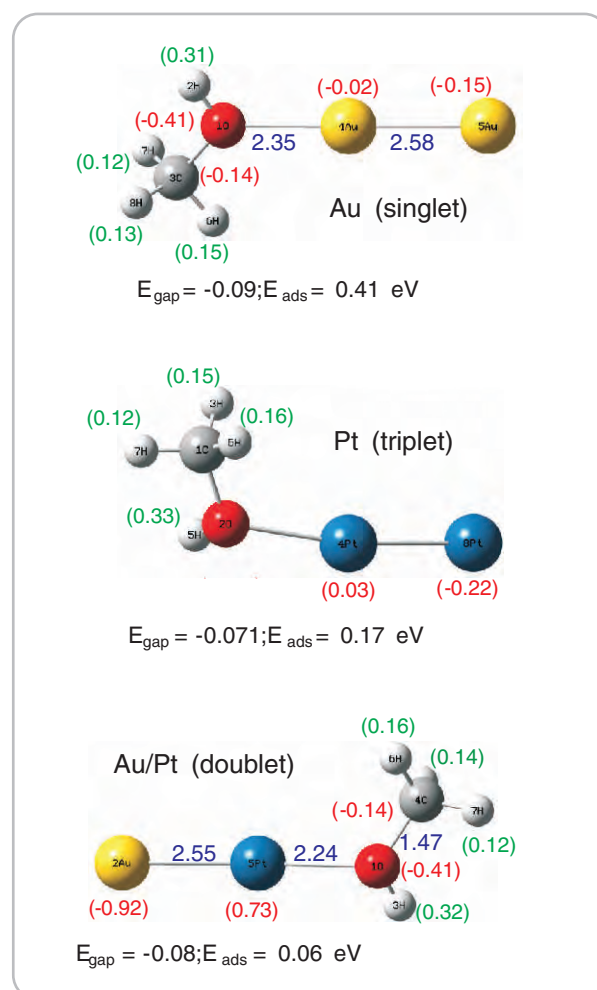


Figure 3. CH<sub>3</sub>OH adsorbed Au/Pt bimetallic subnano-cluster complex at their most stable spin states and their adsorption energies.

Microreactor Engineering



The micro-reactor engineering provides a unique opportunity to revitalize the present status of chemical industry and to enhance its benefits to the society. These micro-reactor technologies have created new platforms for conducting chemical synthesis effectively. With NCL's strengths in synthesis, catalysis, analysis, engineering and direct relevance with the industrial research, NCL has established a Centre of Excellence on Microreaction Technology (CoE). CoE has decided to use the logo as given here.



The CoE is a long term programme where the advantages of miniaturization and continuous flow will be explored and extended towards the understanding science of small devices and further use it to develop new technologies. The CoE will run a few interdisciplinary projects with the focus to use the microreaction technology for developing detailed

understanding about various applications, where the different aspects of the microreaction technology are expected to be useful. Initially, the CoE will be operational until April 2010 and then may be extended up to 2013 depending upon the performance of different proposed projects evaluated in periodic evaluations. Currently, the

CoE is an internal network of activities among the scientists from various divisions having an inclination towards exploring the viability of the continuous flow approach for specific scientific pursuits and depending upon the need and viability, in the due course, it may include research group(s) from other CSIR labs. The individual projects are periodically evaluated by a monitoring committee comprising faculties from different distinguished academic institutes. A team of scientists from NCL, working in this CoE is encouraged to submit new proposals from time to time for their evaluation to the monitoring committee. The CoE is coordinated by Chemical Engineering and Process Development (CEPD) Division. A team of scientists from different divisions (CEPD, Polymer Science Engineering, Organic Chemistry, Physical and Materials Chemistry Division) in NCL proposed a few joint projects to explore the applicability of microreaction technology for specific objectives. The inclusion of the new proposals under CoE is decided by the Director, after the recommendations of the monitoring committee.

In the first year, there are four projects that have been considered under the CoE: (1) Understanding hydrodynamics and scale-out strategies using microreactors, (2) Microreactor based process development for nitration and hydrogenation reactions, (3) Continuous process for functionalized nanoparticles and their scale-up, (4) Microreaction technology for development of hydrogel based prototype diagnostic disposable devices. The work has resulted in the four publications in the peer-reviewed journals.

Understanding hydrodynamics and scale-out strategies using microreactors

**PI: A. A. Kulkarni, V. V. Ranade**

**Members :** V. S. Kalyani, PA-II, C. M. Karale, SRF, Apoorva Kumar Srivastava, IIT-Kanpur, Project Student

Although the microreactors are being used for laboratory scale R&D in a significant way, the transfer of the technology from lab scale to the industrial scale is largely hampered due to the absence of the information about the scale-up or scale-out strategies. Hence in the proposed work we aim at identifying the strategies for scale-up.

Two-phase flow in mini-channels (1 mm x 1.5 mm x 430 mm and 1.5 mm x 0.5 mm x 430 mm serpentine channel geometry) made in different materials (SS 316, PMMA and Teflon) was studied at different flow rate ratio (0.66, 1.0 and 1.56) of the two immiscible fluids. A dual syringe pump was used to pump the fluids (air-water and water-kerosene) through the channels. For characterization of the two phase flow, experiments were carried out to measure the slug size

distribution and relevant hydrodynamic properties, pressure drop across a single serpentine unit (i.e. one sinusoidal unit that includes two 180° return bends connected by a straight portion of 20 mm) and also the residence time distribution of water. In all the cases, the effect of material of fabrication on the hydrodynamics was significant.

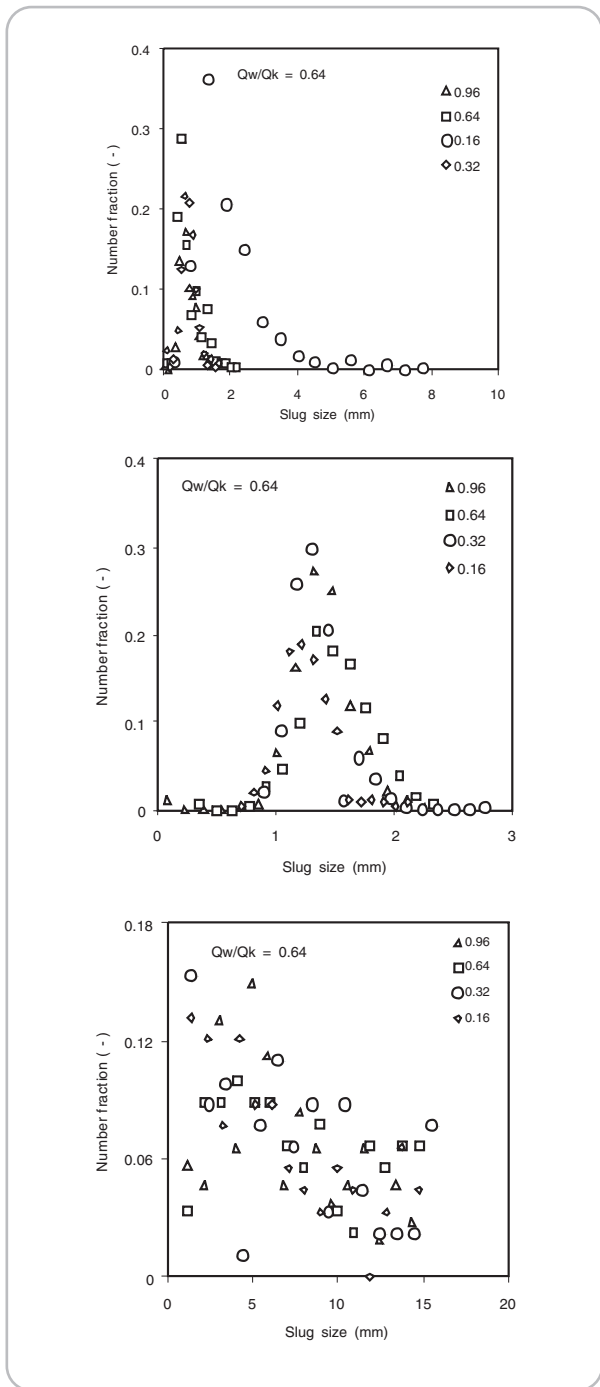
Apart from flow rates and flow rate ratio of the two fluids, the slug size distribution was seen to have a strong effect of the channel orientation (vertical, horizontal) and also the flow direction (up-flow and down-flow). In the RTD studies, the response curve observed at the end of the channel was significantly different than the published literature. The reasons for such observations are discussed in detail.

The experimental results of pressure drop and heat transfer confirm that including the entrance effects, the conventional theory is applicable for water flow through micro-channels. The present results highlight the importance of accounting for common phenomena that are often negligible for

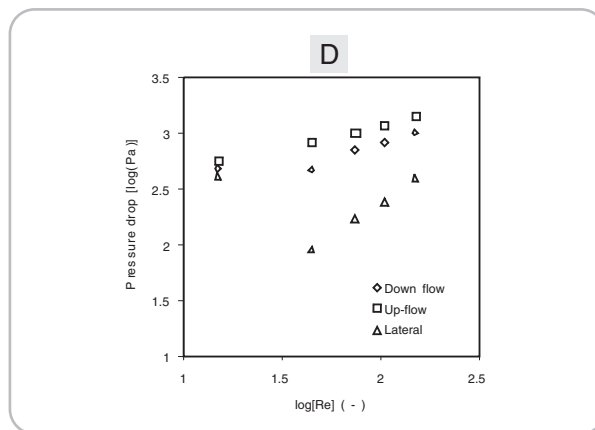
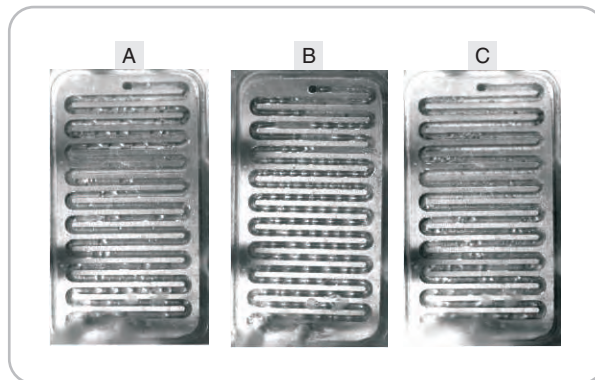


Microreactor Engineering

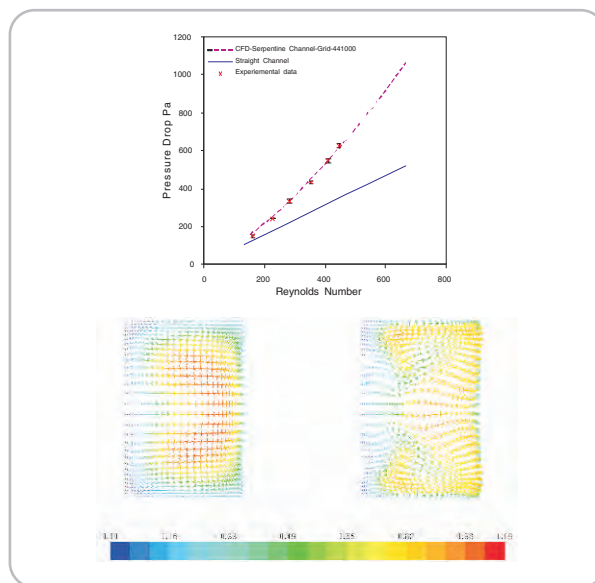
standard flows such as accounting for profile of inlet velocity, axial heat conduction, conjugate heat transfer, effect of the design inlet and outlet manifolds [Ind. Eng. Chem. Res., 2009, 48, 8193].



Slug size distribution observed on the serpentine channel. (Left to right: PMMA, SS316, PMMA plate with 1.5mm channel width). The legends indicate the water flow rate  $Q_w$  in (ml/min).  $Q_w/Q_k$  indicates the water to kerosene flow rate ratio.



Typical slug distribution seen on the SS316 plate for the vertical orientation of the plate. The flow is from bottom to top. A) 6 ml/min, B) 10 ml/min, C) 14 ml/min, D) Effect of plate orientation on pressure drop.



Pressure drop through single serpentine channel and velocity vectors plot at the inlet and outlet of the bed

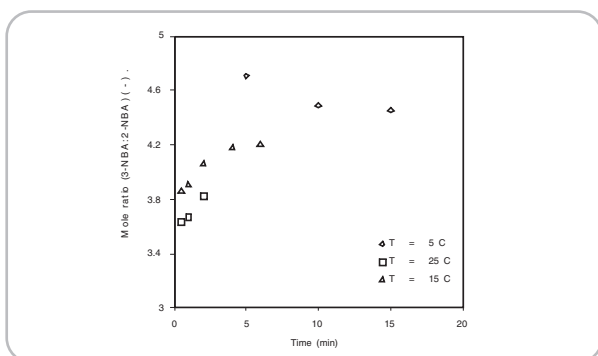


Microreactor based process development for nitration reactions

PI: R. A. Joshi, Dr. R. R. Joshi, A. A. Kulkarni

Members : N. T. Nivangune, PA-II, V. S. Kalyani, PA-II

**Continuous flow nitration of benzaldehyde:** The nitration of benzaldehyde can be carried out in a safe manner in continuous mode using microreactor system. Choice of a micromixer was seen to affect the performance of this two phase reaction significantly. The reaction time could be brought down to 30 s by increasing the reaction temperature and thereby taking advantage of higher heat transfer area. The effect of inlet composition to the micromixer on the product composition is illustrated to indicate the possibility of achieving variability in the product composition from time to time. Further scope of process intensification is also discussed.

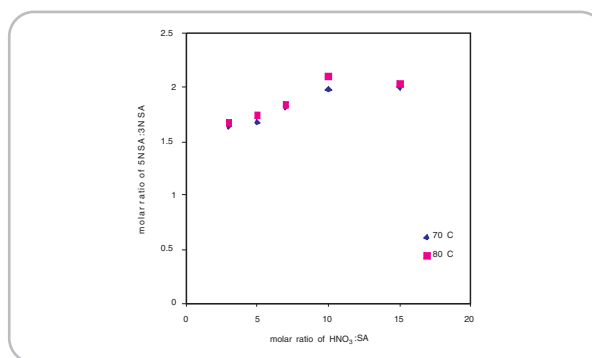


Effect of temperature on the outlet product composition. The inlet composition is fixed at nitric acid to sulfuric acid, mol/mol ratio 0.6:1 and nitric acid to benzaldehyde mole ratio 3.5:1.

The observations from above experiment indicate that on further increasing the temperature of the system, the continuous flow nitration of benzaldehyde can be carried out in a time span of few seconds. This also would mean that preheated reactants if mixed at the desired temperature using a micromixer would help to achieve an instantaneous reaction leading to the complete conversion of the reactants. Thus, having a suitable micromixer with sufficient mixing length would help to eliminate the residence time tube thereby opening several different options for scaling out of miniaturized system for this reaction.

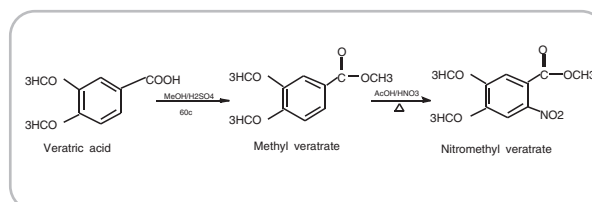
**Nitration of salicylic acid at higher temperature:** Although nitrating mixture contains nitric acid and sulfuric acid, usually, handling of sulfuric acid and its separation from the product mixture is always an issue. In view of this, here we demonstrate the nitration of two aromatic

substrates leading to important pharmaceutical intermediates using a nitrating mixture of nitric acid and acetic acid at higher temperatures. The effect on the % yield of the desired isomer has been improved by choosing the right combination of temperature and residence time.



Effect of temperature on the molar ratio of 5NSA:3NSA with respect to increasing molar ratio of HNO<sub>3</sub>:SA it is observe that the selectivity of 5NSA is increases with respect to temperature and molar ratio of HNO<sub>3</sub>:SA

**Nitration of methyl veratrate:** For the case of nitration of veratric acid, it is necessary to carry out the esterification of substrate with methanol in presence of sulfuric acid. This step was carried out in batch mode. On synthesizing methyl veratrate, it was used as a substrate for further nitration.



In batch mode, at 40°C, the complete conversion of the substrate could be achieved in 20 minutes, and at 50°C, it required only 10 minutes. The reaction time can be further reduced by increasing the temperature; however this becomes irrelevant for batch operation as batch mode is not suitable for such time scales. Continuous flow nitration of methyl veratrate was carried out in SS316 tubular microreactor. The residence time was varied by changing the flow rates. The experiments were carried out at higher temperature (50 – 80°C) and the samples at the tube outlet were quenched by urea and methanol solution. The product at the outlet 2-nitro methyl veratrate was confirmed by NMR. The experiments showed that at 80°C, complete conversion of the substrate could be achieved in less than 30 s, which is not realistic in batch mode [Org. Proc. Res. Dev., 2008, 12, 995; 2009, 13, 999].

Microreactor Engineering



Continuous process for synthesis of functionalized nanoparticles and their scale-up

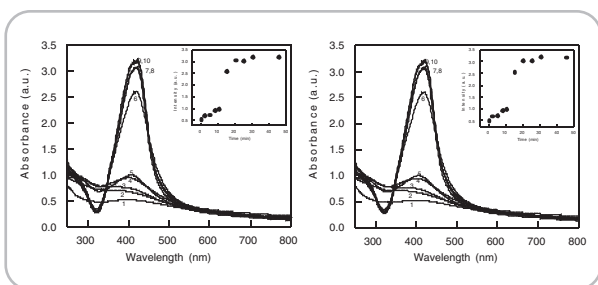
PI: B. L. V. Prasad, Dr. A. A. Kulkarni

Members : V. Ravi Kumar, JRF, M. B. Kasture, SRF

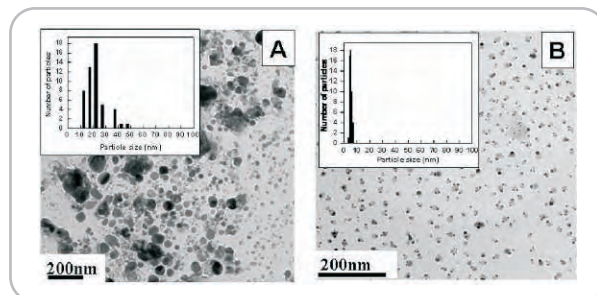
Continuous flow synthesis of nanoparticles has a lot more advantages than the conventional methods. The proposal aims at developing processes for the same to achieve the synthesis at relatively larger scale. Initial studies will be done on the model systems and later the attention will be focused on Co nanoparticles. In order to develop a synthesis protocol and methodology for the nanoparticles, initially, the studies were done for the model systems viz. synthesis of Ag and Au nanoparticles. On finalizing the synthesis strategy, the miniaturized device will be extended for the continuous flow synthesis of Co nanoparticles.

**Continuous process for Ag nanoparticles:** Synthesis of Ag nanoparticles was achieved by adding KOH to the sophorolipid and AgNO<sub>3</sub> mixture. In a typical experiment 10 mL of 10<sup>-3</sup> M concentration of sophorolipid was taken and to it 1mL of 10<sup>-2</sup> M AgNO<sub>3</sub> was added so that the final concentration of AgNO<sub>3</sub> is 10<sup>-3</sup> M. Initially the reaction was carried out using oleic acid and linoleic acid sophorolipid at different temperatures i.e. RT, 40, 60, 80 and 90°C. UV-visible recorded for the samples show that the reaction is faster at higher temperature than at lower temperatures. A sharp surface plasmon peak centered around 420 nm is observed for higher temperature (90°C) for both OA-SL and LNA-SL. All the UV-visible was recorded after 5 min of reaction. Figure shows temperature dependent UV-visible spectra for OA-SL and LNA-SL reduced/capped Ag nanoparticles.

From the UV-visible we observe that in case of OA-SL reduction occurs even at 80°C while for LNA-SL reduction occurs only at 90°C. The reaction in case of SA-SL the reaction is complete within 5 min while in case of OA-SL it takes around 20 min for completion of reaction as indicated by saturation of UV-visible peak in both cases. Transmission electron microscopy (TEM) result show that the particles size obtained at lower temperature are irregular and larger in size that the particles synthesized at higher temperatures.



Time dependent UV-visible study for Ag nanoparticles synthesized using (A) OA-SL and (B) SA-SL as reducing and capping agent.

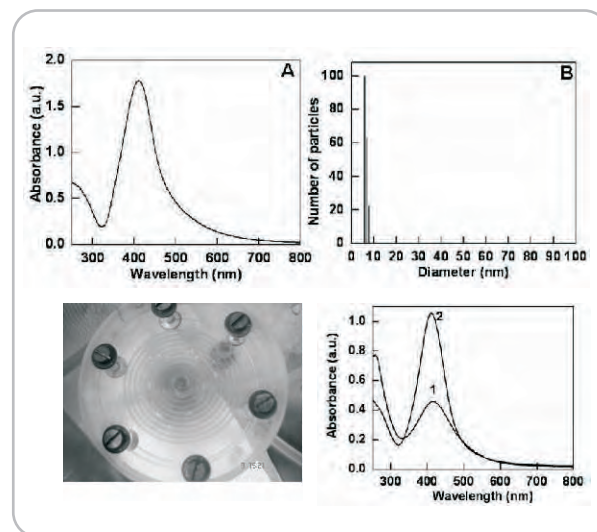


TEM images for silver nanoparticles synthesized using oleic acid sophorolipid as capping/reducing agent. (A) for the experiments carried out at 40 °C and (B) are for reaction carried out at 90 °C. Inset shows the particles size distribution.

The experimental setup for the synthesis of Ag nanoparticles in micro channels consists of two syringe pump, water bath, microreactor, syringes. Mixture of SA-SL+ AgNO<sub>3</sub> was taken in one syringe and KOH in the second syringe. Both the syringe was placed on the syringe pump and attached to SS tube through a T-junction.

The inner diameter of the SS tube was 1mm and the length was 1 M. The flow rate was calculated such that the residence time was 5 min. the flow rate was maintained at 0.027 ml/m. obtained product was analyzed by UV-visible, DLS and TEM.

Keeping the same set up and changing the SS tube with acrylic circular disc we performed set of experiments where we monitored the synthesis of Ag nanoparticles as a function of changing flow rate. For all the reactions SA-SL was used as capping /reducing agent.



(A) UV-visible of Ag nanoparticles synthesized using SA-SL as reducing/capping agent in SS tube with flow rate 0.027 ml/m. (B) Particle size distribution obtained from DLS measurements which indicates the average particle size to be 7 nm. (C) Spiral microreactor (D) UV-visible for Ag nanoparticles synthesized in circular disc at different flow rates 1ml/m (curve 1) and 100 l/m (curve 2)

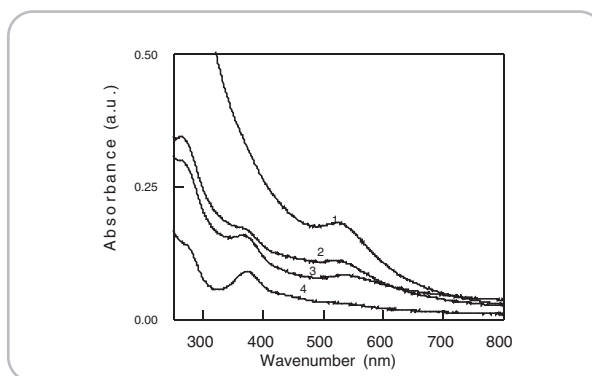
Microreactor Engineering



In order to overcome the possible mixing related non-idealities in particle size distribution, we developed a disk shaped spiral microreactor for the continuous flow synthesis of nanoparticles. The spiral structure helps to generate secondary circulating flow in the channel that keeps the particles continuously circulating thereby avoiding the effects of residence time distribution across the channel cross-section.

*Co-synthesis of bimetallic Au-Ag nanoparticles:* An attempt was made to synthesis of Au-Ag bimetallic nanoparticles in circular disc micro channels. Photographs recorded of the disc after the synthesis of Au-Ag nanoparticles show that Ag nanoparticles are deposited near the inlet while Au nanoparticles are deposited at outer channels. The secondary flow lifts the smaller particles and deposits the larger particles at the center and the centrifugal force leads to deposition of smaller Au particles at the outer channels and Ag nanoparticles at the inlet. From the UV-visible graph we see that at flow rate of 1mL/m only peak corresponding to Au is observed while at the intermediate flow rate that of 500 $\mu$ L/m and 200 $\mu$ L/m SPR peaks corresponding to Au at 520 nm and Ag at 420 nm are observed. At lower flow rate only Ag peak at 420 nm is observed. Form the batch reaction we observe that reduction of Au<sup>3+</sup> to Au<sup>0</sup> by SL is faster than Ag<sup>+</sup> to Ag<sup>0</sup> in presence of KOH. At the higher flow rates when the two solutions are mixed SL reduces Au ions and form Au

nanoparticles. Since the residence time is less and some amount of KOH is already used for reduction of Au ions the formation of silver nanoparticles may not take place and we observe peak corresponding to only Au at flow rate of 1 mL/m. As the flow rate decreases the peak corresponding to Au nanoparticles decreases while peak corresponding to Ag nanoparticle increases. Detailed studies are being carried out to understand the preliminary results that are observed from TEM images [J. Chemical Sciences, 2008, 120, 515].



UV-visible graph for Au-Ag bimetallic nanoparticle system at flow rates of 1mL / m (curve 1), 500 L / m (curve 2), 200L / m (curve 3) and 100L / m (curve 4)



## RESOURCE CENTERS

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## Catalyst Pilot Plant



Heterogeneous catalysis is of fundamental importance in the chemical industry and in other technologically relevant applications. Catalyst Pilot Plant (CPP) is well equipped with all the facilities required to produce range of solid catalyst/catalytic support materials such as silica based micro- and meso- porous molecular sieves, spinels, oxide composites and supported metal catalysts used in a range of industrial processes. CPP is well supported by various physico-chemical characterization facilities. CPP offers R & D services via different models of collaboration such as contract research, consultancy and technical services. The R & D activities were aimed at development of catalyst or support / synthesis route / catalytic process / protocol for characterization and scale up studies.

### Contractual R & D project activities

- ✦ Development of catalyst for tert-butyl amine from isobutylene and ammonia
- ✦ Formulation, characterization and scale-up of a process for the preparation of solid acid catalysts for bisphenol-A
- ✦ Physico-chemical properties of fresh and spent AACL catalysts
- ✦ Development of a continuous process for biodiesel and biolubricant
- ✦ Development of non-infringing catalyst process for the productions of DDM
- ✦ Bulk preparation, characterization and supply of catalysts

### Services offered

Chemical analyses by AAS, supply of D.M. Water, raw materials and finished catalysts to research community

## Center for Materials Characterization

Center for Materials Characterization (CMC) houses some of the most sophisticated equipment utilized for R & D projects of the Laboratory. The Center is run by core member scientists of the Center as well as by the affiliate scientists from other divisions of NCL. This is perhaps the only Center in India having wide range of facilities under one roof. The centre also undertakes contract research projects in niche areas from Govt and other (industry) agencies.

- ✦ The core member scientists of the Center have the expertise in the following areas:
- ✦ Single crystal X-ray crystallography of small organic molecules
- ✦ Powder X-ray diffraction of crystalline and semicrystalline materials
- ✦ Electron microscopy (scanning and transmission) of soft and hard materials
- ✦ Surface spectroscopy of catalytic, inorganic and polymer materials
- ✦ Mass spectrometry of organic and biomolecules
- ✦ Measurement of magnetic properties of materials.

### The Resource Center is equipped with following facilities:

- ✦ **X-ray diffractometry** (Bruker SMART APEX CCD single crystal X-ray diffractometer, Philips Xpert Pro PW-3040, Pan analytical Xpert Pro powder diffractometer)
- ✦ **Scanning electron microscopy** (Leica Stereoscan 440 SEM , FEI Quanta 200 3D with EDXS)
- ✦ **High resolution transmission electron microscopy** (Tecnai F 30 with 300kV FEG;FEI make)
- ✦ Electron spectroscopy (ESCA 3000 system)
- ✦ **Mass spectreoscopy** (LC- MSPE SCIEX, HR-MS, and MALDI-TOF-MS)
- ✦ **Magnetic measurements** (EG & G PAR 4500 vibrating sample magnetometer)

### Annual utilization of CMC facilities

No. of samples analysed	In-house	Outside
	15613	201
Total no. of samples	15814	
Total earning from outside samples, (in Indian Rupees)	26 lakhs (approx.)	

## Central NMR Facility



This Resource Center provides NMR support to all the scientific activities of the laboratory. The scientists associated with this Resource Center also carry out research activities on application of NMR spectroscopy in diverse areas of chemical, biological and materials sciences. The Center maintains and operates four Bruker Avance NMR spectrometers operating at 200, 300, 400 and 500MHz. Although the primary users of this facility are from the research community within the laboratory, the facility is open to researchers in other educational institutions and industries. Apart from the technical support, the Center also plays an integral part in the basic and applied research activities of the Laboratory.

### The scientists of the Center have expertise in the following areas

- ✦ Solid and solution state NMR methodology development.
- ✦ Structural elucidation of organic and bio-organic molecules
- ✦ Micro structural analysis of polymers
- ✦ NMR of molecular self assemblies
- ✦ NMR of gels
- ✦ Protein- ligand binding studies
- ✦ NMR in Biotransformations
- ✦ Protein-nucleic acid interactions
- ✦ Diffusion by pulse field gradient NMR
- ✦ Application of solid-state NMR in Materials Science (polymers, molecular sieves, layered oxides, bio-materials, nanomaterials etc.)
- ✦ Identification of polymorphs by solid state NMR
- ✦ Molecular dynamics in polymers using solid-state NMR
- ✦ NMR instrumentation and maintenance
- ✦ Computational NMR (density matrix numerical simulations, powder spectral simulations and *ab initio* calculations), simulation techniques.
- ✦ Micro imaging

### Facilities Available

The **AV-500** has a standard bore (54 mm) magnet with a field of 11.75 T and is a three channel spectrometer equipped for solution and solid state NMR. This is equipped

with a QNP probe ( $^{31}\text{P}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  and  $^1\text{H}$ ), a 5mm inverse broad band probe ( $^{95}\text{Mo}$ - $^{31}\text{P}$ ) with gradients, a 10 mm high temperature  $^{13}\text{C}$  probe for polymer characterization, a 5mm triple resonance TXI probe with gradients ( $^{13}\text{C}$ ,  $^{15}\text{N}$ ,  $^1\text{H}$ ) and a 5mm broad band BBOF probe with gradients ( $^{109}\text{Ag}$ - $^{31}\text{P}$  and  $^1\text{H}$ ,  $^{19}\text{F}$ ) for the solution state NMR and a broad band 4mm CP/MAS probe, a 4mm HRMAS probe and a Doty 4mm triple resonance probe for solid-state NMR.

The **AV-400** has a standard bore (54mm) magnet with a field of 9.39 Tesla and is a two channel spectrometer for solution state NMR. This has a broad band ( $^{95}\text{Mo}$ - $^{31}\text{P}$ ) observe (BBO) probe with gradients,  $^1\text{H}$ - $^{13}\text{C}$  inverse (SEI) probe with gradients, high temperature (SEX)  $^{13}\text{C}$  probe and a broad band observe probe (BBFO) with gradients ( $^{109}\text{Ag}$ - $^{31}\text{P}$  and  $^1\text{H}$ ,  $^{19}\text{F}$ ).

The **AV-300** has with a wide bore (89mm) magnet with a field of 7.05T and is three channel spectrometer exclusively for solid state NMR and micro-imaging. This has a 4mm triple resonance probe ( $^{31}\text{P}$ - $^{15}\text{N}$ ,  $^1\text{H}$ ), a 2.5mm MAS probe with STMAS attachment, a 4mm double resonance probe with low gamma nuclei capability, a wide line probe ( $^{109}\text{Ag}$  to  $^{31}\text{P}$ ) and a micro imaging probe with 5-25mm inserts.

The **AV-200** has a standard bore (54mm) magnet with a field of 4.7 T and is a two channel spectrometer which is used for routine solution state NMR and is equipped with a 60 carousel auto-sampler. This has a QNP ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$  and  $^{19}\text{F}$ ) probe and a dedicated  $^1\text{H}$  probe.

### Annual utilization of NMR facilities

No. of samples analysed	In-house	Outside
	23741	662
Total no. of samples	24403	
Total earning from outside samples, (in Indian Rupees)	26 lakhs (approx.)	

### Digital Information and Knowledge Resource Center



NCL deploys tools of information technologies to help its scientists to be in the forefront in their chosen area of research. DIKRC through Network Administration Unit (NAU), Knowledge Resource Centre (KRC) and Chemoinformatics contributes to the NCL's success as a leader in R&D by bringing together information, knowledge, tools and systems for informed decision making for research and management.

#### Digital Information and Resource Center

Digital information and resource center (DIRC) is responsible for planning, installations, enhancement, operation, setting up and maintenance of IT infrastructure of the laboratory including computers, servers and network components, data storage services as well as management of time and access control system. The center also provides well secured Internet and e-mail services for the NCL staff. The center is continuously in the process of upgrading the infrastructure to provide recent technology to the LAN / WAN users.

Center enhanced its existing Internet Bandwidth from 34 (1:4) Mbps shared leased line to 34 (1:1) Mbps dedicated leased line, standard leased line on fail safe OFC link with Ethernet connectivity to fulfill internet requirements, which may be broadly classified as data upload / download using FTP, accessing other networks by building a VPN, Internet browsing, mails Download as well as Video conferencing.

In this year, center has installed content delivery device that offers content caching, hosting, content replication and other content-based services. It has capability of filtering, blocking, reporting millions of web pages in various categories. It will also help in meeting the risks of internet use and offering maximum protection by identifying and classifying known and emerging internet security threats.

This year, eleven L3 switches were installed. Autosensing on each non-SFP port detects the speed of the attached device and automatically configures the port for 10/100. They support inter-VLAN IP routing for full Layer 3 routing between 2 or more VLANs. All the rooms in the NCL guest house (15, with built-in wireless network cards to support WI-FI connectivity) as well as common rooms of GJ hostel (5, wired connectivity) and new hostel (3, wired connectivity) were provided with Thin-clients. Twelve wireless network devices were installed to provide wireless connectivity in the conference halls / lecture halls of various divisions

Pre-wimax / Wi-Fi technology was installed to connect area of NCL colony and establish wireless network. DIRC also deployed a new web-based 'Time attendance and Access control Management system'.

#### Knowledge Resource Centre

Knowledge Resource Center (KRC) / Library provides seamless access to information resources print as well as Electronic format. KRC homepage provides links to all the subscribed E-resources and also information about the services offered. The homepage was modified and updated continuously.

#### Print collection

KRC as on March 2009, has a total collection of 1.38 lakhs,

which includes books and bound volumes of journals. During this year, 564 books were purchased and 250 Indian and foreign print journals were subscribed. KRC subscribed to 55 electronic journals. Research students submitted 84 theses and link has been provided on intranet to the awarded theses. Electronic Resources: Being the part of CSIR consortium project, access was provided to more than 3300 journals from 10 publishers. Access to databases like Web of Science, Delphion, DII Micropat was also available under consortium project. During this year KRC subscribed to Springer E books on Biomedical and Life Sciences (2005-2008). Access to Scopus, Annual Reviews, Methods in Enzymology series, Chemical Abstracts on CD, India Patents and Chemical Business News Base was continued.

#### Services

Information related services like document delivery of journal articles, patents, searching of specialized online databases and translation of scientific documents were provided to 12 pharmaceutical companies. Membership to the KRC is also open to research students and faculty members of colleges and universities and to the industries. This year 242 outside members referred the library.

Annual Events: A book exhibition was arranged for providing an opportunity to readers to browse latest books and select books of their choice for purchase. Training programs to know the E-resources were conducted for Scientists and Research fellows. Publisher's experts worked as resource persons. This helped to maximize the use of the available resources.

KRC's RFID system is now working satisfactorily. One additional self checkout station with drop box is positioned to save the time of members while issue / return of books. Inventory wand is purchased to find out misplaced books and bound volumes of journals. Radio Frequency Identification (RFID) system for KRC helps for self check-outs by members, stock verification, misplaced documents search and documents security.

#### Chemoinformatics

The java based chemoinformatics software tools such as Chemstar, Texthra, J-Proline, Scaffoldpedia, 3D Chemeye and Chemscreener were developed.

ChemStar is an opensource based chemical computing toolkit for distributed computing environment. We developed the server/client communication framework as well as an application to distributed computing of chemical properties on a large scale (currently the size of PubChem; about 18 million compounds), using both the Marvin toolkit as well as the open source JOELib package. ChemStar was built on Java RMI, which is also easily adaptable to user demands due to its "plug-in architecture". The complete source codes as well as calculated properties along with links to PubChem resources are available at <http://moltable.ncl.res.in/chemstar/>.

TextHydra is a chemically intelligent textmining tool for building biological networks from medical literature and is capable of handling both chemical and biological data from scientific literature in order to establish link between chemicals and their roles in biological systems. Several standard textmining methods were implemented in this tool like tokenization, part-of-speech tagging, dictionary lookup, chemical name

## Digital Information and Knowledge Resource Center



recognition, biological term recognition (proteins, genes, diseases, organisms etc.) and extraction of relations between them. The program reads plain text (for example abstracts from PubMed) containing both chemical and biological data and transforms them into meaningful relationships through annotation, classification, interpretation of chemical names as molecules and build biological networks.

J-Proline is a tool for analysis of protein ligand complexes. It is based on open source architecture compatible for distributed computing environment. The similarity scores and alignment data generated computational methods were used to build the protein-protein network, heatmaps and other statistical analysis for identification of selectivity of the ligands towards protein targets. The ligands with common scaffolds were identified and used for virtual library generation and screening against biological targets using in-silico methods. In order to overcome the time constraints for computational tasks the program is implemented on distributed environment which was previously used successfully for ChemXtreme and ChemStar cheminformatics applications.

Scaffold translator is compatible for distributed computing environment to handle massive computational tasks. Over a million molecular scaffolds were extracted from over 50 million diverse molecular structures of Pubchem to build a repository named Scaffoldpedia. The Scaffoldpedia is suitable for identifying molecules which are very novel in terms of their molecular frameworks and also to identify similar compounds from published literature and patents.

3D ChemEye is an optical chemical structure recognition tool for automatic transfer of chemical structure images into 3D

molecular structures for scientific computing. Chemical structures are stored as textual names or bitmap images of structures. Extracting molecular structure for reusability in vector graphics format back from these bitmap images is a challenging task. 3D ChemEye is a cheminformatics application designed to convert images of graphical chemical representation into truly computable formats in both 2D and 3D conformations. Currently this program is capable of reading several image formats like GIF, JPEG, PNG, TIFF, BMP, PDF etc., and able to generate the molecular structures in SMILES, SDF and MOL formats suitable for chemical structure databases. Since the optical recognition is unlikely to be perfect, the attempts are being made to improve the quality of reproducing chemical structures.

ChemScreener was developed to design focused virtual library and In-silico screening for lead likeliness against common protein targets. The role of chemscreener is to reduce the cost and time associated with lead molecule discovery in the early stage of drug design. It consists of several modules to handle large scale molecular structures, extraction scaffolds and functional groups from molecules of biological interest. The virtual synthesis of structures employs a scaffold-appendage based strategy. The core component of this program is to re-assemble large number virtual molecules using combinatorial approach and screen them in-silico for their drug likeliness, lead likeliness and pharmacophore based searching. These molecules were validated for their fitness for ease of synthesis, physicochemical properties and biological activities using simulation and modeling studies. The selected list of 'hits' after docking studies against known protein targets could further validated through experimental methods including chemical synthesis and bio-activity evaluations.

## National Collection of Industrial Microorganisms



The National Collection of Industrial Microorganisms (NCIM) preserves nonpathogenic, industrially important microbial cultures and provides authentic cultures to research institutes, colleges, universities and private organizations on request. The center generated an ECF of more than Rs. 52 lakh during the year by providing cultures to industries and research institutes including testing of samples.

**Preservation of microbial cultures:** The center maintains approximately 3500 microbial cultures of bacteria, yeast and fungi using regular transfer and lyophilization methods. The cultures which are in frequent demand are tested for their purity and biochemical performance.

### Strain improvement for production of L-lactic acid

Protoplast fusion is a useful technique in the improvement of microorganisms. This technique allows the exchange of entire genomes between unrelated genera of microorganisms. It is considered as a classical or fundamental method of gene transfer in which multiple genes can be introduced in contrast to the advanced methods in molecular biology which are suitable for introducing only one or few genes. Recent reports on genome shuffling in *Lactobacillus* proved the success of protoplast fusion approach which generated new population of strains with additional improvements in acid and glucose tolerance. This genome shuffling approach was also used to obtain *Lactobacillus delbrueckii* strain capable of converting starch to lactic acid. It is necessary to optimize the conditions for protoplast formation and regeneration before we proceed to fusion experiments. Hence we tried to standardize the methods of protoplast isolation and regeneration using one of the mutants of *Lactobacillus delbrueckii*, Uc-3. We found that there is no established universal method for protoplast regeneration of all genera of lactobacilli. This could be due to the requirement of suitable osmotic stabilizer for regeneration. However, we found that sucrose was the best osmotic stabilizer for regeneration of protoplasts of lactobacilli since we get more than 30% efficiency of protoplast regeneration in case of all the species of *Lactobacillus* tested. This work will provide a basis for the genetic improvements of *Lactobacillus delbrueckii* using protoplast fusion approach (*Ind. J. Microbiol.* 2009, In Press; *Appl. Environ. Microbiol.* 2008, 74: 333).

### Screening of *Lactobacillus* strains for D-lactic acid production and its improvement

We screened 78 lactic acid producing strains from NCIM and tested them for production of D-lactic acid using L-lactate oxidase enzyme kit. Among them, *Lactobacillus lactis* NCIM 2368, *Streptococcus faecalis var liquifaciens* NCIM 2406 and *Streptococcus salivaris* NCIM 2610 were found to produce D-lactic acid from hydrolyzed sucrose based fermentation medium. Our objective of present work was to develop mutants of all above selected organisms capable of producing enhanced levels of D-lactic acid with higher productivity. Few mutants were selected through UV mutagenesis showing bigger acid formation zones on the selected medium. We examined mutants for their growth and lactic acid production. *Lactobacillus lactis* NCIM 2368 was producing better D-lactic acid (16.0g/l) within 24 h using 100g/l of hydrolyzed cane sugar. This strain was further employed for mutagenesis using UV-irradiation. This protocol resulted in isolation of improved strain, RM-2 producing D-lactic acid 49g/l in 24 h with enhanced productivity (2.0g/l/h).

### Prostaglandin intermediate preparation of 4(R)-hydroxy cyclopent-2-en1(S)-acetate

4(R)-hydroxy cyclopent-2-en1(S)-acetate is an important intermediate in the synthesis of cyclopentanoid natural products, for example, prostaglandins, prostacyclins, thromboxanes, and recently in the synthesis of some anti-HIV drugs. The desymmetrization of mesodiacetate using most of the efficient enzymes, except PLE, shows pro-S preference yielding 4(S)-hydroxy configuration. It is possible to get desired 4(R)-hydroxy configuration from 4(S)-hydroxy configuration which involves additional steps and the use of diethylaluminium chloride or DIBALH which are costly and hazardous and hence not recommended for large scale. A yeast, *Trichosporon*, was identified from our culture collection which has pro-(R) preference yielding 4-(R)-hydroxycyclopent-2-en1-(S)-acetate from meso-cyclopent-2-en-1,4-diacetate albeit with low enantioselectivity. Detailed medium engineering investigations resulted in enhanced enantio-selectivity of the enzyme affording the right enantiomer with 85% optical purity (**U.S. patent No. 6,448,051 B1**). The patent has been licensed to one of the pharmaceutical industries, interested in the production of 4(R)-hydroxy cyclopent-2-en1(S)-acetate which is an important intermediate in the synthesis of cyclopentanoid natural products.

### Lipase from *Aspergillus niger* NCIM 1207

Chitosan and its derivatives have been used as affinity matrices for purification of lipase from *Aspergillus niger*. A total of 10 different chitosan derivatives were prepared and screened for lipase adsorption. Among them, TMA-cross-linked deacetylated chitin was selected as ideal support for adsorption. It adsorbed the lipase selectively, yielding approximately 5-fold purification of the crude lipase with 70% yield. Further 9-fold purification occurred on eluting through sephacryl-100. These results suggest that chitosan derivatives can be used as inexpensive biopolymer matrices for the purification of lipases for industrial applications (*Int. J. Biol. Macromol.*, 2008, 43: 422).

### Novel highly acidic phytase from *Aspergillus niger*

Phytases are the enzymes used for reduction of phytates in food and animal feed. They increase the bioavailability of phosphate and liberate the chelated minerals from the feed.

Novel highly acidic phytase production by *Aspergillus niger* NCIM 563 was studied under submerged fermentation conditions using statistical methods, namely, Plackett-Burman design and response surface methodology. Plackett-Burman design identified glucose,  $MgSO_4$ , KCl,  $MnSO_4$  and incubation period as five important parameters for phytase activity. Response surface methodologies and full factorial central composite design suggest that glucose,  $MgSO_4$ ,  $MnSO_4$ , KCl at concentrations of 8 %, 0.1 %, 0.005 %, and 0.1 % along with a 13- day incubation period, respectively, resulted in maximum phytase production. As compared to the one variable approach, which gave phytase production of 68,000 U/L, the optimization experiments using statistical methods gave a 3.8-fold increase (282%) in its production, that is, 2,59,800 U/L. Thus, phytase production was quadrupled due to optimization using statistical methods. Even though various high activity recombinant phytases are reported in the literature the phytase from the present study is more promising in poultry feed due to its high activity at pH 2.5 than others (*J. Ind. Microbiol. Biotechnol.*, 2009, 36:373).

## NCL Innovations



NCL Innovations (NCLI) was founded to champion the cause of technology innovations within the organization. The immediate goal of NCLI shall be to build and rejuvenate for NCL various component parts of a world-class ecosystem supporting the development and enrichment of commercially and socially useful knowledge (technology), protection and capture of value, exploitation of know-how, and the setting up of new commercial and social enterprises based on NCL know-how. Thus, NCLI will bring a fresh and renewed focus to and champion the cause of technology development and acceleration, technology commercialization (in concert with Business Development Division) and new venture development.

NCLI continue to run programs and activities in the following areas:

1. Technology acceleration, building innovation networks and creating a conducive culture (activities promoting technology innovation/ innovators from idea creation to proof-of-concept stage)
2. Intellectual property (activities and institutional systems to effectively and efficiently file for and manage intellectual property)
3. Technology commercialization (activities and institutional initiatives aimed at marketing, negotiating and facilitating the commercialization of intellectual property and technology)
4. Public-private partnership (build longer-term research and technology development partnerships with private entities that leverage NCL expertise and resources for creating intellectual property)
5. New venture development (activities, institutional policies and mechanisms to facilitate the creation of more technology enterprises using NCL know-how, expertise or involvement of NCL staff, students and alumni)
6. Developing the NCL Innovation Park as a home for technology innovation activities in partnership with private entities.

The NCLI team combines backgrounds in science, engineering/ technology, business and intellectual property/ law consisting of: Dr V Premnath, Dr V V Panchanadikar, Mr AD Kulkarni, Dr Magesh Nandagopal, and Ms Mousumi Khan.

### Quick-view of key emphasis areas

1. Venture Center: Mentoring support for Venture Center's first year of DST-NSTEDB funding. Help build a management team and organizational systems for Venture Center.
2. Intellectual Property Group: Taking over the erstwhile "Patent Cell" and putting in place entirely new systems, contracts etc and getting the activities back on track.
3. Consolidation and strengthening of NCL-TEC and student-led activities.
4. NCLI Seminar Series
5. First steps in technology/ IP marketing
6. Networking, skills up-gradation and strengthening group competencies.

### Venture Center

Under the mentorship of NCLI, the Venture Center took important, giant strides and is reported separately in the report.

### NCL Innovation Park – a home for public-private partnerships in the making

NCLI continued exploring longer-term public-private partnerships for NCL in the areas of materials, energy and bio-resource value additions and significant progress has been made in conceptualization of operational models.

### Intellectual Property Group

During the year, NCLI officially took the Intellectual Property Group (IPG) under its umbrella. Although the IPG shall operate independently, NCLI was charged with rethinking the role and activities of the IPG and chart a course for its future. The IPG is a service group that aims to help scientists and students strategize, protect, secure, valorize and extract value from intellectual property emerging out of their work while also championing the cause of inventions, inventors and the spirit of invention within NCL. The IPG (in partnership with Venture Center) conducted a "Preparatory Course for the Patent Agent Exam" primarily targeting young students and project staff at NCL and URDIP.

#### Scope of activities

- ✦ Patent administration (Receiving house for disclosures, patentability assessment, drafting, preparation of forms, prosecution support, correspondences with IPMD)
- ✦ Records, databases, business process automation (Records, databases, tracking sheets, generation of reports for Director/CSIR-HQ/ IPMD/ PSC, ICT systems, ERP)
- ✦ Research support (Reports for planning IP and research projects – such as patent landscapes, freedom-to-practice, infringement assessment, prior-art reports)
- ✦ Portfolio and investment management (Decisions – should we file? Portfolio planning & focus. Where should we file? How much will it cost? Maintenance decisions)
- ✦ Policy, strategy and institutional mechanisms (IP policy, strategic framework for the organization)
- ✦ Awareness, training and promotion (Awareness and education campaigns, workshops, lectures, etc, prizes and recognitions)
- ✦ Marketing, valuation and licensing (Publicity and active marketing, negotiations, valuation and pricing, licensing agreements)
- ✦ Material transfer agreements (Receiving house for in-bound and out-bound requests, IP-related approval, signing authority)

#### Key achievements

- ✦ The IPG was relocated to the Room 275 in the Director's wing. The room was refurbished and equipped for smooth operations.
- ✦ NCLI made large and dramatic departures in the patent administration and management systems/ processes at NCL. New formats and processes were introduced. New decision making processes were introduced. The considerable backlog of cases accumulated during the previous 18 dysfunctional months was addressed.
- ✦ IPG signed a contract with M/s Gnanlex Hermeneutics for patentability assessments and patent drafting. The arrangement also included support of one staff member from M/s Gnanlex for discussions with scientists and addressing of patent related queries. This arrangement reduced the burden of scientists in drafting patents considerably and also brought objectivity to filing decisions.
- ✦ With the help of M/s Gnanlex, IPG started offering patent

## NCL Innovations



related strategic research services including prior art search reports, patent landscapes and infringement assessments.

- ✦ NCLI changed decision making processes to a more objective process based on patentability assessments and an attractiveness assessment rather than a committee based process. This reduced decision making time and enabled fast processing of applications.
- ✦ The IPG set-up IT-enabled systems and tracking systems that improved efficiencies and reliability despite having a skeleton staff at the IPG. IPG began reorganizing and updating records and databases in view of future needs.
- ✦ Significant efforts were made to regain confidence amongst scientists and IPMD-Delhi. Mechanisms were developed to efficiently interface with IPMD-Delhi. Consequently, 50 new disclosures were received from scientists during FY 2008-09. Queries from IPMD were handled efficiently.
- ✦ The IPG took the first steps in portfolio management along with other NCLI staff. NCLI is working with IPG to group the IP portfolio into clusters and start marketing the IP during FY09-10.
- ✦ The IPG enthusiastically promoted the CSIR Invention Award for School Children, 2008.
- ✦ The IPG began facilitation of Material Transfer Agreements (MTA) for scientists.

### Invention activities

- ✦ Value addition of bioresources; Renewable polymers
- ✦ Controlled delivery of active agents using polymeric materials
- ✦ Nano-structured and micro-structured materials
- ✦ Other specialty applications of polymers (membranes, enzyme immobilization etc)
- ✦ New organic and bio-organic molecules as potential drugs, antifungal agents etc
- ✦ Alternative energy
- ✦ Agro-biotechnology

### NCL Technology and Entrepreneurship Club and related activities

Dr. Keki Gharda generously donated Rs 5.00 lakhs to support the activities of the NCL-TEC. Student activities relating to Technology and Entrepreneurship saw considerable growth and ran several activities during the year:

- 7 Feb 2009: Seventeen students from NCL participated in the E-Summit at IIT-Bombay.



Kranthi demonstrating a prototype of his product idea

- 3 Dec 2008: Young entrepreneur, Kranthi Kiran Vistakula (CEO, Dhama Apparel Innovation Pvt Ltd) gave a demonstration of his technology innovation in the Evening with Entrepreneur Series.
- 1 Sep 2008 – 27 Feb 2009: The Venture Center along with NCL-TEC organized Concepto 2008 – A Technology Idea Competition – which was open to NCL and IISER students. The prizes were distributed to prize winners on the National Science day. As preparation for this competition, two mentoring sessions were arranged wherein NCL technologists shared their real-world experiences developing and commercializing technology. The NCL Research Foundation (NCL-RF) agreed to support prizes for Concepto 2008 – Technology Idea Competition. NCL-RF agreed to give prizes to the extent of Rs 70,000. Prizes worth Rs 12500 were eventually distributed.
- 22-23 Aug 2008: Organized a two-day workshop on IP and Patenting, along with GMCC and Indian Patent Office.
- 18 June 2008: Prof George Whitesides (Harvard University) spoke on “Commercializing New Science”.
- 7-8 May 2008: Organized two lectures on IP and Patent Law/Procedures by Mrs Srividya Ravi (Gnanlex Hermetics).



Prof Whitesides addressing questions from attendees

NCLI facilitated the participation of 18 students from NCL in the CSIR's Fifth Technology Led Entrepreneurship Program (TLEP) run by IIM-Bangalore at IICT-Hyderabad during 2-28 June 2008. NCL's contingent was the largest in the Program. NCLI again actively promoted the TLEP Program in early 2009 to send 15 applications from NCL for the 6th TLEP scheduled for 1-26 June 2009.

Sarvesh Kumar Soni reached the stage First short-list and Elevator Pitch for the business plan on “Nutraceuticals - To reduce risk of old-age neurodegenerative diseases” organized by Power of Ideas, Business Plan Competition by Economic Times (Jan-June 2009).

### Events and learning opportunities organized by NCLI

NCLI also organized other events towards furthering the group's other goals:

*Innovation and Technology Enterprise Lecture Series*, which is a public lecture series, aims to present exemplary cases of research-based innovation translated into business ventures - the associated ideas, the people and the

## NCL Innovations



experiences - in order to inspire, energize and inform Indian scientists, technologists and business people.

29 Sep 2008: Dr Keki Ghada (Founder and CMD, Ghada Chemicals) delivered the 4th Innovation & Technology Enterprise Lecture on "Entrepreneurship and Innovation – A Personal Perspective".

**NCLI Seminar Series** shall present talks by people who have excelled in building institutions and institutional mechanisms/systems to promote technology, technology commercialization and new venture development -- goals that are important for "NCL Innovations".

13 Feb 2009: Prof Shai Vyakarnam (University of Cambridge) delivered the 5th NCLI Seminar titled "The journey from science to enterprise: Key lessons from Cambridge".

5 Feb 2009: Ms Susan Searle (CEO, Imperial Innovations Group PLC) delivered the 4th NCLI Seminar titled "The best practices in R&D commercialization – Success stories from Imperial College London".

19 Dec 2008: Dr Faruq Marikar (Nanobiz LLC) delivered the 3rd NCLI Seminar titled "The future of the chemical industry".

11 Dec 2008: Prof Amit Ray (JNU) delivered the 2nd NCLI Seminar titled "Public funded research and technology transfer: Implications of the Bayh-Dole Act and its Indian equivalent".

NCLI also organized and facilitated learning opportunities for NCL scientists and staff during the year.

28 June – 4 July 2009: NCLI (along with Venture Center) facilitated the participation of Dr K Guruswamy, NCL in the Ignite 2009 program at the Centre for Entrepreneurial Learning at University of Cambridge. Funding support was arranged through the British Council and NCL.

### Networking and human resource strengthening/ planning

NCLI operate at the interface of Science/ Technology, Business and Law – a domain where there is considerable shortage of ready skills in the country. NCLI is actively pursuing a policy of continuous up-gradation of skills of its staff, strengthening and broadening exposure and capabilities of its members while also actively seeking out well trained personnel to join its ranks. Furthermore, NCLI realizes the

importance of networking for technology commercialization professionals and thus encourages its staff to network with various communities - science, entrepreneurship, intellectual property etc.

essionals and thus encourages its staff to network with various communities - science, entrepreneurship, intellectual property etc.

### Contributions to CSIR-level thinking and systems relating to technology commercialization

One of the goals of NCLI is to participate in and contribute to the shaping of policies, procedures and rules at the CSIR and NCL levels that have a direct impact on technology development and acceleration, technology commercialization and new venture development.

### NCLI staff contributions in FY 2008-09 included

Dr Premnath participated in discussions rethinking IP management and technology commercialization within CSIR. Dr Premnath provided insights into the mechanisms involved and possible re-organization strategies.

Dr Premnath also joined a high-level team for a study visit of Singapore's Biopolis and Australia's CSIRO (Sydney and Melbourne) during 6-13 March 2009. These study visits explored practices of A-STAR and CSIRO regarding intellectual property management, technology planning, technology commercialization and new venture development.

### Technology acceleration and commercialization

NCLI also participated in technology transfer / licensing discussions during the year:

- Godavari Sugar Mills (In this agreement, NCLI suggested an innovative new arrangement for risk-reward sharing through a milestone payment linked to future valuation of the company.)
- Hyca
- Hygeia
- One key area where NCLI wishes to focus is in facilitation of the ideation process and idea mining process within NCL. NCLI began some work in this direction during the year and hopes to scale up activities as more human resources are allocated to the group.
- NCLI facilitated the availability of IP research reports to scientists prior to starting projects.
- NCLI project with BRBNMPL directly contributed to the filing of one invention disclosure.



## National Repository of Molecules

In early 2005, NCL took the initiative to create National Repository of Molecules (NRM) as a unique facility within CSIR system. At NCL, several hundred new organic compounds are synthesized and at present there is no centralized facility for collection of organic compound in India especially from academic and research institutes. The molecular repositories helps the researchers to learn and connect indigenously developed new compounds available for screening against known/ unknown diseases and thereby accelerate the drug discovery research programmes. The NRM facility will facilitate collection of molecular samples across participating regional molecular repositories (RMR) which includes CSIR, DST, DBT, government sponsored organizations / laboratories and other academic institutions / universities across the country. The NRM has a collection of about 1600 organic compounds.



The objective of this facility is to collect samples of single organic molecules prepared as a part of PhD program by researchers especially from publicly funded research projects. In order to accommodate several thousands of physical collection of organic molecules at low temperature, a dedicated cold room was also established at NRM. Chemoinformatics tools using bar-coding system are employed for managing the inventory electronically.

In order to accommodate the wide molecular diversity and to compare with synthetic compounds, pure fractions of biological active ingredients of medicinal plants of Indian origin are also included in the programme. A web-server is linked to dedicated database server for handling NRM molecular data and other associated information (<http://www.ncl-india.org/nrm>).

The state-of-the-art chemoinformatics tools for creating molecular fingerprints integrated with web-server enable the users and administrators to search the molecules using sub-structure, exact-structure and similar structures over the web in a secured environment. This will facilitate research community and other collaborators from pharmaceutical sector (under non-disclosure agreement, NDA) to get access to the samples and available associated data for further biological screening studies on several drug targets. It is also proposed to expand the collection by including natural products and their derivatives.

### Road Map

- + Connecting academic research with pharma industry
- Development of comprehensive database of chemical structures and their bioactivity profiles.
- + Support drug discovery research through networking of chemists and biologists
- + Seek new lead bio-active molecules through NRM facility
- + Organize awareness workshops and promote NRM activities

### Expansion of NRM to facilitate

- + Testing new molecules against several disease related biological targets

- + Patenting the active compounds (IPR and confidentiality issues)
- + Selection and prioritization of active compounds for licensing
- + Networking with other participating research laboratories, universities and pharma industries.
- + Robust automatic inventory management system for handling samples and data
- + Revenue generation for self-sustained activity of NRM

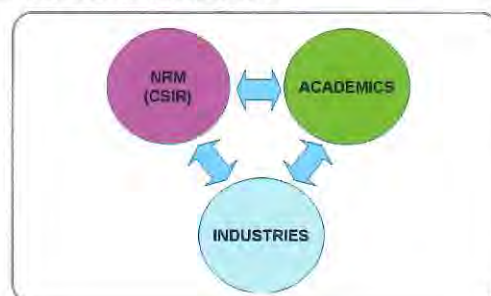
By creating such centralized facility, it is also possible to bridge the gap between experimental chemists and biologists in understanding the function of small molecules in biological systems in the context of chemical-biology interface. The biological assays made available from repository would greatly help future drug discovery research programs in the country.

### Activities proposed at NRM

To connect with biological screening facilities (in-house / external) under NDA to acquire biological data on the available molecular collection. The screening data will be collated and analyzed and promising compounds will be selected for further SAR, in-vivo studies, pharmacokinetics, formulation and further investigational new drugs enabling studies.

Facilitate generation of IP (patents / publications) with due credit to sample depositors and collaborators supporting biological screening. The Pharmacological profiles of lead compounds, Screening data and IP rights will be available to Pharma companies for in-licensing and the revenues generated through such licensing deals shall be shared by the PIs, the national facility, depositors, host institute and sponsoring agency.

It is also proposed to compile all the available information about the samples in the inventory along with chemical structures in standard file formats, spectral data (IR, NMR, Mass, UV, X-ray etc.) physico-chemical properties, biological activity profile data, literature citation (publications, patents, PhD theses, scientific reports etc.) in the electronic format with full search features as an information product priced at nominal cost. This would be updated periodically with the growth of samples at Molecular Repository. This information product is expected to facilitate the researchers to compare their experimental data with available analytical data, interpretation of chemical structures, modeling and predictive studies on the molecules of interest.





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## Business Development



Business Development Division (BDD) takes care of various aspects of business planning, contracts management, strategy consulting, intellectual property and event management. A Significant portion of NCL's budget is generated through contract R&D services, consultancy and technology licensing. The division is staffed with engineers and management graduates who work as technology facilitators interfacing with scientists, industry, government, financial institutions, other statutory agencies, etc.

### Business Facilitation

The NCL is constantly exploring opportunities to work with industrial customers on challenging research problems which have an impact on their performance. The NCL realizes that it is the industrial customer that keeps research relevant to and focused on real world problems and opportunities. Great emphasis is placed, therefore, on understanding customer's needs, clearly defining deliverables and meeting customer's expectations.

The BDD undertakes a mapping of skill sets and patent portfolio available at The NCL and contacts industrial customers relevant under the context. It then plays a technology facilitation role through discussions related to project proposals, pricing issues and contracts management. The NCL believes in the credo that NCL wins only if its customer wins. Consequently, The NCL constantly aims at building a win-win relationship with all its customers. During the year NCL worked with 39 Indian and 15 foreign customers.

### Event Management and Exhibitions

The Division assists in planning, coordination and organisation of various events such as conferences, memorial and endowment lectures, and CSIR HRDG programmes. The NCL also actively participates in the exhibitions related to scientific achievements organized by other agencies. The Division coordinated development of The NCL Diamond Jubilee Logo and video highlighting sixty years journey of NCL.

The NCL participated in the Chemspec India 2008 held at NSE Complex, Mumbai during April 9-10, 2008. The CSIR Programme on Youth for leadership in Science (CPYLS) for meritorious students of Standard was organized during December 17-18, 2008. Besides organized a CSIR HRDG was organised for science teachers on faculty improvement and motivation at Deogiri College, Aurangabad during Jan. 29-31, 2009.

### Management Information System

MIS Group handles all activities related to Project Management System. The activities can be broadly classified as follows:

- ◆ Assistance to scientists in preparation of project proposals as per CSIR guidelines
- ◆ Coding of new projects and preparation of new project Initiation note for circulation to all concerned departments

- ◆ Allocation of funds to the projects and circulation of challange to all concerned
- ◆ Preparation and raising of invoices for Industrial Projects
- ◆ Extension of projects in consultation with scientists
- ◆ Issuing of completion Certificate of Projects
- ◆ Calculation and payment of service tax for consultancy and technical services projects to Central Excise Department
- ◆ Maintenance of service tax records as per CSIR guidelines for consultancy and technical services projects
- ◆ Providing audit Information on NCL projects
- ◆ Laboratory budget preparation/ allocation / monitoring
- ◆ Preparation of financial and performance reports of NCL
- ◆ Developing appropriate systems for MIS functions
- ◆ Providing Information on projects to MC/RC Meetings
- ◆ Management of NCL Research Foundation and its activities
- ◆ General assistance in the management and smooth functioning of the Laboratory

Efforts are being made continuously to streamline the procedures relating to project initiation, monitoring and closure. Many of the activities have been computerized. There is an efficient system to track the receipt of funds for various projects, monitoring cash flows, project monitoring, publication profiles etc.

A web enabled project management information system was developed in-house to support the activities of the group. This system takes care of the financial aspects (receipts, budgeting) of projects from initiation to completion. It stores all the important information about the project:

- ◆ Project information
- ◆ Funds receipt
- ◆ Party information
- ◆ Staff deployed
- ◆ Project installments

The system provides for generating a range of reports to enable the management to review the status. The MIS portal offers access window to PMIS for the scientific staff, project leader, HOD's and management teams. The site offers hierarchical login to different users. This enables to control the information depending on the requirements of the user and prevents unauthorized viewing. Apart from PMIS, the site also provides information on performance of NCL, Divisional performance, various proforma for downloading, about NCL research foundation activities etc. This portal will be the driving force for providing financial information to NCL Scientists.

The PMIS is a centralized document management system holding all project records at one place. The project records are available to the concerned scientists through an MIS website (24 x 7 hours). The MIS group creates all the project records internally and same is made available on the MIS website to the scientists. The scientists are

## Business Development



provided with a login and password to access their project records directly from their desktops. All project documents such as agreements, project proposals, project initiations, challans, and funds received and due are available on the fly as and when the records are created by the MIS group. In addition, there is an upload facility for the scientists to upload interim and final reports submitted to the client and project output summary into the PMIS system.

Therefore, all financial and scientific reports are centralized and stored in the MIS server and all project records can be created as when required. PMIS creates important reports for management for decision making. The External cash flow reports, Lab reserve earnings, detailed project break up, dollar earnings, funds due from project are some of the important management reports available to HOD' s and Director. In addition, queries can be created to pull out information from the database as and when required. The PMIS sends alert mails, whenever a payment is due. This helps the MIS group to raise an invoice and collect the funds in time. An alert mail is also sent to the scientists, whenever a report to the client is due and scales up the alerts to HOD and the Director, if the request is not complied.

### Budget Planning

Budget Planning is a significant management tool adopted by the laboratory to manage & control the resources of the laboratory. It helps to utilize the resources for the development and growth of the laboratory to achieve the aims set by the management of the laboratory.

The MIS is responsible for the budgeting exercise of the laboratory. the MIS along with the Director make a detailed plan to meet the overall budgetary requirements of the laboratory. They are further broken down to different budget heads and the expenditure is matched with the available resources of the laboratory.

With over all plan in hand, the MIS calls for the budgeting requirements known as 'Operational Budget' for the divisions and resource centers at the beginning of the financial year. The budget mainly covers equipment maintenance within the divisions and common equipment for the laboratory, divisional office requirements for office equipment, consumables and small scientific equipments required in the divisions. The requirements are compiled into appropriate formats and studied. The allocations are made based on resource planning and overall budgeting principles developed within the laboratory. The budgets are then projectised with project codes and then released to budget centers.

The budgets are booked through stores, which maintain the expenditure for all budget centers. The MIS along with the Director monitor the expenditure twice in a year in the months October and March. Corrective measures are undertaken if the expenditure is more or too less than the allocated resources.

### Indian Customers

- ✦ Aquatech Systems (Asia) P. Ltd.
- ✦ Bilag Industries P. Ltd.
- ✦ Biopore Surgicals
- ✦ Borax Morarji Ltd.
- ✦ Centaur Chemicals P. Ltd.
- ✦ Ciba Research (India) Pvt. Ltd.
- ✦ Dharpur Sugar Mills Ltd.
- ✦ Dow Chemicals International Pvt. Ltd.
- ✦ East India Pharmaceuticals Works Ltd.
- ✦ Engenious Engineering Pvt. Ltd.
- ✦ FDC Ltd.
- ✦ Godavari Sugar Mills Ltd.
- ✦ Godrej High Care Ltd.
- ✦ Godrej Sara Lee Ltd.
- ✦ GMM Pfaudler Ltd.
- ✦ Gharda Chemicals Ltd.
- ✦ Gujarat Narmada Valley Fertilizers Co. Ltd.
- ✦ Hemani Intermediates Pvt. Ltd.
- ✦ Hindustan Polyamides & Fibers Ltd.
- ✦ Hygeia Laboratories
- ✦ Indian Oil Corporation Ltd.
- ✦ IPCA Laboratories Ltd.
- ✦ Kirloskar Oil Engines Limited
- ✦ Larsen & Toubro Ltd.
- ✦ Lupin Research Park
- ✦ Merloni TermoSanitari (India) Ltd.
- ✦ Ranbaxy Laboratories Ltd.
- ✦ Radhe Renewable Energy Development Pvt. Ltd.
- ✦ Reliance Industries Ltd.
- ✦ S C Johnson Products Pvt. Ltd.
- ✦ Sandoz Private Limited
- ✦ SRF Ltd.
- ✦ Sud-Chemie India Pvt. Ltd.
- ✦ Sumitomo Chemical India Pvt. Ltd.
- ✦ Syngenta India Ltd.
- ✦ Tata Chemicals Ltd.
- ✦ Torrent Pharmaceuticals Ltd.
- ✦ USV Ltd.
- ✦ Vinati Organics Limited (Mumbai)

### Foreign Customers

- ✦ Alcoa Inc.
- ✦ BASF Catalysts LLC
- ✦ Benefuel Inc.
- ✦ Celanese Ltd.
- ✦ Colgate Palmolive Company
- ✦ Dow Corning Ltd
- ✦ Eastman Chemical Company
- ✦ INVISTA
- ✦ Johnson & Johnson Vision Care, Inc.
- ✦ The Procter & Gamble Company
- ✦ Reviva Pharmaceuticals Inc.
- ✦ Sabic Innovative Plastics Inc.
- ✦ Solvay Solexis
- ✦ UCB Pharma S. A.

### Human Resource Management



The Human Resource Management (HRM) Unit promotes the competencies of the employees to enable the laboratory to achieve its mission. During the year, HRM Unit continued efforts to improve the productivity of the organization.

#### Training programmes arranged for NCL staff

The Unit conducted nine training programmes. Of these, two programmes were conducted off-campus and others in house.

Six programmes of two-day each for thirty-two store and purchase officers/staff members were conducted by the Pune branch of Indian Institute of Materials Management on July 25 & 26, 2008, August 08 & 09, 2008, September 19 & 20, 2008, October 17 & 18, 2008, November 28 & 29, 2008, and February 06 & 07, 2009. The programmes focused on the basics of purchase parameters such as specifying requirements and planning supply, appraising and short-listing suppliers, obtaining and selecting offers, negotiation, preparing the contracts, managing the contracts; during training programmes. These programmes will have direct impact on the working of all the members of stores and purchase. The participants appreciated all the programs as it is helpful to them in day-to-day work.

A Management Development Programme (MDP) of three-day duration was conducted National Institute of Construction Management and Research (NICMAR), Pune on 'Computerized MS Project Management' for twenty staff members of Engineering Services Unit on March 06, 13 & 24, 2009. The programme was on the use of softwares namely, Microsoft Project Management. The staff be starts starting to use this software in their daily works. Hence they are being trained in utilizing it to fullest extent. All the staff members are ready to implement this software in their daily work.

Two off-campus programmes of one-day each for thirty support staff members per program were conducted by Credence Management Services, Pune on 'Self-development' on October 13, 2008 and March 02, 2009. The programme focused on management games, touched upon the importance of team work as well as on the importance of team members by requesting them to apply their mind and then completing the assigned task. All the participants enjoyed the programme as they could learn many new things through management games.

#### Short Term Summer/Winter Project

About 380 students pursuing the courses such as M.Sc., M.Pharm., B.E., M.E., B.Tech., M.Tech. at various Indian institutes including IITs, IISERs, and NITs were trained at the NCL. The students for the short term projects worked normally for the period of two months to one year.

#### Guest workers

Twenty-eight guest workers worked at NCL during the year including ten fellows of various Indian science and engineering academies, one KVPY Fellow and four fellows from abroad two each from France and Iran.

#### Institutional visits

NCL receives many requests throughout the year from various academic and research institutes including PG colleges to visit NCL facilities. The Unit coordinated twenty-four institutional visits during this year. These visits were mainly of students pursuing professional courses in agricultural, medical, engineering sciences, besides basic and applied sciences from postgraduate colleges located across India.



## Human Resource Management



## NCL Scientists recognized by different universities as research guides (2008-09)

Name	University
Dr. Adikane, H. V.	Pune
Dr. Agrawal, D. C.	Pune
Dr. Ahmad, Absar	Pune
Dr. Anil Kumar	Pune
Dr. Argade. N. P.	Pune, Mumbai
Dr. Asha, S. K.	Pune
Dr. (Mrs.)Asthana, Saroja	Pune
Dr. Avadhani, C. V.	Shivaji University; Pune
Dr. Badiger, M. V.	Pune
Dr. Bastawde, K. B.	Shivaji University; Pune, Kolhapur
Dr. Bhadbhade, M. M.	Pune; Bhavnagar
Dr. Bhat, Suresh	IIT- Mumbai
Dr. Bhattacharya, A. K.	Pune
Dr. Borate, H. B.	Pune
Dr. Chavan, S. P.	Pune
Dr. Chumbhale, V. R.	Shivaji University; Pune, Kolhapur; Swami Ramanand Tirth University, Nanded; Amravati University
Dr. Deshmukh, M. N.	Osmania
Dr. Deshpande, M. V.	Pune; Shivaji University; Kolhapur; North Maharashtra University, Jalgaon; Bharathi Vidyapeeth, Pune
Dr. Deshpande, S. B.	Pune
Dr. Dongare, M. K.	Pune; Mumbai
Dr. Gadre, R. V.	Pune
Dr. (Mrs.)Gaikwad. Sushama Mugutarao	Pune
Dr. Gaikwad. A. G.	Pune
Dr. Ganapathy. S.	Pune
Dr. (Ms.)Garnaik, B.	Pune
Dr. Giri, A. P.	Pune
Dr. Gokhale, D. V.	Pune; Shivaji University, Kolhapur
Dr. Gopinath. C. S.	Pune
Dr. (Mrs)Gupta. Vidya	Pune; Mumbai
Dr. Gupte, S. P.	Pune
Dr. Guruswamy, K	Pune; IIT-Mumbai; UICT, Mumbai
Dr. Halligudi, S. B.	Pune; Bhavnagar
Dr. Hegde. S. G.	Shri Ramanand Tirth University, Nanded

Name	University
Dr. Hotha, Srinivas	Pune
Dr. Idage, B. B.	Pune
Dr. Iyer, Suresh	Pune
Dr. Jaganathan, R.	Pune
Dr. Jayaraman, V. K.	Pune
Dr. (Mrs)Jog, J. P.	Pune; Shivaji University, Kolhapur
Dr. John, C. K.	Pune
Dr. (Mrs)Joshi, S. P.	Pune
Dr. Joshi, N. N.	Pune
Dr. Joshi, P. N.	Swami Ramanand Tirth University, Nanded
Dr. Joy, P. A.	Pune
Dr. Kalkote, U. R.	Pune
Dr. Karthikeyan, M	Pune
Dr. Kelkar, A. A.	Pune
Dr. Khan, B. M.	Pune
Dr. Khan, M. I.	Pune; North Maharashtra University, Jalgaon
Dr. Kharul, U. K.	Pune; Mumbai
Dr. Khire, J. M.	Pune
Dr. (Mrs)Kolar, Lalitha Sunilkumar	Pune
Dr. Krishnan, S.	Pune
Dr. Kshirsagar Suresh Tukaram	Pune
Dr. Kulkarni, B. D.	Pune; Mumbai; Nagpur; Shivaji University, Kolhapur
Dr. Kulkarni, M. G.	Pune; Mumbai
Dr. Kulkarni, M. J.	Pune
Dr. Kulkarni, R. A.	Pune
Dr. (Mrs)Kumar, V. A.	Pune
Dr. Lele, A. K.	Pune; Mumbai; IIT Mumbai
Dr. (Mrs) Mayadevi, S.	Pune; Mumbai; and Shivaji University, Kolhapur
Dr. (Ms)Deshmukh, Sumedha Sharad	Pune
Dr. Mukherjee, S. N.	Pune
Dr. Mulla, I. S.	Pune
Dr. Mulla, S. A. R.	Pune
Dr. Naik, Rajan H.	Pune; and Yashwantrao Chavan Maharashtra Open University, Nashik
Dr. Pal, Sourav	Pune



NCL Scientists recognized by different universities as research guides (2008-09)

Name	University
Dr. Pandey, Ganesh	Pune; Osmania University, Hyderabad; Shivaji University, Kolhapur
Dr. (Mrs.)Pawar, Pushpa V.	Shivaji University, Kolhapur
Dr. Pedireddi, V. R.	Pune
Dr. Ponrathnam, S.	Pune
Dr. (Mrs)Pore, V. S.	Pune
Dr. (Mrs)Prabhune, Asmita	Pune
Dr. Prasad, B. L. V.	Pune
Dr. Prasad, S. D.	Pune
Dr. (Ms)Pundle, Archana	Pune
Dr. (Mrs)Puranik, V. G.	Pune
Dr. Radhakrishnan, S.	Bharati Vidyapith, Pune,
Dr. Rajamohanan, P. R.	Pune
Dr. Ramana, C. V.	Pune
Dr. Ramesh, C.	Pune
Dr. Ranade, V. V.	Pune; Mumbai
Dr. (Mrs)Rao, Mala	Pune; Shivaji University, Kolhapur
Dr. Rathna, GVN	Pune
Dr. Ravi Kumar, V.	Pune
Dr. Ravi, Venkatanarayanan	Pune
Dr. (Mrs.)Rele, M. V.	Pune
Dr. Rode, C. V.	Pune; Swami Ramanand Tirth University, Nanded
Dr. Saini, D. R.	Pune; BHU, Varanasi BVP, Pune
Dr. Sanjayan, G. J.	Pune
Dr. Sarkar, Dhiman	Pune
Dr. Satyanarayana. C. V. V.	Pune
Dr. (Mrs)Seetalaxman. R.	Pune
Dr. Shashidhar, M. S.	Pune
Dr. Singh, A. P.	Pune
Dr. Singh, R. P.	Pune
Dr. Sivaram, S.	Pune; Mumbai; IIT-Mumbai
Dr. Srinivas, D.	Pune, Bhavnagar
Dr. Sudalai, A.	Pune
Dr. Suresh, C. G.	Pune
Dr. Suryavanshi Gurunath	Pune
Dr. (Mrs.)Tambe, A. S.	Pune
Dr. Tambe, Sanjeev	Pune

Name	University
Dr. (Mrs)Tare, V. S.	Shivaji University, Kolhapur; North Maharashtra University, Jalgaon Yashwantrao Chavan Maharashtra Open University, Nashik
Dr. Tewari, R.	Pune
Dr. (Mrs.)Thengane, S. R.	Pune
Dr. Thomas Daniel	Pune; Shivaji University, Kolhapur
Dr. Thulasiram H. V.	Pune
Dr. Tripathi, P. K.	Pune
Dr. (Ms)Umbarkar, Shubhangi Bhalchandra	Pune
Dr. Varma, A. J.	Pune
Dr. Vijayamohan, K.	Pune
Dr. Wadgaonkar, P. P.	Pune; Shivaji University, Kolhapur
Dr. Waghmare, Kashinath	Pune



## Publication and Science Communication

Publication and Science Communication (PSC) Unit builds a positive image of the Laboratory by establishing communication between the Laboratory and its external and internal stakeholders. The Unit informs and educates the stakeholders about the mission of the Laboratory, guiding principles and values through various means such as web, print and electronic media.

### External Communication

The Unit creates and manages NCL websites ([www.ncl-india.org](http://www.ncl-india.org); [www.ncl.res.in](http://www.ncl.res.in)); prints annual reports and brochures; communicates impact making work from the laboratory in the form of R&D features; prepares walkthrough video for general information to its stakeholders from scientific community, industry and public.

During the year, brochure on Combi Chem-Bio Resource Center was prepared. Besides NCL input for the CSIR brochure covering the themes - 'Healthcare-Affordable for all', 'Healthcare- Discovery to development' were provided. Six R&D features covering impact making work from the NCL were prepared.

Being a one-point contact for press/media and releases, the Unit issued press releases, attended press queries, provided customised reports on request to the stakeholders, and co-ordinated interviews with NCL scientists on request from science magazines/ newspapers / electronic media.

Press releases were also issued on awards/ medals / recognitions granted to the staff. Reports covering various events such as the National Science Day, the Technology Day, the NCL Foundation Day, the CSIR Foundation Day, Memorial and Endowment Lectures, symposia / conferences were prepared and released to the press, *CSIR News*, *CSIR Samacha*, besides uploading at the NCL websites. Interviews with the Director and ten scientists were co-ordinated with the editor of *Chemical Industry Digest* and the interviews were published in the March and the April 2009 issues of the magazine in two parts under the series 'Rediscover National Chemical Laboratory'.

Advertisements in *Nature* (India edition) and *Chemical and Engineering News* were released in Oct.- Nov. 2008 for scientific recruitment. A web page for receiving online applications for the scientific posts was developed.

To meet the CVC guidelines, a new application for uploading Purchase Orders was developed. A separate page was developed for announcing temporary vacancies.

Scientist profiles were updated on business and academic web sites and new scientists were encouraged to prepare their profiles for uploading at the web sites.

The organisers of various conferences were assisted to manage the conferences by launching the website for the particular conference. During the current year organisers of the following events were given various types of support for organising the events smoothly : '19th National Symposium on Catalysis: Catalysis for Sustainable Energy and Chemicals', '3rd CRSI - RSC Symposium and 11th CRSI National Symposium in Chemistry', 'An EMBO Conference - Recent Developments in Macromolecular Crystallography', 'International workshop on The Booroola fecundity (FecB) mutation: Science and Practice', 'Indo-Korean Symposium in Organic Chemistry', 'Indo-Russian Joint Workshop on Catalysis for Bio-mass Conversion and Environmental Engineering', 'The deMon Developers' 9th Annual Workshop on Density Functional Theory, Present and Future', and 'Indo-German Workshop in Micro-reaction Technology'.

### Internal Communication

Development of new applications is done continuously and the concerned office secretaries / users are trained for updating the pages. Memos from CSIR Hq, DG-CSIR, other Government Agencies, and from within the NCL are announced using intranet portal [ncl@home](mailto:ncl@home), besides announcement of events and lectures. During the year the web pages of Quarterly Reports of NCL Medical Centre, Stores and Purchase department, Safety, institutional committee were prepared / modified. Reports that were published in print media and which appeared in electronic media, for instance NCL in news, CSIR general science articles, photos of major events, audio of the inaugural function of major events, science day posters, press notes were archived.



### Publications Database

R&D work at the NCL results in more than 400 research papers annually. To manage publication database, a publication management software developed in-house is used. Databases from Web of Science, Scopus and JCR are used for the purpose. The software is used to generate customized reports. The Unit also provided NCL publication database to NISCAIR for CSIR Research Output database. The Unit managed multimedia facilities including video conferencing, public address system, video and still photography, and also prepared guidelines for external agencies for using the auditorium and the lecture hall.



### Research Planning and Audit



Research Planning & Audit (RP&A) Unit has been involved in areas of project planning, project monitoring, budget, interaction with auditors, liaison with CSIR, etc. Technical and scientific audit of all on-going projects is a key activity. Highlights of the major activities are listed below.

#### In-house Projects

RP&A Unit is associated with the screening, evaluation and providing funding for the new projects within the Lab. During the year, fresh proposals were invited and reviewed. In addition, monitoring and review of existing In-house research programmes was undertaken. During the year four review meetings / seminars were conducted to audit the technical and scientific performance of several projects.

Five scientists who joined the NCL during the year were given a start-up annual grant of Rs. 6 lakh for 2 years. In addition, the start-up grants to six scientists (who joined in the previous year) were continued into the second year. The total funding to all In-house projects (including start-up grants) during 2008-09 was Rs. 84 lakh.

It is observed that during the year, the In-house projects produced more than twenty publications in peer-reviewed journals, while about seventeen are under the process of publication. Besides, the research work has also helped train several M.Sc and M.Tech. students as summer trainees. In addition, the initial work taken as a part of the In-house projects has led to the initiation of four public funded (DST/DBT) projects, the sponsorship of an industrial project and four technical services projects.

#### Projects under 11th Five-year plan

RP&A Unit acts as a nodal agency for the coordination and implementation of the network projects within the NCL, with

CSIR and other participating labs. The NCL is the Nodal Laboratory for two Network Projects (NCL-IGIB joint research initiative, and Hydrogen energy initiatives). In addition, creation of Centers of Excellence in Micro-reactor Engineering and Scientific Computing has been a major highlight.

**The Annual plan** 2009-10 was prepared for the CSIR. The comprehensive report basically covers project wise achievements (outputs and outcomes) against the objectives and targets set out in project proposals, and a summary of the financial information and future plans of work etc. for 11<sup>th</sup> Five-Year Plan projects, Non-network projects of the Lab with a consolidated accomplishment and performance of the Lab for the year 2008-09 and projections for the next year.

#### Research Council Meetings

The Unit conducted two RC meetings and which were followed by actions and implementation of recommendations. The Unit also made presentations to the RC on the "Status of In-house projects 2008-09".

#### Liaison with CSIR

The Unit consolidated performance reports on two major network projects, and research utilization data of NCL were sent to CSIR on a quarterly basis. This involved providing current status on all on-going projects, highlighting the work done, major achievements in basic and applied science, outputs (patents - applied for and granted) and funds generated through technical services, etc. Response to certain queries under the RTI has also been provided to the CSIR.

## Safety Management



The NCL maintains a comprehensive safety programme. It has devised procedures and protocols to see that the risks arising out of handling, use, storage and disposal of chemicals are minimized.

In order to ensure this action, the NCL has a statutory Safety Committee which is chaired by the Director, and has senior scientists as from various divisions as members. Besides, there are nine Divisional Safety Committees to handle safety related issues at the division level. The Divisional Safety Committee holds formal meetings periodically in addition to the informal discussions with staff and research students.

The Divisional Safety Committee conducts regular inspections of the laboratories and storage areas. The inspection checklist includes items such as laboratory house keeping, personal protection, chemical inventory and storage, gas cylinder storage, electrical and mechanical equipment, emergency safety equipment etc. The report is categorized into action points and is submitted to Head, Safety Management and to the Director with remarks on actions taken and to be taken.

### Fire safety audit

The NCL invited National Safety Council, Mumbai to conduct its fire and safety audit, to physically observe and comment on the hazards and associated risks, systems and preparedness to respond in an emergency, and also to recommend solutions to the observed lacunae. A draft report on the same has been received.

### Orientation and Training

Newly joined research students, project assistants and scientists were briefed through an orientation programme to sensitize them of the safety in chemical laboratories, initiatives taken by the safety unit, information sources and facilities; their duties and responsibilities. Live demonstration and hands-on practical training for handling small fires and the use of portable fire extinguishers was organised twice during the year and more than 130 scientists and students attended the demonstration. Two scientists were deputed to attend a conference on chemical safety and risk assessment at IICT, Hyderabad.

Based on the leadership roles and contributions to lab safety, IUPAC, has given a mandate to Head, Safety Management NCL, to undertake safety awareness programmes and to improve safety, health and environment in India. In this context he attended a two-week programme on aspects of health and safety at Novozymes A/S in Denmark.

### Facilities

Each laboratory is equipped with a fire extinguisher and an eyewash station. In addition there is a common facility (within 15 m) for a safety shower and a fire blanket. The safety equipment is inspected on a regular basis by the laboratory staff. Engineering services personnel test fume hoods on a regular basis. A 24-hour access to emergency telephones is provided.

### Up-gradation of infrastructure and systems

The health, safety and environment is protected and the systems are refined and upgraded on a continuous basis.

- ✦ Safety solvent storage cans and solvent storage cabinets have been procured and distributed to researchers all over the lab.
- ✦ LPG leak detectors have been installed at a few select locations and are being monitored for their efficacy.
- ✦ Heating mantles, earlier used for distillation of flammable solvents, have been replaced with water baths.
- ✦ Six new books on fire and safety have been procured and a monthly periodical has been subscribed for the NCL library, which already has more than 400 books and documents related to safety.

### Assistance to outside agencies

- ✦ Public awareness programme and lectures on various aspects of safety, accident prevention and mitigation, disaster management are also organized for various educational and industrial establishments.
- ✦ Liaison with College of Military Engineering, Pune for participation in their officer-training programme.
- ✦ MSDS for several chemicals was provided to outside agencies on request.

## Engineering Services



The Unit comprising Mechanical, Electrical and Civil Engineering as well as Glass Blowing sections provides support to the laboratory in various ways. This year, the project of adding eight numbers of type V quarters (Area -1860 sq ft each) was completed and construction of new Polymer and Advanced Materials building is going on.

The garbage composting facility was set up in the NCL campus and the NCL is the first government. organization in Pune to take this initiative regarding garbage disposal management system. According to the new guidelines of Pune Municipal Corporation (PMC), the garbage generated by institutions and housing societies is required to be segregated into wet and dry garbage, and the disposal of the wet garbage has to be done at the place of generation.

The NCL, one of the biggest establishments in Pune spread over 475 acres of land generates garbage to the tune of one ton per day. As a first step in garbage disposal management, the NCL engaged SWACHCH, a PMC approved cooperative of waste pickers for house-to-house collection of garbage and segregating the same into wet and dry garbage. The non recyclable dry garbage is disposed by the PMC.

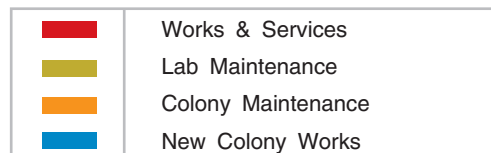
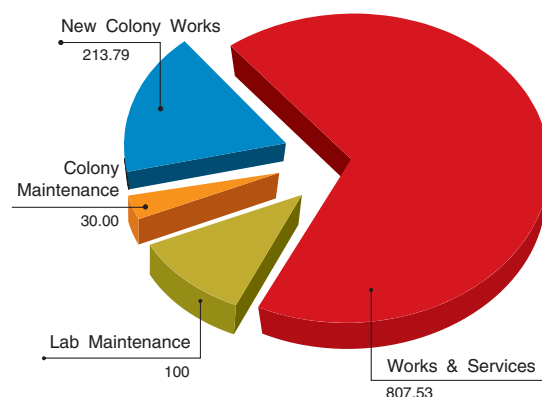
The NCL uses mechanical composting system in an area spread over 10,000 sq ft. The composting machine processes 50 kg of wet garbage in one batch in 15 minutes. With the aid of this machine, the wet garbage is converted into compost in two weeks. This way from the garbage of one ton, about 300 kg of wet garbage is gets converted into compost. The compost is being used in the gardens of the NCL as manure. The Unit continued its efforts in developing and renovating various parts of the NCL Innovation Park including Venture Center Library and Lab Block.

The Glass Blowing Section provides the glassware and the modified set-up for the scientific community. During this financial year, about sixty special set-up / apparatus with innovative ideas as per the need of the research were prepared. Besides, about 1500 fabrications such as distillation sets, filtration sets, reaction units, etc. were made. The section

also carried out about 2030 various jobs involving repairs, maintenance and petty works. The section added more than Rs. 10.2 lakh to the Lab Reserve Fund.

Category	Expenditure (Rs in Lakh)
Works & Services	807.53
Lab Maintenance	100.00
Colony Maintenance	30.00
New Colony Works	213.79
<b>Total</b>	<b>1151.32</b>

### Expenditure, Rs. 1151.32 Lakh



## Communication Group

Video Conferencing system procured centrally by CSIR Hq. was commissioned in Chemical Engineering conference room. The ISDN BRI lines were made functional from Omni PCX Enterprise communication system redundancy hardware for this purpose. To avoid failure on account of PRI lines, a BSNL ISDN PRI line in redundancy was laid and routed up to redundancy hardware location and two PRI lines (out of four) were rerouted on redundancy hardware

A dedicated node of 400 telephone lines for new Polymer and Advanced Materials building was commissioned near the 'G' wing of this up-coming building to take care of telephone requirements. These lines have been made functional from the redundancy hardware.

The challenging and complicated work of uprooting all

telephone connections in the main building basement area was taken up. Since the beginning of the NCL, all telephone lines in the main building were routed from basement through boxes, and tag blocks, and then through the corresponding ducts in the rooms / labs. It was cumbersome for day-to-day maintenance. Rerouting of all numbers from respective floors and wings associated with floors was taken up. This was completed for NCIM basement wing, Organic Chemistry Division ground floor wing, Physical and Materials Chemistry Division, Director's wing, Business Development Division wing and Administration wing.

Emergency numbers services have been programmed for dialing telephone numbers of ambulance, medical centre doctor, lift service providers, engineering services as well as Venture center of NCL Innovation Park area.

## वित्त एवं लेखा

यह विभाग प्रयोगशाला के नियमित स्टाफ, कनिष्ठ शोधछात्र/वरिष्ठ शोधछात्र, अनुसंधान सहयोगी, परियोजना सहायक, एमरिटस वैज्ञानिकों के अलावा लगभग 500 से अधिक बाहरी वित्तीय सहायता प्राप्त परियोजनाओं एवं लगभग 850 पेन्शनभोगियों आदि के वित्त एवं लेखा का प्रबन्धन करता है। सम्पूर्ण खातों (इम्पैक्ट) तथा इससे सम्बन्धित रजिस्ट्रों का रखरखाव किया गया तथा इम्पैक्ट आँकड़े प्रत्येक मास/वर्ष में सीएसआईआर मुख्यालय को प्रस्तुत किए गए। बैंक समाधान विवरण को अद्यतन किया गया (समायोजित कुल राशि - रु. 2734.386 लाख तथा लेनदेन की कुल संख्या 1292)। सेवा कर विभाग द्वारा इस वित्तीय वर्ष में केन्द्रीय वेट भी लागू किया गया।

1 निधि की उपयोगिता	
सीएसआईआर अनुदान राशि	
परियोजनाएँ	(रु. लाख में)
नेटवर्क (आगे ले जाई गई राशि सहित)	2052.932
गैर-नेटवर्क	7771.345
नमिटली परियोजनाएँ	233.035
ईएमआर एवं वैज्ञानिक पूल	544.172
प्रयोगशाला आरक्षित निधि	1544.762
बाहरी वित्तपोषित परियोजनाएँ	1533.833
विविध/फुटकर जमा राशि	63.290
बाहरी संगठनों द्वारा किया गया भुगतान	114.215
प्रायोजित सम्मेलनों/संगोष्ठियों हेतु जमा राशि	7.004
<b>कुल</b>	<b>13864.588</b>

2 प्रयोगशाला आरक्षित निधि का अर्जन	
वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर से भिन्न) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	258.774
अन्य लेखाशीर्षों से	493.012
<b>कुल</b>	<b>751.786</b>

3 31. 3. 2008 को अतिरिक्त निधि का निवेश	
(रु. लाख में)	2600.000

4 आपत्ति पुस्तिका मदों का निपटारा	
वर्ष के दौरान किए गए समायोजन	(रु. लाख में)
निजी	1203.578
यात्रा भत्ता/छुट्टी यात्रा रियायत	8.041
स्थानीय	6.407
<b>कुल</b>	<b>1218.026</b>
मदों की संख्या	284

5 निम्न प्रकार के वाउचर तैयार किए गए	
भुगतान	16558
प्राप्त राशि	4341
टी.ई.	369
<b>कुल</b>	<b>21268</b>

## भण्डार एवं क्रय

भण्डार एवं क्रय अनुभाग एनसीएल के लिए वैज्ञानिक/विश्लेषणात्मक, अत्याधुनिक उपकरणों के अलावा रसायनों, विलायकों, उपभोग्य वस्तुओं, अतिरिक्त पुर्जों आदि की खरीद करके उन्हें उपलब्ध कराता है। उक्त वस्तुएँ अनुसंधान एवं विकास कार्य हेतु प्रयोगशाला के बेंच स्तर के वैज्ञानिकों को जारी की जाती हैं। यह विभाग सामग्री प्राप्त करने, उसे जारी करने, उसका हिसाब रखने, सामग्री का अभिलेख रखने एवं अनुपयुक्त मदों/वस्तुओं के निपटारे हेतु वर्षभर अपनी कार्ययोजना पर कार्य करता है। भण्डार एवं क्रय विभाग प्रयोगशाला को सामग्री एवं सेवाएँ उपलब्ध कराने हेतु सतत रूप से कार्य करता है। यह विभाग सुचारु रूप से कार्यनिष्पादन हेतु विभिन्न विभागों एवं एजेन्सीयों जैसे - सीमा शुल्क एवं केन्द्रीय उत्पाद शुल्क से छूट हेतु डीएसआईआर के साथ, चुंगी (ऑक्ट्राई) से छूट प्राप्त करने के लिए पुणे नगर निगम, आयातित सामग्री समय पर प्राप्त होने के लिए सीमा शुल्क प्राधिकारी, मुम्बई/पुणे के साथ समन्वय स्थापित करता है तथा भारतीय स्टेट बैंक एवं माल वहन करने वाले एवं कार्गो क्लियरिंग एजेन्टों के साथ भी समन्वय बनाए रखता है ताकि प्रयोगशाला हेतु खरीद/प्राप्त की जाने वाली सामग्री समय पर उपलब्ध हो सके।

इस विभाग द्वारा पूरे किए गए कार्य/गतिविधियों के स्वरूप को दर्शाने हेतु मूल्य (रुपयों में) के साथ संख्यात्मक संकेतक

	संख्या		मूल्य (रु. करोड़ में)	
	2007-08	2008-09	2007-08	2008-09
कुल प्राप्त एवं निष्पादित माँगपत्र	2045	1817	47.00	57.11
कुल दिए गए ऑर्डर (आयातित)	900	849	24.99	28.63
कुल दिए गए ऑर्डर (स्वदेशी)	871	729	8.78	12.24
कुल प्राप्त सामग्री (आयातित)	971	1009	15.76	19.11
कुल प्राप्त सामग्री (स्वदेशी)	1836	1575	6.05	9.78
ऑनलाइन माँगपत्र	2086	0.96*	1517	0.90*
स्थानीय खरीद (ऑनलाइन आर सी सहित)	9683	3.11	14046	4.09
भण्डार से जारी की गई कुल सामग्री	36126	0.83	35340	0.64
वित्त वर्ष 2008-09 में समायोजित बकाया शेष			9.10	15.43
सीमा शुल्क छूट से प्राप्त राशि का उपयोग			16.57	19.22
उत्पाद शुल्क छूट से प्राप्त राशि का उपयोग			1.64	6.49
वर्ष के दौरान सूचना उत्पाद विकास एवं अनुसंधान यूनिट हेतु खरीद की गई सामग्री			0.83	0.65

\* ऑनलाइन रेट कॉन्ट्रैक्ट मदों को छोड़कर

## भण्डार एवं क्रय

खरीदे गए प्रमुख उपकरण /अन्य वस्तुएँ

मदें	मूल्य (रु. लाख में)
एन्टरप्राइज प्रबन्धन सूचना प्रणाली	230.50
ऑटोमेटेड डीएनए सिन्थेसाइजर	50.00
प्रयोगशाला फर्नीचर एवं हूड	619.61
टाइम अटेंडन्स	20.00
फ्लेमबल स्टोरेज कैबिनेट्स	37.00
माल्डी उपकरण	606.70
कॉन्फोकल लेज़र स्कैनिंग माइक्रोस्कोप	143.50
4 स्तरीय जल शुद्धिकरण प्रणाली	27.50
स्पेअर्स फॉर एनएमआर स्पेक्ट्रोमीटर	111.00
आईसीपी-ईईएस सिस्टिम	110.00
इन्डिपेन्डन्ट स्टेशन सरफेस एरिया एनालाइजर	31.00
एलेक्ट्रोफोरेसिस सिस्टिम	23.50
बैंच टॉप फरमेन्टेशन ऐण्ड बायोरिएक्टर सिस्टिम	23.30
ऑटोमेटेड रियल टाइम पीसीआर सिस्टिम विथ टीएलडी	48.00
ट्रान्सजेनिक ग्लास हाउस	27.00
अल्ट्रा लो वर्टिकल फ्रीजर	21.70
वर्सटाइल मोलेक्यूलर इमेजिंग सिस्टिम	49.00
ऑटोमेटेड एचपीएलसी फॉर प्रोटीन प्युरीफिकेशन	51.00
पैरेलल रिएक्शन स्टेशन	25.70
एनालिटिकल कम प्रिपरेटिव एचपीएलसी	30.20
स्टिडी स्टेट स्पेक्ट्रोफ्लुओरीमीटर	33.00
सरफेस प्रोफाइलर	37.00
ईडीएस माइक्रोएनालिसिस सिस्टिम	27.00
जीपीसी सिस्टिम	20.00
सोलार सेल कैरेक्टराइजेशन यूनिट	22.50
इलेक्ट्रोकेमिकल वर्कस्टेशन विथ आरडीई	21.50
माइक्रोसॉफ्ट डाइनामिक्स	58.40

## वर्ष के दौरान किए गए अन्य कार्य

- 4 प्रेस निविदाएँ जारी की गईं ।
- 11 बोली-पूर्व बैठकें आयोजित की गईं ।
- 30 मर्यादित निविदाएँ वेबसाइट पर अपलोड की गईं ।
- अनुपयुक्त वस्तुओं के निपटान से रु. 18,58,781/- की राशि प्राप्त हुई ।
- भारतीय पदार्थ प्रबन्धन संस्थान, पुणे शाखा द्वारा भण्डार एवं क्रय अनुभाग के स्टाफ हेतु छह मापदण्डों (मॉड्यूल्स) पर प्रयोगशाला में ही प्रशिक्षण कार्यक्रम आयोजित किया गया ।
- सूचना उत्पाद विकास एवं अनुसंधान यूनिट हेतु वर्ष के दौरान रु.65.00 लाख की सामग्री खरीद की गई ।

## Finance and Accounts

The department deals with the financing and accounting of more than 500 approx. externally funded projects and about 850 number of pensioners, besides the regular staff, JRF / SRF, RAs, PAs, Emeritus Scientists etc. Maintenance of full accounts (IMPACT) and its related registers and IMPACT data was submitted to CSIR HQ monthly / annually. Updated the Bank reconciliation statement (Total amount adjusted : Rs. 2734.386 lakh; No. of transactions: 1292). CEN VAT was claimed this financial year from Service Tax Department.

## 1 Funds Utilization

Projects	(Rs. in lakh)
CSIR Grant	
Network (including C/F)	2052.932
Non - network	7771.345
NMITLI Projects	233.035
EMR & Scientist Pool	544.172
Laboratory Reserve	1544.762
Externally Funded Projects	1533.833
Misc. Deposits	63.290
Payment on behalf of outside bodies	114.215
Deposits for Sponsored conf. /seminars	7.004
Total	<b>13864.588</b>

## 2 Generation of Lab Reserve (Rs. in lakh)

Through earning of interest on investment of surplus funds (other than CSIR) during the year	258.774
From other heads	493.012
Total	<b>751.786</b>

## 3 Investment of surplus funds as on 31.3.2008 (Rs. in lakh)

2600.000

## 4 Clearance of OB items

Adj. made during the year	(Rs. in lakh)
Private	1203.578
TA/LTC	8.041
Local	6.407
Total	1218.026
No. of items	284

## 5 Following types of vouchers were generated

Payment	16558
Receipt	4341
TE	369
Total	<b>21268</b>

## Stores and Purchase

The department takes care of procurement of scientific/ analytical, highly sophisticated instruments for the laboratory as a whole and also chemicals, solvents, consumables, spares etc. These items are issued to the bench level Scientists for their R&D activities. The department works with plan of action throughout the year to procure the materials, issuing, accounting, record maintenance and disposal of unserviceable items. It works with sustainable performance to provide goods and services to the laboratory. It co-ordinates with various other departments/ agencies such as DSIR for custom duty and central excise duty exemption and Pune Municipal Corporation for obtaining octroi exemption, Mumbai/ Pune Customs Authorities for timely clearance of imported consignments, and with State Bank of India and freight forwarding and cargo clearing agents.

#### Numerical indicators along with value (in Rupees) to indicate nature/type of Work/ activities completed

Item	Numbers		Value (Rs.in Crore)	
	2007-08	2008-09	2007-08	2008-09
Total indents received and processed	2045	1817	47.00	57.11
Total orders placed (imported)	900	849	24.99	28.63
Total orders placed (indigenous)	871	729	8.78	12.24
Total consignments received(imported)	971	1009	15.76	19.11
Total consignments received (Indigenous)	1836	1575	6.05	9.78
On-line indents	2086	0.96*	1517	0.90*
Local Purchases (including on-line RC)	9683	3.11	14046	4.09
Total Stores Issues	36126	0.83	35340	0.64
Outstanding balance adjusted during the Financial year 2008-09			9.10	15.43
Utilization of Custom Duty Exemption during Financial year 2008-09			16.57	19.22
Utilization of Excise Duty Exemption During Financial year 2008-09			1.64	6.49
URDIP Procurement for the year 2008-09			0.83	0.65

\*- Online RC indents

#### Major equipment / other items purchased

Item	Value (Rs.in lakh)
Enterprise management information system	230.50
Automated DNA synthesizer	50.00
lab furniture & hoods	619.61
Time attendance	20.00
Flammable storage cabinets	37.00
MALDI equipment	606.70
Confocal laser scanning microscope	143.50
4 Stage water purification system	27.50
Spares for NMR spectrometer	111.00
ICP-AES system	110.00
Independent station surface area analyzer	31.00
Electrophoresis system	23.50
Bench top fermentation & bioreactor system	23.30
Automated real time PCR system with TLD	48.00
Transgenic glass house	27.00
Ultra low vertical freezer	21.70
Versatile molecular imaging system	49.00
Automated HPLC for protein purification	51.00
Parallel reaction station	25.70
Analytical cum preparative HPLC	30.20
Steady state spectrofluorimeter	33.00
Surface profiler	37.00
EDS microanalysis system	27.00
GPC system	20.00
Solar cell characterization unit	22.50
Electrochemical workstation with RDE	21.50
Microsoft dynamics	58.40

#### Other jobs carried out during the year

- ✦ 4 Press Tenders issued
- ✦ 11 Pre-bid meetings were conducted
- ✦ 30 limited tenders uploaded on website
- ✦ Rs.18,58,781/- were been realized from disposal of unserviceable items
- ✦ An In-house Training Programme was conducted by Indian Institute of Materials Management, Pune branch for Stores & Purchase staff on six modules
- ✦ URDIP procurement for the year 2008-09 valued at Rs. 65.00 lakhs



## ANNEXURES

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## Biological Sciences

**Barreto M.S., Nookaraju A., Joglekar A.M., Karibasappa G.S., Agrawal D.C.**

Variability among vitis vinifera cultivars to *in vitro* propagation  
*Acta Horticulturae*  
785, 127-140

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DNA profiling of the grape varieties grown in India using ISSR markers  
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Influence of pretreatment of agriculture residues on phytase production by *Aspergillus niger* NCIM 563 under submerged fermentation conditions  
*African Journal of Biotechnology*  
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Utilization of molasses sugar for lactic acid production by *Lactobacillus delbrueckii* subsp. *delbrueckii* mutant Uc-3 in batch fermentation  
*Applied and Environmental Microbiology*  
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Integrated process for extraction and purification of alcohol dehydrogenase from Baker's yeast involving precipitation and aqueous two phase extraction  
*Biochemical Engineering Journal*  
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**Savergave L.S., Dhule S.S., Jogdand V.V., Nene S.N., Gadre R.V.**

Production and single step purification of cyclodextrin glycosyltransferase from alkalophilic *Bacillus firmus* by ion exchange chromatography  
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*Biocontrol Science and Technology*  
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Comparative Biochemical And Structural Characterizations of Fungal Polygalacturonases  
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Synthesis of chimeric tetrapeptide-linked cholic acid derivatives: Impending synergistic agents  
*Bioorganic and Medicinal Chemistry Letters*  
18(20), 5512-5517

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A serine protease inhibitor from hemolymph of green mussel, *Perna viridis*  
*Bioorganic and Medicinal Chemistry Letters*  
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Use of response surface optimization for the production of biosurfactant from *Rhodococcus* spp. MTCC 2574  
*Bioresource Technology*  
99(16), 7875-7880





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Immobilization of *Candida rugosa* lipase on poly(allyl glycidyl ether-co-ethylene glycol dimethacrylate) macroporous polymer particles  
*Bioresource Technology*  
99(9), 3623-3629

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*Carbohydrate Research*  
343(8), 1287-1296

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*Carbohydrate Research*  
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*Chemical Biology and Drug Design*  
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*Current Science*  
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Rapid and high biodegradation of phenols catalyzed by *Candida tropicalis* NCIM 3556 cells  
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First asymmetric total synthesis of penarolide sulfate A1  
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Taxol and 10-deacetylbaicatinIII induce distinct changes in the dynamics of caveolae  
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*Fish and Shellfish Immunology*  
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De novo shoot regeneration from root cultures of *Garcinia indica* Choiss.  
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Structure-activity relationship of a hemagglutinin from *Moringa oleifera* seeds  
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Induction of somatic embryogenesis in tamarind  
*International Journal of Plant Developmental Biology*  
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Rapid *in vitro* propagation of grapevine cv. Crimson Seedless - Influence of basal media and plant growth regulators  
*J. Applied Hort.*  
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*In vitro* regeneration of 'Green Sweet' apple via nucellus-raised callus  
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83(4), 447-452

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T-antigen binding lectin with antibacterial activity from marine invertebrate, sea cucumber (*Holothuria scabra*): Possible involvement in differential recognition of bacteria  
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*Journal of Microbiological Methods*  
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*Plant Cell, Tissue and Organ Culture*  
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*Vitis - Journal of Grapevine Research*  
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*World Journal of Microbiology and Biotechnology*  
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*World Journal of Microbiology and Biotechnology*  
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*Acta Materialia*  
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*Applied Catalysis A: General*  
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*Applied Catalysis A: General*  
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*Asian Journal of Chemistry*  
20(4), 3289-3291

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*Asian Journal of Chemistry*  
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New Strategy for the Synthesis of Pyrrolidine Derivatives  
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Title	Inventors	Country / Region	Patent No.
Novel dicarbanionic initiator, a process for the preparation and use thereof	Gnanou, Y., Matmour, R., More, A.S., Wadgaonkar, P.P.	SG	145403
A new process for the synthesis of micron/nanosized inorganic materials	Sastry, M., Rautaray, D.	US	7455823
Novel polymeric hindered amine light stabilizers based on end functionalized polyolefins and preparation thereof	Singh, R.P., Reddy, K.R.	EP	1863872
A high temperature stable non-noble metal catalyst, process for production of syngas using said catalyst	Choudhary, V.R., Mondal, K.C., Mamman A.S.	US	7432222
Oligomers and preparation thereof	Kulkarni, M.G., Khandare, J.J.	EP	1699833
A process for the preparation of beta-hydroxy-delta lactone using novel intermediates	Ghorpade, S.R., Kalkote, U.R., Chavan, S.P., Bhide, S.R., Ravindranathan, T.	EP	1234884
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An improved process for liquid phase oxidation of toluene to benzaldehyde.	Chaudhari, R.V., Rajurkar, K.B., Tonde, S.S., Rane, V. H.	US	7411099
An improved process for preparing carbamates	Srinivas, D., Srivastava, R., Ratnasamy, P.	US	7405319
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A novel catalytic formulation and its preparation	Mahajan, A.N., Chaudhari, R.V.	AU	2001258725
Process for recovery of highly pure acrylonitrile	Barve, P.P., Ghike, S.M., Shinde, R.W., Gupte, M.Y., Joshi, C.N	CN	ZL03826408.0
Process for crosslinking of polyallylamine hydrochloride	Kulkarni, M.G., Kanawade, T. S., Benjamin, S.B.	US	7388056
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Process for preparation of conducting polyaniline	Radhakrishnan, S., Deshpande, S.D.	EP	1701991
An improved process for the production of cyclic carbonates	Srinivas, D., Srivastava, R.	US	7375224

## Foreign Patents Granted

(1-1-2008 TO 31/12/2008)



Title	Inventors	Country / Region	Patent No.
An improved catalytic process for the production of pyridine and picolines (NCL-JOL)	Rajiv Kumar, Joshi, P.N., Chaphekar, G.M., Niphadkar, P.S., Agarwal, A., Verma, P.K., Singh, K.S.	US	7365204
Process for the preparation of cyclic carbonates using zeolite based catalysts	Srinivas, D., Srivastava, R.	US	7365214
bisphenols compounds and process for preparation there of	More, A.S., Wadgaonkar, P.P.	US	7446234
A process for polymerization and copolymerization of olefins	Sensarma, S., Sivaram, S.	EP	0878483
A novel catalytic formulation and its preparation	Chaudhari, R.V., Mahajan, A.N.	CN	ZL01823320.1
pH sensitive polymer and a process for preparation there of	Kulkarni, M.G., Menjoge, A.R.	AU	2003288706
Oligomers and preparation there of	Kulkarni, M.G., Khandare, J.J.	AU	200300704
Process for Producing Lubricants	Darbha Srinivas, Rajendra Srivastava, Paul Ratnasamy	EP	1733788
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Title	Inventors	Patent No.
A process for the preparation of enzymatically degradable polymers	Lele, B.S., Padmaja, T., Kulkarni, M.G.	226581
A process for the preparation of novel polyesteramide membranes	Razdan, U., Joshi, S.G., Kulkarni, S.S. (Ex.), Kharul, U.K.	226551
A process for the preparation of aliphatic-aromatic compatibilizers (jointly with IFCPAR, France)	Gopakumar, T.G., Ponrathnam, S., Rajan, C.R., Fradet, A.	226544
An improved process for the preparation of hydroxystigmasta-22-en/hydroxystigmastan 6-ones	Massey, A.P., Pore, V.S., Hazra, B.G.	226260
A process for the preparation of 2-aryl-4-hydroxy-cyclopent-2-en-1-ones	Gurjar, M.K., Wakharkar, R.D., Borate, H.B., Shinde, P.D., Mahajan, V.A., Jadhav, V.H., Wagh, A.M.	226070
An improved process for the preparation of 4-nitro-o-xylene	Dongare, M.K., Patial, P.P., Malshe, K.M.	225778
A process for the preparation of polymer films having high solvatochromic effect	Radhakrishnan, S., Valiyavalappil, S.	225687
A process for the preparation of a catalyst useful for the preparation of mixture of alkylphenols	Rao, B.S., Mathew T.	225321
A process for the preparation of metal sulfide nanoparticles	Mukherjee, P., Mandal, D., Ahmad, A., Sastry, M., Rajiv Kumar	224812
An improved process for the preparation of enantiomerically pure 3-phenyl-3-hydroxypropylamine	Pradeep Kumar, Pandey, R.K.	224384
A low temperature process for the production of hydrogen from methane or methane rich hydrocarbons and steam using GRP VIII metal oxide containing solid catalyst in tow parallel reactors	Choudhary, V.R., Rajput, A.M., Banerjee, S.	224382
A composition for hybrid seed production, process for the preparation of such composition and use thereof	Mahajan, V., Nagarajan, S., Deshpande, V.H., Kelkar, R.G., Lahoti, R.J., Ramalingam, S., Bulbule, V.J.	223253
A process for the preparation of an optically active alkyl 4-phenyl-2-[(trifluoroacetyl)amino] butanoate	Wakharkar, R.D., Borate, H.B., Waske, P.A., Gurjar, M.K.	222598
An improved hydrocarbon gas sensing instrument	Ramgir, N.S., Chaudhary, V.A., Vijaymohanam, K.P., Mulla, I.S.	222259
A process for the preparation of novel disperse dyes from naphtho [1,8-cd] dithiole	Srinivasan, K.V., Daniel, T., Lahoti, R.J., Swamy, V.P., Rajagopal, R.	221993
A process for preparation of an electrode useful for electrocatalytic oxidation of alkenes	Radhakrishnan, S., Adhikari, A.	221723
An improved process for the preparation of a mixture of alkyl phenols	Rao, B.S., Sreekumar, K., Jyothi, T.M.	221632

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Title	Inventors	Patent No.
A process for the preparation of poly bis (naphthalimido) sulphides	Yemul, O.S., Yemul, S.O., Ponrathnam, S., Rajan, C.R.	221645
A process for the preparation of bisphenol-A	Narayanan, S.V., Gopinathan, S., Unny, I.R., Deshpande, S.S., Degaonkar, M.P., Gopinathan, C.	221522
A process for the preparation of aziridines	Ali, S.I., Khisti, R.S., Dalavoy, V.S., Pardhy, S.A., Sudalai, A.	221469
A process for the preparation of surface modified zinc oxide sensor material useful for sensing ammonia gas	Aslam, M., Chaudhary, V.A., Mulla, I.S., Vijayamohanam, K.P.	221212
A process for the preparation of para nitro toluene	Dongare, M.K., Dagade, S.P., Kadam, V.S., Ratnasamy, P.	221052
An improved process for the preparation of Barium Titanyl Oxalate	Date, S.K., Potdar, H.S., Deshpande, S.B., Kholam, Y.B., Deshpande, A.S., Patil, A.J.	220791
An improved process for the preparation of microporous crystalline titanium silicate	Dongare, M.K., Patil, P.T., Malshe, K.M.	220788
A process for the preparation of conductive processable, polyaniline gel in water	Rethi, M., Rajan, C.R., Ponrathnam, S.	220750
A process for the preparation of alkaline protease	Laxman, R.S., More, S.V., Rele, M.V., Rao, B.S., Jogdand, V.V., Rao, M.B., Deshpande, V.V., Naidu, R.B., Manikandan, P., Kumar, D.A., Kanagaraj, J., Ramalingam, S.	220333
An improved process for the preparation of nitroxyl radicals	Phukan, P., Dalavoy, V.S., Sudalai, A.	220173
A process for the preparation of copper bound catalyst on polymer support (Continuation of NF-338/96)	Skaria, S., Rajan, C.R., Ponrathnam, S., Ghadge, V.B.	220150
A process for the preparation of aluminosilicate zeolite of type Na-P (jointly with NALCO)	Shiralkar, V.P., Joshi, P.N., Shiralkar, S.G., Seth, M.M., Mishra, C.R.	219882
An improved process for the preparation of nano-composite cathode materials for high energy density rechargeable lithium batteries	Ganguly, P., Kholam, Y.B., Bandopadhyay, K., Natarajan, N., Vijayamohanam, K.P.	218201
A process for the preparation of cellulase free xylanase	Lachke, A.H., Sathivel, C.	218343
A process for the preparation of ultra filtration membranes based on polyacrylonitrile and its copolymers	Kulkarni, S.S., Shinde, M.H., Musale, D.A.	218226
A process for the preparation of an improved rhodium catalyst	Balaji, B.S., Chanda, B.M.	218335
An process for the isolation of novel thermophilic Saccharomyces sp.	Sivaraman, H., Prabhune, A.A., Sahasrabudhe, T., Srinivasan, M.C.	218129



Title	Inventors	Patent No.
A process for the preparation of a nanosized colloidal metal particle	Mukherjee, P., Mandal, D., Ahmad, A., Sastry, M., Rajiv Kumar	218355
A novel membrane process for the production of hydrogen peroxide by non-hazardous direct oxidation of hydrogen by oxygen using a novel hydrophobic composite Pd-membrane catalyst	Choudhary, V.R., Sansare, S.D., Gaikwad, A.G.	218339
A process for the preparation of a nanosized noble metal catalyst useful for the selective preparation of aliphatic diols	Rode, C.V., Telkar, M.M., Chaudhari, R.V.	218357
An improved process for the preparation of naphtha [1,8-cd] dithiole	Srinivasan, K.V., Daniel, T., Lahoti, R.J., Swamy, V.P., Rajagopal, R.	218350
An improved process for the preparation of microencapsulation of active ingredients in polymers	Vishwanathan, B.N., Thomas, P.A., Kulkarni, M.G., Mashelkar, R.A.	218111
A process for decolourisation of molasses based distillery effluent (NCL-VSI, Pune)	Dongare, M.K., Sankpal, N.V., Gunjal, B.B., Nimbalkar, D.S.	218309
A process for the preparation of a novel crystalline zirconium containing aluminophosphate, Zr-APO-11	Dongare, M.K., Hegde, S.G., Sabde, D.P., Kamble, K.R.	217841
An improved process for the preparation of 1,4 butenediol	Chaudhari, R.V., Rode, C.V., Jaganathan, R., Telkar, M.M., Rane, V.H.	217636
A method for preparation of mycolytic enzymes containing mainly chitinase	Deshpande, M., Desai, M., Chitnis, M., Patil, R.	217783
A process for the preparation of polymeric adsorbents	Joshi, V.P., Kulkarni, M.G., Mashelkar, R.A.	217331
A process for the preparation of novel derivatised macroporous beaded copolymer as affinity chromatography supports (NCL, HAL, Pune & DBT, New Delhi)	Ghadge, V.B., Ponrathnam, S., Rajan, C.R., Deshpande, B.S., Sudhakaran, V.K., Shewale, J.G.	217160
An improved process for the removal of colour and degradation of industrial waste mainly containing aromatic compounds	Sahasrabudhe, N.A.	217114
An improved process for the deposition of a conducting polymer film on an insulating substrates having interdigitated electrodes	Radhakrishnan, S., Deshpande, S.D.	216983
An improved process for preparation of a poly propylene moulding compound having high impact and high tensile strength	Radhakrishnan, S., Saujanya, C.	216973
An improved process for the preparation of carboxylic acids	Suryavanshi, G., Sawaikar, D.D., Pardhy, S.A., Sudalai, A.	216936



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Title	Inventors	Patent No.
An improved process for the treatment of agro based black liquor waste to produce potable water	Moghe, P.P., Panchanadikar, V.V., Untawale, A.G., Dhargalkar, V.K.	216746
A process for the synthesis of reactive polymers and copolymers from vinylbenzyl methacrylate	Baskaran, D.	216747
A process for the preparation of novel derivatised macroporous beaded crosslinked polymer useful as affinity chromatography supports [NCL, HAL, Pune and DBT]	Ghadge, V.B., Ponrathnam, S., Rajan, C.R., Mujawar, S.K., Shewale, J.G.	216785
An improved process for the production of hydroxy phenyl ketones	Chaube, V.D., Singh, A.P.	216704
A process for the preparation of thermoprecipitating affinity polymers	Vaidya, A.A., Lele, B.S., Kulkarni, M.G., Mashelkar, R.A.	216559
An improved process for the preparation of stable aqueous urethane dispersions	Ramanathan, L.S., Raut, K.G., Srinivasan, S.R., Sivaram, S.	216277
An improved process for the preparation of starch based polyesters	Varma, A.J., Kokane, S.P., Deshpande, P., Paradkar, A., Choudhary, N.	216245
A process for the activation of perovskite-type oxide	Choudhary, V.R., Banerjee, S.	216276
A device useful for operating gas cylinders having leaky cylinder valves	Balakrishnan, S., Parande, M.G.	216121
An improved process for preparation of hexagonal mesoporous silica catalyst	Sathaye, S.D., Soni, H.S., Jacob, N.E., Agashe, M.S., Belhekar, A.A.	216097
An improved process for decolourisation of agro-industry effluents to produce colourless effluent	Gokarn, A.N., Joshi, A.P., Chaturvedi, N.S., Akolkar, L.P., Sankpal, N.V.	215820
An improved process for the preparation of aralkylated aromatic compounds	Choudhary, V.R., Jana, S.K., Kiran, B.P.	215824
An improved process for the preparation of dihydroxydiphenyl methanes	Singh, A. P., Dagade, S.	215816
A process for the preparation of mixture of 19-hydroxy eicosatetraenoic acid and 20-hydroxy eicosatetraenoic acid	Nori Krishnamurti, Deekshitula Bhaskara Rohinikumar	215843
Improved process for the preparation of saturated carboxylic acids and their esters	Chaudhari, R.V., Seayad, A., Seayad, J.	215748
A process for the preparation of chromium containing molecular sieve	Chaudhari, K., Das, T.K., Sivasanker, S., Chandwadkar, A.J.	215802
A process for preparation of ultrathin films of metal phthalocyanines	Sathaye, S.D., Patil, K.R., Paranjape, D.V.	215776
An improved process for the preparation of polyurethane spherical particle	Ramanathan, L.S., Sivaram, S.	215710



Title	Inventors	Patent No.
A process for producing polycondensable macromonomer	Ramanathan, L.S., Sivaram, S.	215723
A device for sensing ammonia gas using surface functionalized zinc oxide as sensor	Aslam, M., Chaudhary, V.A., Mulla, I.S., B.S., Kulkarni, M.G., Mashelkar, R.A., Vijayamohan, K.P.	215705
An improved process for the preparation of carboxylic acids	Dalavoy, V.S., Pardhy, S.A., Sudalai, A., Ramaswamy, A.V.	215765
An improved process for the selective preparation of catechol or mixture of catechol and hydroquinone from phenol	Yadav, N.K., Kulkarni, B.D., Khomane, R.B.	215670
A process for the preparation of molecularly imprinted polymers useful for separation of enzymes	Vaidya, A.A., Lele	215686
Novel hydrophobic multicomponent catalyst useful for direct oxidation of hydrogen to hydrogen peroxide	Choudhary, V.R., Sansare, S.D., Gaikwad, A.G.	215677
An improved process for the preparation of purified metal sulphide nano particles	Lachke, A.H., Gole, A.M., Sathivel, C., Sastry, M.	215660
An improved process for the preparation of aromatic polyesters	Kharul, U.K., Kulkarni, S.S.	215506
An improved process for the preparation of 1,4-butanediol	Panse, D.G., Gumaste, V.K., Deshmukh, A.R.A.S., Bhawal, B.M., Sarkar, A.	215481
A process for the preparation of hyperbranched polymers and copolymers	Baskaran, D.	215492
A process for the preparation of supported copper catalyst	Gopinathan, S., Gopinathan, C., Unny, I.R., Deshpande, S.S., Degaonkar, M.P., Sajanikumari, C.S., Joseph, T.	215575
A process for the preparation of supported solid catalysts useful for Friedel-Crafts reactions	Choudhary, V.R., Jana, S.K., Kiran, B.P.	215581
An improved process for the preparation of porous crystalline silico aluminophosphate molecular sieve	Sinha, A.K., Sivasanker, S.	215579
An improved process for production of propylene and ethylene by non-catalytic oxycracking of propane or propane-rich C2-C4 paraffins	Choudhary, V.R., Rajput, A.M., Rane, V.H.	215333
An improved process for 1,4-butanediol	Panse, D.G., Gumaste, V.K., Deshmukh, A.R. A.S., Bhawal, B.M., Sarkar, A.	215236
An improved process for the preparation of dihydroxy alkenes	Sawaikar, D.D., Suryavanshi, G., Sudalai, A.	215245

## Indian Patents Granted

(1-1-2008 TO 31/12/2008)



Title	Inventors	Patent No.
A process for the preparation of novel monomers based on disubstituted cycloalkanones	Raju, S.V.N., Subramaniam, S., Srinivasan, K.V., Rajan, C.R., Ponrathnam, S.	215169
An improved process for the preparation of bis(halo-naphthalimido) alkylenes	Yemul, S.O., Yemul, O.S., Ponrathnam, S., Rajan, C.R.	215158
An improved process for the preparation of alkyl 2-acyl/carbalkoxy-3-(substituted amino) acrylates	Deshmukh, A.R.A.S., Panse, D.G., Bhawal, B.M.	215148
A process for the simultaneous production of styrene oxide and benzaldehyde	Saji, P.V., Ratnasamy, C., Gopinathan, S.	215099
A process for the preparation of polymeric adsorbents by precipitation polymerization	Joshi, V.P., Kulkarni, M.G., Mashelkar, R.A.	215140
A process for the preparation of compatibilized polymer blends	Gopakumar, T.G., Ponrathnam, S., Rajan, C.R., Fradet, A.	215019
An improved process for the preparation of aralkylated aromatic compounds using heterogeneous catalyst	Choudhary, V.R., Jana, S.K., Kiran, B.P.	215038
A single step process for the preparation of poly(oxyalkylene)-alpha, omega-dicarboxylic acids	Lele, B.S., Kulkarni, M.G.	215035
An improved process for the preparation of ultrathin/thin films of metallic compounds	Sathaye, S.D., Patil, K.R., Paranjape, D.V.	215039
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A process for the manufacture of cyclohexanoneoxime	Robert, Raja, Ratnasamy, P.	214109
A Process for the Preparation of Protease Inhibitor Using Novel Alkalo Theromphilic Bacillus SP.	Chandravanu Dash, Sangita Uday Phadtare, Absar Ahmad, Vasanti Vishnu Deshpande, Mala Balchandra Rao	215711 215711
A Process for the Preparation of Polyesteramides	Kelkar AA, Kulkarni SM, Chaudhari RV	217629
An Improved Process for the Treatment of Spent Wash Using Marine Alga to Produce Potable Water	Moghe; Pramod Prabhakar (Pune); Panchanadikar; Vinita Vinay (Pune); Untawale; Arvind Gajanan (Goa); Dhargalkar; Vinod Kashinath (Goa)	215771

## PhD Theses



## IIT, Mumbai

Author	Title	Guide
Mujumdar, K.S.	Modeling of Rotary Cement Kilns	Ranade, V.V. & Mehra, A.

## Kalyani University

Author	Title	Guide
Chatterjee, B.	Synthetic Studies Towards Amphidinolide W and Heliconols A- C	Gurjar, M.K.
Maity, P.K.	Synthesis of Biologically Active Multicyclic Frameworks via [3+2] Cycloaddition and Studies Towards the Total Synthesis of Palau' Amide	Gurjar, M.K.
Mondal, M.A.	Studies Toward the Total Synthesis of Aspercyclide A-C, Macrocin A and 4-Epi-Stagonolide B by Employing Ring Closing Metathesis Reaction	Gurjar, M.K.

## Osmania University

Author	Title	Guide
Boddeti, I.	Cycloisomerizations of Sugar Derived Alkynols and Toward the Total Synthesis of Didemnerinolipid B and Some Functionalizes Nortropane Alkaloids	Deshmukh, M. N.
Karumudi, B.	Synthetic Studies Toward Eupomatilone-6, 4-O- $\beta$ -D-Galactosyl Maltose and Amphidinol-3	Gurjar, M. K.
Raghupathi, N.	Studies Toward the Total Syntheses of Skipped Polyol Natural Products: Strictifolione, 6R-6-[(4R,6R)-4,6-Dihydroxy-10-Phenyldec-1-Enyl]-5,6-Dihydro-2H-Pyran-2-one, Marinomycin A. (+)-Cryptocarya Diacetate	Gurjar, M. K.
Ramesh, D. K.	Synthesis of Macrolides by Protecting Group Directed Ring-Closing Metathesis (RCM) and Studies on Lipoic Acid Caminoside A.	Gurjar, M. K.
Reddy, C. N.	Studies Toward the Total Synthesis of Carba Analogue of Motif C of M.tb Cell Wall AG Complex, Integrastatins And A Double_Suzuki Approach for Synthesis of Substituted Diarylmethylenefluorenes	Gurjar, M. K.

## University of Mumbai

Author	Title	Guide
Pardeshi, V. C.	Study Towards Genetic Diversity and Genetic Basis of Prolificacy in Important Sheep Breeds of India	Gupta, V. S. (Ms)

## PhD Theses



## University of Pune

Author	Title	Guide
Amalraj, S. F.	Structure and Properties of Conducting Polymers Modified with Functional Molecules	Radhakrishnan, S.
Atul Kumar	Penicillin V Acylase from <i>Rhodotorula aurantiaca</i> (NCIM 3415): Studies on Biochemical and Biophysical Characterization of the Enzyme	Pundle, A.
Badhe, Y. P.	Process Modeling and Optimization Using Artificial Intelligence and Machine Learning Formalisms	Kulkarni, B. D.
Bairagi, A. S.	Studies on Arylation and Carbonylation Reactions using Palladium Complex Catalysts	Chaudhari, R. V.
Balakrishnan, M.	Synthetic Studies Towards Amaryllidaceae Alkaloids: An Intramolecular Aza- Michael Addition Approach	Pandey, G.
Banu, S.	Molecular Marker Based Genetic Diversity in Symplocos SPP. from the Two Biodiversity Hotspots in India	Gupta, V. S. (Ms)
Barreto, M, S.	In Vitro Plant Regeneration and Transformation Studies in Grape ( <i>Vitis vinifera</i> L.)	Agrawal, D. C.
Bhange, D.	Structural Studies of Silicate and Metallosilicate Molecular Sieves of MFI Type Using Non Ambient Powder X-ray Diffraction Techniques	Ramaswamy, V. (Mrs)
Bharadwaj, K. C.	Synthesis of Polyhydroxy Cyclic Amines as Potent Glycosidases Inhibitors	Pandey, G.
Biradar, A. V.	Cyclopentadienyl Molybdenum Acetylides Complexes as Novel Catalyst for Oxidation Reactions	Umbarkar, S. B.
Bordoloi, A.	Hybrid Inorganic-Organic Materials and Nanocomposites: Synthesis, Characterization and Catalytic Applications in Organic Transformations	Halligudi, S. B.
Burgula, S.	Synthetic Studies Toward the Skipped 1,3-polyol Natural Products and Some Pd-Medicated Reactions of Sugar Alkynols	Deshmukh, M. N.
Chandra kiran, N.	Synthetic Studies Toward the Total Synthesis of Aflastatin A, Brugierol A and Preparation of Some 10-Diarylmethylidene Anthraquinones	Gurjar, M. K.
Chatterjee, S.	Towards the Total Synthesis of Multiplolide A, Feigrisolide B and Pandangolide 1 using Chiron Approach and Exploration of Click Reaction in Crystal Engineering	Gurjar, M. K.
Depan, D.	Novel Designing of Chitosan Based Nanocomposites for Tissue Engineering and Drug Delivery Applications	Singh, R. P.
Dharap, Y. V.	Facile Synthesis of Azeridines using Copper Hydrotalcite under Microwave Irradiation, Synthesis of 3-Substituted -2(1H)- Quinolinones Catalyzed by Hydrotalcite like Anionic Clays, Rearrangement of Alpha- Pinene Epoxide to Campholenice Aldehyde with Modified Beta Zeolite Catalyst and Regioselective Nitration of Phenols with New Phosphorous Based Ionic Liquids	Chanda, B.M.(Mrs.)
Dumbre, D.K.	Selective Liquid Phase Alcohol Oxidation and Heck- Type Coupling Reactions Using Heterogeneous Catalysts	Wakharkar, R.D.(Ms) & Choudhari, V.R.



Author	Title	Guide
Emmanuvel, L.	Asymmetric Synthesis of Bioactive 1, 2- Aminoalcohols and Methodologies Involving Dihydroxylation of Olefins, Esterification and Iodination of Aromatics	Sudalai, A.
Gholap, A.R.	Application of Ionic Liquids/Ultrasound Towards the Study of Cross-Coupling Reactions, Multi-Component Reactions; Synthesis of Enaminones/PD Enaminone Complexes and their Applications; Studies Towards the Synthesis of Novel Biologically Active Nitrogen Heterocycles	Sirivivasan, K.V.
Gogoi, S.	Studies on Total Synthesis of Bioactive Natural Butyrolactones	Argade, N.P.
Gowda, N.M.	Purification and Characterization of a Lectin From Marine Invertebrate, Sea Cucumber ( <i>Holothuria scabra</i> )	Khan, M.I.
Gupta, M.K.	Photo and Thermo Latent Initiators for Cationic Polymerization	Singh, R.P.
Gupta, S.K.	Isolation, Cloning and Characterization of Lignin Biosynthesis Pathway Gene(s) 4- Coumarate Co A Ligase (4CL) from <i>Leucaena leucocephala</i>	Khan, B.M.
Haval, K.P.	Synthesis of Natural and Unnatural Dialkyl Substituted Maleic Anhydrides and Related Natural Products	Argade, N.P.
Ingle, R.	Selective Oxidation of Alkanes and Alkenes by Polyoxometalates Using Green Oxidants	Manikandan, P.
Jagdale, A.R.	Enantioselective Synthesis of Bioactive Molecules via Asymmetric Reductions, Dihydroxylations of Olefins and Synthetic Methodologies Involving Reduction of Esters, Halogenation of Ketones and Hydroarylation and Arenes	Sudalai, A.
Kadam, V.S.	Synthesis and Characterization of Novel Hydrophobically Modified Polymers and Organogelators	Badiger, M.V.
Kakade, B.A.	Synthesis, Functionalization And Wetting Behavior of Carbon Nanotubes	Vijaymohanana, K.
Kashyap, S.	Synthesis of Glycosides, Saccharides and Glycoconjugates via Alkyne Activation	Hotha, S.
Kendhale, A.M.	Design, Synthesis and Conformational Studies of Foldamers with Novel Backbones	Sanjayan, G.J.
Khan, A.	Biochemical Studies on Some Aspects of Nitrogen Metabolism in Mycobacterium SP.	Ganesh, K.N.
Khan, M.S.	Study of Natural and Synthetic Protease Inhibitors and their Biological Activities	Khan, M.I.
Kumar, A.P.	Polymeric Materials From Cellulose and Its Derivatives: Preparation, Characterization and Durability of their Blends and Composites	Singh, R.P.
Kumbharkar, S.C.	Structure Gas Permeation Property Correlations in Polybenzimidazoles and Related Polymers	Kharul, U.K.
Lohokare, H.R.	Investigations in Ultrafiltration Membranes Based on Polyacrylonitrile and AB Polybenzimidazole	Kharul, U.K.
Mahima, S.	Template-Assisted Synthesis and Characterization of High Aspect Ratio Metallic Nanostructures	Vijayamohanana, K.

## PhD Theses



Author	Title	Guide
Malwadkar, S.S.	Supported Metal Catalysts for the Preferential Oxidation of Carbon Monoxide and Partial Oxidation of Methane	Satyanarayana, C.V.V.
Manoj, K.	Investigation of Polymorphism in inositol Derivatives: Synthesis, Crystallographic Studies & Analysis of Intermolecular Interactions.	Bhadbhade, M.M. & Shashidhar, M.S.
Marivel, S.	Supramolecular Synthesis of Some Organic and Metal Organic Complexes by Co-crystallization	Pedireddi, V.R.
Murali, C.	Studies Directed Towards the Synthesis, Associated Reaction Mechanisms and Structure of Inositols and their Derivatives	Shashidhar, M.S.
Naidu, V. S.	Asymmetric Dihydroxylation and Jacobsen's Hydrolytic Kinetic Resolution Methods to the Synthesis of Naturally Occuring Amino Alcohols and Lactones	Pradeepkumar
Pal, R.	Synthesis Studies Towards Superstolide A, Centrolobine and Some Radical Rearrangement	Gurjar, M. K.
Palaskar, D. V.	Controlled Synthesis of End-Functionalised Polymers and Block Copolymers	Wadgaonkar, P. P.
Pandey, S. K.	Enantoselective Total Synthesis of Biologically Active Natural Products Employing Hydrolytic Kinetic Resolution (HKR) and Asymmetric Dihydroxylation	Pradeepkumar
Pandit, S. S.	Genetic Analysis of Aplhonso Mango Flavor Biogenesis	Gupta, V. S.(Mrs).
Parambadath, S.	Heterogenized Nitrogen Containing Metal Complexes over SBA-15 for Asymmetric Transfer Hydrogenation Reaction	Singh, A. P.
Pathak, A. B.	Synthetic Studies Towards Camptothecin, Its Analogues and Other Biologically Active Compounds	Chavan, S. P.
Pawar, K. D.	<i>In vitro</i> Production of Secondary Metabolites from Cultured Cell/Tissue and Molecular Characterization of Calophyllum inophyllum (L)	Thengane, S. R.
Potewar, T. M.	Studies on Synthesis of Biologically Active N- Heterocycles: Development of Environment Friendly Synthetic Methodologies	Srinivasan, K. V.
Prabhakaran, P.	Exploring Multiple Hydrogen-Bonding Interactions in the Design of Novel Molecular Architectures	Sanjayan, G. J.
Rahaman, H.	Synthesis Studies toward Amphidinolide C and Some Biologically Active Natural Products	Gurjar, M. K.
Rajurkar, K. B.	Studies in Catalysis and Reaction Engineering Aspects of Multiphase Catalytic Reactions	Chaudhari, R. V.
Reddy, P. S.	Design and Synthesis of Supramolecular Adducts of Nucleobases and Nucleosides	Pedireddi, V. R.
Sahoo, G.	Synthetic Studies toward Prototype Resin Inhibitors, Basiliskamides and Decarestrictine C1	Gurjar, M. K.
Sahoo, S.	Chiral Metal Complexes Anchored onto Mesoporous Silica as Heterogeneous Catalysts for Asymmetric Organic Transformations	Halligudi, S. B.

## PhD Theses



Author	Title	Guide
Saikia, L.	Synthesis and Catalytic Activity Studies of Functionalised Mesoporous Silica Materials	Srinivas, D.
Salunke, D.B.	Design Synthesis and Bio-evaluation of Steroidal Conjugates: A Study Directed Towards The Development of Novel Lead Molecules.	Pore, V. S. (Ms), Hazra, B. G.
Satpute, D.B	Effect of Electrolytes on Thermodynamics of Amino Acids in Aqueous and Non-Aqueous Media	Anilkumar
Seetha Lakshmi,N.(Ms)	Supramolecular Synthesis of Organic and Coordination Assemblies Utilizing Some Aromatic Boronic Acids	Pedireddi, V. R.
Shah, P.P.	Synthesis, Characterization and Catalytic Activity of Ordered Sn, AL-SBA-15 and Immobilization of Ntn-Hydrolase Family Enzymes on SBA-15 Mesoporous Molecular Sieves	Ramaswamy, V.(Ms)
Shanbhag, G. V.	Studies on Hydroamination Reactions Usinig Heterogeneous Catalysts	Halligudi, S. B.
Sharath, B.	Structure and Kinetics of Gamma Glutamyl Transferases from Bacillus Species	Prabhune, A.(Mrs)
Shingate, B. B.	Stereoselective Syntheses of Steroidal Unnatural C(20R) Aldehydes by Ionic Hydrogenation: Syntheses of Naturally Occurring 20-EPI Cholanolic Acid Derivatives	Hazra, B. G.
Singh, S.	Somatic Embryogenesis and Genetic Transformation in Peanut	Hazra, S. (Ms)
Singh, S. K.	Bio-Inspired Metal and Metal-Oxide Nanoparticles: Synthesis, Characterizations and Applications	Prabhune, A(Ms) & Prasad, B. L. V.
Sreekant, D.	Secondary Metabolites from Endophytic Fungi: Isolation, Purification, Characterization and Bioassay	Khan, M. I.
Srinivas, D.	<i>De Novo</i> Designed Foldamers Based on Biotic and Abiotic Building Blocks	Sanjayan, G. J.
Sunil Kumar	Studies on Metal Tolerance in Plants	Hazra, S. (Ms)
Tiwari, K.N.	Asymmetric Desymmetrization Approach for the Construction of Enantiopure (+)-7-Azabicyclo[2.2.1] HEPT-2-one: Application in the Synthesis of Biologically Active Alkaloids	Pandey, G.
Tripathi, A.	Synthesis of Fused Tricyclic Compounds from Glycals & Click Chemistry Inspired Imaging of Microbes	Hotha, S.
Venkatesan, K.	Novel Organic Transformations for the Thermal / Sonochemical Synthesis of Important Intermediates and Biologically Active Molecules	Srinivasan, K.V.
Vysabhatar, R.	Synthesis of Cyanuryl, 8-Substituted Adeniny PNA Analogues and Biophysical Studies of their DNA/RNA Hybridisation Properties	Ganesh, K.N.
Yadav, A. K.	Studies Towards The Total Synthesis of Radicamine B, Quercitols, Dolastatin 19 and Developing New Process for Sucralose	Gurjar, M. K.
Yellol, G.S.	Studies Towards the Total Synthesis of Amphidinolide X, Ecosanoid and Solandelactone	Gurjar, M. K.

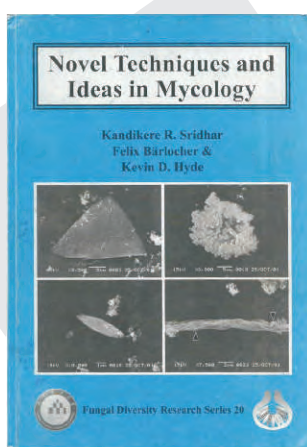


## Books / Chapter In Books



## Chapter in books

- + 'Engineered ZnO Nanostructures: An Excellent Field Emitter for Next Generation Devices', N.S. Ramgir, M.A. More, D.S. Joag and I.S. Mulla in *Metal Oxide Nanostructures and their Applications*, American Scientific Publishers.
- + 'Bioethanol from Lignocellulosic Biomass Part-I: Pretreatment of Substrates', R. Seeta Laxman and A.H. Lachke in *Plant Based Biofuels*, (Ed.) Ashok Pandey, CRC Press, Boca Raton, Florida, USA, pp. 121-139.
- + 'Bioethanol from Lignocellulosic Biomass. Part-III: Hydrolysis and Fermentation' Ramakrishnan Anish and Mala Rao in *Plant Based Biofuels*, (Ed.) Ashok Pandey, CRC Press, Boca Raton, Florida, USA, pp. 159-173.
- + 'Biosynthesis of nanoparticles by *Fusarium oxysporum*', A. Ahmad, S. Senapati, M. I. Khan, R. Kumar and M. Sastry in *Novel techniques and Ideas in Mycology*, (Ed.) K.R. Sridhar, F. Baerlocher and K.D. Hyde, Fungal Diversity Press, Thailand, pp. 77-94.
- + 'Electroantennogram responses of *T. chilonis* Ishii and *Chrysoperla carnea* to plant volatiles: Need for molecular aspects of Sensory physiology in insects, A. Sen and R. Raina in *Dimensions of Molecular Entomology*, Orient Longman', New Delhi, 2007, pp. 110-121.
- + 'Toxic effects of non-edible oil seed extracts on yellow fever mosquito *Aedes aegypti* (L)', Pushpa Pawar, Vijay Tungikar and Swati Joshi in *Microbiology Applications and Current Trends*, (Ed). P. C. Trivedi, Pointer Publishers, Jaipur, 2007, pp 229-36.
- + 'Template Synthesis and Catalysis of Metal Nanoclusters in Ordered Mesoporous Silicas', Paresh L. Dhepe and Atsushi Fukuoka in *Metal Nanoclusters in Catalysis and Materials Science: The Issue of Size-control*, (Ed). B. Corain, G. Schmid and N. Toshima, Elsevier, 2008, 383-390.
- + 'Recent advances in the production of hydrogen as a renewable source of energy by way of semiconductor-mediated and visible-light-induced photocatalytic splitting of water', Narendra M. Gupta and Aparna S. Deshpade in *Renewable Energy*, (Ed). A. D. Vyas, U. S. Mirdha and M. Yyas, McMillan Publishers, Delhi, 2009, pp. 141-151.
- + 'The biotechnological applications of dimorphic yeasts', N. Doiphode, C. Joshi, V. Ghormade, M. V. Deshpande in *Yeast biotechnology – Diversity and applications*, (Ed.) Satyanarayana and Kunze, Springer, New York, USA, 2009, pp.635-650.
- + 'Status of microbial pesticides in India', S. Chavan, M. Kulkarni and M. V. Deshpande in *Review of Plant Pathology*, Vol. 4, (Ed.) Prof. S. M. Reddy and H. N. Gour, Sci. Publishers, Jodhpur, 2008, pp.393-420.
- + 'Selective alkylation of organic substrates on spinels', M. Vijayaraj, T. Mathew and C. S. Gopinath, in *Heterogeneous Catalysis Research Progress*, (Ed.) Mathias B. Gunther, Nova Science, New York, 2008, pp. 145-191.



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 M.B. Rao, A. Kulkarni

## Academic Collaborations



NCL has collaborative projects with many leading national and international academic and scientific institutes. NCL scientists individually or as a team also have international collaborative programmes with leading research groups from abroad.

### Institute to Institute Collaborations

External Institute	Field(s) of Collaboration	NCL Nodal Scientist(s)
Bharati Vidyapeeth University Poona College of Pharmacy, Pune	Biotechnology, Polymer and Materials Science Engineering, Nanomaterials (Design and Development)	Dr. S. Sivaram
Center of Excellence in Polymer Science, Karnatak University, Dharwad	Polymer Science	Dr. M.G. Kulkarni
Centre for Development of Advanced Computing (C-DAC), Pune	Parallelisation of Coupled-Cluster Electronic Structure Theory, Parallelisation of Optimization Technique, and Biodiversity	Dr. Sourav Pal
Centre for Development of Advanced Computing (C-DAC), Pune and ERNET India	Promoting High Level Research with the help of GRID Technology and its Applications	Dr. Sourav Pal
Gwangju Institute of Science and Technology (GIST), Republic of Korea	Organic Materials, Photonic Polymers and Hybrid Materials	Dr. S. Sivaram
Institute of Genomics and Integrative Biology, Delhi	Research at the interface of Chemistry and Biology	Dr. H.V. Thulasiram
National Center for Cell Science, Pune & National Institute of Oceanography, Goa	Exploitation of Biomedical Potentials of Fungal Extracts of Specific Tissues Related to Hitherto Unattained Aspects of Peptide/ Protein Fractionation, Purification and Bioactivity Testing from Fungi	Dr. Islam Khan
National Institute for Applied Sciences, Lyon (INSA, Lyon), France	Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Mr. Sanjay Nene
National Institute of Food and Agro Industries, Massy, France	Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Mr. Sanjay Nene
RMIT University, School of Applied Sciences, Melbourne, Australia	Catalysis, High Field Solid State NMR Studies and Nanoscience / Nanotechnology	Dr. S. Sivaram
The Ohio State University Research Foundation (OSURF), Columbus, Ohio, USA	Materials Science Engineering and Nanotechnology	Dr. K. Vijayamohan
The Tokyo University of Science, Japan	Chemical Sciences	Dr. S. Sivaram
Universidade Federal do Parana, Brazil	Bio-diesel, Bio fuel, biomass conversion, and polymeric composites	Dr. S. Sivaram
University of Applied Sciences, Hochschule Anhalt HAS, Kothen, Germany	Biochemistry, Bioprocess Technology and Bioengineering (Design and Development)	Mr. Sanjay Nene

## Academic Collaborations



External Institute	Field(s) of Collaboration	NCL Nodal Scientist(s)
University of Science and Technology, Lille (USTL), France	High Field Solid State NMR Studies, Catalysis, Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Dr S. Ganapathy
Vasantdada Sugar Institute, Pune	Zeolite assisted Ethanollic Fermentation	Dr. Asmita Prabhune
Hanyang University, Seoul, S. Korea	Collaborative Research Activities	Dr. S.B. Ogale
The University of Rome	Polymer chemistry and Physical chemistry of Macromolecules	Dr. S. Sivaram
National Institute for Applied Sciences, Lyon (INSA, Lyon), France	Indo-French Unit for Water and Waste Technologies Project	Mr. Sanjay Nene
University of Turin, Italy	Catalysis and spectroscopy of catalyst surfaces	Dr. D. Srinivas

## Scientist-to-Scientist International Collaborations

Project Title	NCL Partner(s)	External Partner(s)
Catalytic reaction engineering using ionic liquids	Dr. A. A. Kelkar	Prof. Henri Delmas ENSIACET, Toulouse, France
Synthesis of novel heterogeneous catalysts for asymmetric oxidation catalysis	Dr. A. P Singh	Dr. Stéphane Ménage DR CNRS Lab, Laboratoire de Chimie et Biochimie des Centres Redox Biologiques (CBCRB), 17 rue des Martyrs, CEA-Grenoble, 38054 GrenobleCedex 9 France
A Continuous process for the synthesis of monocrystalline polysaccharide nanoparticles	Dr. Amol Kulkarni	Prof. Wim Thielmans University of Nottingham UK
Hydrodynamics of High solid concentration three phase slurry reactor for GTL	Dr. Amol Kulkarni	Prof. Tiefeng Wang Key Laboratory of Reaction Engineering Tsinghua University, Beijing, China
Stability analysis and performance of microreactors for exothermic nitration reactions	Dr. Amol Kulkarni	Prof. Achim Kienle Max-planck Institute of Dynamics of Complex Technical Systems Magdeburg, Germany
Synthesis and surface modification of magnetic core-noble metal shell nanoparticles for biological applications	Dr. B.L.V. Prasad	Prof. Mathias. Brust University of Liverpool UK

## Academic Collaborations



Project Title	NCL Partner(s)	External Partner(s)
Development of PP-clay nanocomposites and detailed investigations on the effect of drawing on the structure and morphology	Dr. C. Ramesh	Dr. Taweechai Amornsakchai, Mahidol University, Bangkok, Thailand
Study on crystalline transition in nylons using HTFTIR	Dr. C. Ramesh	Prof. K. Tashiro, Department of Macromolecular Science, Graduate School of Science, Osaka University, Japan
Towards an understanding of NO <sub>x</sub> management for ethanol addition to gasoline	Dr. C.S. Gopinath	Prof. Michael Bowker, Wolfson Nanoscience Laboratory and Cardiff Catalysis Institute, School of Chemistry, Cardiff University, U.K.
Interactions in nano-magnet arrays	Dr. Pankaj Poddar	Prof. W. Schwarzacher University of Bristol UK
Evaluation and improvement of the durability in a composite insulator: study of the degradation/ stabilization of epoxy fiber glass composites coated with elastomers	Dr. R. P. Singh	Prof. J.L. Gardette Laboratoire De Photochimie Moleculaire et Macromoleculaire (LPMM) Universite Blaise Pascal, Cedex, France
		Prof. J.Lacoste, ENSCCF, France
		Dr. Emmanuel Brocard Sediver, St.Yorre, France
Synthesis of functionalized polyolefins and its durability improvements: Novel approach to stabilization against photochemical degradation	Dr. R. P. Singh	Dr. Maria das Mercedes Marques, Instituto Superior Technico, Centro de Qumica Estrutural II Lisboa Cedex, Portugal
Modeling of zeolite framework relaxation	Dr. Sourav Pal	Dr. Francois Fajula (PI) Dr. Annick Goursot (Co-PI), ENSCM, Montpellier, France
Synthesis and study of ionic liquids possessing complexing cations or anions: towards novel task-specific extractants for metal ions and organic compounds.	Dr. Thomas Daniel	Dr. Igor V. Pletnev Leading Research Scientist Chemistry Dept, Lomonosov Moscow State University Russia
Synthesis of novel ionic liquids and their application to Dye-sensitised solar cells.	Dr. Thomas Daniel	Prof. Michael Graetzel Director, Laboratory of Photonic and Interfaces, Institute of Chemical Science and Engineering, EPFL Lausanne. Switzerland
Improved productivity, profitability and sustainability of sheep production in Maharashtra through genetically enhanced prolificacy, growth and parasite resistance	Dr. Vidya Gupta	Stephen Walkden-Brown, Associate Professor in Animal Health and Production Centre for Animal Health and Welfare W49 School of Rural Science and Agriculture

## Academic Collaborations



Project Title	NCL Partner(s)	External Partner(s)
		University of New England, Armidale, NSW 2351 Australia
		Dr. Jill Maddox Senior Research Fellow Centre for Animal Biotechnology School of Veterinary Science University of Melbourne, Victoria 3010 Australia
Improving rust resistance in wheat suitable for marginal rain-fed and semi arid zone of central and peninsular India through molecular markers	Dr. Vidya Gupta	Prof. Beat Keller Institute of Plant Biology University of Zurich, Zollikerstr,107, CH-8008, Zurich Switzerland
Increasing the efficiency of production and nutritional value of chickpea	Dr. Vidya Gupta	Fred J. Muehlbauer USDA-ARS 303 Johnson Hall Washington State University Pullman, WA 99164-6434, USA
		T.J. Higgins Deputy Chief CSIRO Plant Industry
		John Gatehouse, Reader in Biological Sciences, School of Biological and Biomedical Sciences, University of Durham, South Road, Durham DH1 3LE, UK.
Potential antidiabetic agents:synthesis and enzymatic evaluation of sugar-derived inhibitors of glycogen phosphorylases	Dr. Vincent Paul	Dr. László Somsák Department of Organic Chemistry University of Debrecen, Debrecen, Hungary
Novel method for the synthesis of enantiomerically pure $\gamma$ -amino acids and its application towards to antispastic drug Baclofen and epileptic drug Pregabalin	Dr. Vincent Paul (PI) Dr. Hotha Srinivas (Co - PI)	Prof. José Mario Ordóñez Palacios (PI) Centro de Investigaciones Químicas- Universidad Autónoma del Estado de Morelos Av. Universidad 1001 62210 Cuernavaca, Mor. (Mexico)
		Dr. Mario Fernández Zertuche(Co-PI) CIQ-UAEMAv. Universidad 1001 62210 Cuernavaca, Mor. Mexico

## Deputations Abroad



## Business Development activity

**Wadgaonkar P. P.**

Italy,  
11 - 24 May 2008

**Raja T.**

Taiwan,  
09 - 14 June 2008

**Srinivas D.**

Taiwan,  
09 - 14 June 2008

**Joshi A. R.**

USA,  
10 - 22 Nov 2008 and 09 -13 Feb 2009

## Bilateral / Collaborative / Exchange programmes

**Satyanarayana CW.**

Japan,  
01 - 30 May 2008

**Anil K. Kinage.**

UK,  
02 June - 04 July 2008

**Vincent Paul Swamy.**

Germany,  
24 June - 07 July 2008;  
Mexico,  
11 - 24 Mar 2009

**Joshi A. R.**

Thailand,  
07 Aug-06 Sep 2008 and  
25 Feb - 10 Mar 2009

**Srinivas Hotha**

Hungary,  
13 - 24 Oct 2008

**Rode C. V.**

Japan,  
11 Oct - 01 Dec 2008 and 04-12 Mar 2009

**Kelkar A. A.**

Germany,  
24 Nov - 16 Dec 2008

**Ajith Kumar T. G.**

Germany,  
19 - 29 Jan 2009

**Bhattacharya A. K,**

Italy,  
07 - 13 Mar 2009

**Anil Kumar**

France,  
16 Mar - 06 Apr 2009

**Ogale S. B.**

France,  
23 Mar - 13 Apr 2009

Extra Ordinary Leave / Fellowship / Sabbatical Leave /  
Visiting Professor**Amol A. Kulkarni**

Germany,  
27 Apr - 24 May 2008

**Patil K. R.**

Spain,  
01 May - 30 June 2008

## Deputations Abroad

**Prasad B L V**

France,  
15 June - 06 July 2008

**Badiger M. V.**

France,  
01 - 30 Nov 2008

**Moneesha Fernandes**

Italy,  
02 Sept - 01 Dec 2008

**Kinage A. K.**

South Korea,  
01 Dec - 30 Nov 2009

**Sanjayan G. J.**

USA,  
10 Dec 2008 - 09 Dec 2009

## Conferences / Seminars / Symposia / Workshops

**Harle A.**

Germany,  
19 - 21 May 2008

**Shukla P. G.**

UK, Ireland,  
26 Aug - 06 Sep 2008

**Pol H. V.**

Italy,  
15 - 19 June 2008

**Grover G. S.**

Denmark,  
16 - 27 June 2008

**Sivaram, S.**

S. Korea, 28 June - 2 July 2008

**Argade N. P.**

Italy,  
03 - 05 July 2008

**Pandey G. P.**

Italy,  
03 - 05 July 2008

**Sourav Pal**

Poland, USA,  
06 - 18 July 2008;  
Egypt,  
17 - 20 Nov 2008;  
Japan,  
04 - 06 Mar 2009

**Ogale S. B.**

Singapore,  
07 - 21 Aug 2008

**Jadhav A. S.**

UK,  
26 - 29 Aug 2008

**Anil Kumar**

Germany,  
07 - 11 Sept 2008

**Varma A. J.**

Italy,  
18 - 20 Sep 2008

**Gokhale D. V.**

China,  
13 - 15 Dec 2008

**Lele A. K.**

Italy,  
15 - 19 June 2008;  
Australia,  
20 - 27 Jan 2009

**Premnath V.**

Singapore & Australia,  
06 - 12 Mar 2009

**Gupta V. S.**

Australia,  
20 - 29 Aug 2008;  
France,  
17 - 20 Mar 2009

## Deputations Abroad



### K. Vijayamohanam

Germany,  
16 - 20 Mar 2009

### Kharul U. K.

Germany,  
16 - 20 Mar 2009

## Fellows and Students participation in conferences/ research projects

### Nishant R. Gupta

SRF, South Korea,  
22 - 27 June 2008

### Neelam Jagtap

SRF, France,  
01/04 - 30 June 2008

### Ashok Kumar Das Mohapatra

SRF, Taiwan,  
29 June - 04 July 2008

### Suman Sahoo

SRF, South Korea,  
13 - 18 July 2008

### Amti Delori, SRF

Japan,  
23 - 30 Aug 2008

### S. Krishnaswamy, SRF

Japan,  
23 - 30 Aug 2008

### D. F. Gupta, SRF

Japan,  
07 - 10 Sept 2008

### Amit Chaudhari, SRF

Japan,  
07 - 10 Sept 2008

### Sachin Gokhale, SRF

Japan,  
08 - 2 Sept 2008

### Rahul Kar, SRF

Australia,  
14 - 9 Sept 2008

### Tuhina Kelkar, SRF

Australia,  
14 - 9 Sept 2008

### Eldho Mathai, JRF

Germany,  
10 Nov - 07 Dec 2008

### Hamid Shaikh, JRF

Germany,  
10 Nov - 07 Dec 2008



## Lectures / Seminars Delivered by Visitors



Date	Topic	Speaker
01/04/2008	Adventures in catalytic nanospace: Resolving catalytic problems at the atomic scale using STM	Prof. Michael Bowker, Cardiff Univ., UK
24/04/2008	Compositionally tailored thin films and nanostructures of ceramic materials and their exploitation for optical and electronic applications	Dr. R. D. Vispute, Research Scientist, Univ. of Maryland, College Park, USA
05/05/2008	Challenges and potentials of ionic polymer-metal composites as dynamic sensors	Dr. M. Luqman, Artificial Muscle Research Centre, Konkuk Univ., Seoul, South Korea
07/05/2008	Solid or liquid? solidification of a nanoconfined liquid under nonequilibrium condition	Prof. S. Patil, Indian Institute of Science Education & Research, Pune
16/05/2008	Water and other liquids: Anomalies and solvation	Prof. Charusita Chakravarty, Dept. of Chemistry, IIT, Delhi
16/05/2008	Morphological and structural characterization of nanocomposites with a polyolefinic matrix	Prof. Valerio Causin, Dipartimento di Scienze Chimiche, Università di Padova, Italy
21/05/2008	Optical and dynamic studies of CdTe quantum dots: Ensemble to single QD	Dr. Abhijit Mandal, Dept. of Physical Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata
21/05/2008	Single molecule dynamics of plasma membrane Ca <sup>2+</sup> -ATPase by calmodulin proteins	Dr. Abhijit Mandal, Dept. of Physical Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Kolkata
18/06/2008	Commercializing new science	Prof. George Whitesides, Harvard, Cambridge, USA
26/06/2008	On modeling metabolic systems: Cybernetic route	Prof. D. Ramkrishna, School of Chemical Engineering, Purdue Univ., West Lafayette, USA
26/06/2008	Formation of nanoparticulate transition metal complexes with unique functional properties	Prof. Bala Subramaniam, Director, Center for Environmentally Beneficial Catalysis, Kansas Univ., USA
27/06/2008	Intensified olefin hydroformylation in CO <sub>2</sub> -expanded media	Prof. Bala Subramaniam, Director, Center for Environmentally Beneficial Catalysis, Kansas Univ. USA
30/06/2008	Membrane gas separation	Dr. Sudhiar Kulkarni, Senior Scientist, MEDAL, Newport, USA,

## Lectures / Seminars Delivered by Visitors



Date	Topic	Speaker
16/07/2008	Developing photoaffinity labels for enzyme paraoxonase-1: Interplay of experimental and computational studies	Sivaramakrishnan Muthukrishnan, Ohio State Univ., Ohio, USA
21/07/2008	Curcumin? A natural food colorant with multiple bioactive attributes	Dr. P. Srinivas, Head, Plantation Products, Spices and Flavour Technology Department, Central Food Technological Research Institute, Mysore
28/07/2008	A continuum scale global model for czochralski crystal growth process for pure silicon	Dr. Prashant Gunjal, Univ. of Washington St. Louise, USA
22/08/2008	Applications of polarized neutron scattering in thin films research	Dr. Frank Klose, Bragg Institute, ANSTO, Australia
22/08/2008	From RAFT polymerisation to polymers for medical devices; oh yes we need those materials!	Roshan Mayadunne, Senior Research Scientist, Polymeric Biomaterials, CSIRO, Melbourne, Australia
09/09/2008	Hydrogen sensors and nanocrystalline titania for photocatalysis	Dr. Satyajit Shukla, Scientist, NIST, Thiruvananthapuram
09/09/2008	Opportunities in catalysis: An organometallic perspective	Dr. Sumit Bhaduri, Senior Scientific Advisor, Reliance Industries Limited, Mumbai
16/09/2008	Self-assembled block copolymer nanotemplates for nanofabrication	Dr. Bhoje Gowd, Alexander von Humboldt Fellow, Dept. of Nanostructured Materials, Leibniz-Institute of Polymer Research, Dresden, Germany
18/09/2008	Thin film platform for emerging technologies	Dr. Ram Janay Choudhary, UGC-DAE Consortium for Scientific Research, Indore
29/09/2008	Entrepreneurship and Innovation? A personal perspective	Dr. Keki Gharda, CMD, Gharda Chemicals, Mumbai
30/09/2008	Applications of confocal microscopy in material science	B.V.R. Tata, Indira Gandhi Centre for Atomic Research, Kalpakkam
30/09/2008	In situ observations to study phase transformation	Prof. Kamanio Chattopadhyay, Indian Institute of Science, Bangalore
14/10/2008	Interfacial flow processing of biological thin films	Prof. Gerald G. Fuller, Dept. of Chemical Engineering, Stanford Univ., Stanford, USA
16/10/2008	Lipidemia	Dr. Anil Katdare, Cardiologist, N. M. Wadia Institute of Cardiology, Pune
21/10/2008	Low cost multi-parameter OFET sensor for chemical odours	Dr. Arindam Das, Research Associate, Dept. of Astronomy and Physics, Univ. of Sheffield, Sheffield, UK

## Lectures / Seminars Delivered by Visitors



Date	Topic	Speaker
07/11/2008	Development of potent and selective organoruthenium mammalian sterile 20 kinase inhibitors	Dr. Ruchi Anand, IIT, Mumbai
12/11/2008	Nanoslabs: The embryonic precursors hydroconversion over acidic molecular sieves	Dr. Raman Ravishankar, Head, R & D, Eurochem Corporation Pvt. Ltd., Singapore
14/11/2008	Rapid data acquisition methods in biomolecular NMR	Prof. K. V. R. Chary, Tata Institute of Fundamental Research, Mumbai
21/11/2008	Inhibition of glycogen phosphorylase as a potential treatment for type 2 diabetes	László Somsák, Prof. and Head, Dept. of Organic Chemistry, Debrecen Univ., Debrecen, Hungary
24/11/2008	Polybenzimidazole membranes for fuel cell	Prof. Tushar Jana, School of Chemistry, Univ. of Hyderabad, Hyderabad
25/11/2008	Regenerative medicine: Stem cells biology meets materials science and engineering	Prof. Shyni Varghese, Univ. of California, San Diego, USA
03/12/2008	Process mass spectrometer for gas analysis and solvent applications	Richard Shehab, Product Manager, Ametek, USA
05/12/2008	Challenges associated with drug design for Alzheimer's disease	Prof. Kumar Sambamurti, Medical Univ. of South Carolina, Charleston, USA
11/12/2008	Metal-organic frameworks: The emerging family of porous solids	Prof. S. Natarajan, Indian Institute of Science, Bangalore
11/12/2008	Design and synthesis of new materials for anion sensing	Prof. Ivan Stibor, Dept. of Organic Chemistry, Institute of Chemical Technology, Prague, Czech Republic
11/12/2008	Public funded research and technology transfer with special reference to Bayh-Dole Act	Prof. Amit Shovon Ray, Jawaharlal Nehru Univ., New Delhi
17/12/2008	Engineering artificial cartilage tissue: A scaffold design strategy	Prof. Dharendra Katti, IIT, Kanpur
19/12/2008	The Future of the chemical industry	Dr. Faruq Marikar, Director, Nanobiz LLC, Scotch Plains, USA
19/12/2008	Reversible clay supported copper complex for controlled polymer synthesis	Dr. Selvaraj Munirasu, Research Associate, GKSS-Forschungszentrum Geesthacht, Germany
22/12/2008	Molecules to materials: An in situ view of material formation	Prof. Gopinathan Sankar, Royal Institute, London, UK
26/12/2008	Static and dynamic magnetic properties of composite Au-Fe <sub>3</sub> O <sub>4</sub> nanoparticles	Prof. Srinath Sanyadanam, School of Physics, Central Univ. of Hyderabad, Hyderabad

## Lectures / Seminars Delivered by Visitors



Date	Topic	Speaker
26/12/2008	Molecular hydrodynamics at the nanoscale	Prof. Rajesh Khare, Chemical Engineering Department, Texas Tech Univ., Lubbock, USA
02/01/2009	Electron counting rules and the stability of clusters	Prof. Kiran Boggavarapu, Chemistry Department, McNeese State Univ., USA
05/01/2009	Multicomponent diffusion in ternary and quaternary diffusion couples and in multilayered assemblies	Dr. Kaustubh Kulkarni, Process Engineer, Applied Materials, Inc., Santa Clara, USA
07/01/2009	Water structure and dynamics near solutes and interfaces: Implications on	Prof. Shekhar Garde, Chair, Chemical Engineering Department, Rensselaer Polytechnic Institute, Troy, New York, USA
13/01/2009	Functionalization and design of micropores of zeolites and nanopores of mesoporous silica	Dr. Masahiro Fujiwara, Senior Research Scientist, Kansai Center, National Institute of Advance Industrial Science and Technology, Osaka, Japan
05/02/2009	Best practices in R&D commercialization: Success stories from Imperial College London	Susan Searle, Chief Executive Officer, Imperial Innovations Group plc, London, UK
11/02/2009	Nano fillers in reactive foaming - from dispersions to thermosetting nanocomposite foams	Dr. Harikrishnan, Post-doctoral Fellow, Univ. of Minnesota, Minneapolis, USA
12/02/2009	Scriptures: Science and mythology	Prof. Rajesh Kochhar, CSIR Emeritus Scientist, IISER, Mohali
13/02/2009	The journey from science to enterprise	Dr. Shailendra Vyakarnam, Director, Centre for Entrepreneurial Learning, Univ. of Cambridge
16/02/2009	The role of co-crystals in pharmaceutical science and solid-state chemistry? Do they represent multiple paths to new and improved medicines?	Prof. Mike Zoworotko, Univ. of South Florida, Tampa, USA
23/02/2009	Block copolymer supramolecular assemblies: Microphase separation and nanofabrication	Dr. Bhanu Nandan, Dept. of Nanostructured Materials, Leibniz Institute of Polymer Research, Dresden, Germany,
23/02/2009	Microfluidic and nanofluidic technologies for miniaturizing the devices and technologies for biochemical sensing micro-reactors and medical diagnostics	Dr. Subhra Datta, Ohio State Univ., USA
26/02/2009	The rheology microstructure and processing of carbon nanotube suspensions	Prof. Malcolm Mackley, Dept. of Chemical Engineering and Biotechnology, Univ. of Cambridge, UK

## Lectures / Seminars Delivered by Visitors



Date	Topic	Speaker
06/03/2009	Seeing and moving magnetic nanoparticles	Prof. Majetich, Carnegie Mellon Univ., Pittsburg, USA
06/03/2009	Functional magnetic nanostructures: Living on the edge	Prof. Har Srikanth, Univ. of South Florida, Tampa, USA
09/03/2009	Precursor approach to synthesize nanoparticles	Dr. P. Jeevanandam, IIT, Roorkee
12/03/2009	Anaemia	Dr.(Mrs.) Manchanda, Director, KEM Hospital, Pune
12/03/2009	Polymer graphene nanocomposite	Prof. Chris Macosko, Dept. of Chemical Engineering and Materials Science, Univ. of Minnesota, Minneapolis, USA
16/03/2009	Novel polymer shelled microbubbles for diagnostic and therapeutic purposes	Prof. Gaio Paradossi, Dipartimento di Scienze e Tecnologie Chimiche, Università di Roma Tor Vergata, Rome, Italy
16/03/2009	Semiconductor sensitized solar cells: Aspects of different deposition techniques	Dr. Shaibal K. Sarkar, Dept. of Chemistry and Chemical Engineering, Univ. of Colorado, Boulder, USA
18/03/2009	Polymer-solvent compounds: Phase diagrams structures, properties	Prof. J. M. Guenet, Institut Charles Sadron Strasbourg, France
20/03/2009	Playing with interactions in polymeric systems	Dr. Soumyadeb Ghosh, Staff Scientist, GE India Technology Centre, Bangalore
20/03/2009	Novel eco friendly, flame retardant styrenics	Dr. Satish Gaggar, Principal Scientist, SABIC Innovative Plastics, Parkersburg, USA
23/03/2009	Infectious diseases: The ways to tackle	Dr. Jayanta Haldar, Post-Doctoral Research Associate, Departments of Chemistry and Biological Engineering, MIT, Cambridge, USA
25/03/2009	Cellulose, silk and epoxy based carbon nanotubes composites	Dr. Sameer Rahatekar, Post-doctoral Fellow, NIST, Gaithersburg, USA
26/03/2009	Key challenges in biomass gasification	Dr. Ashish Chaurasia, Imperial College, London
30/03/2009	Polyisobutylene-based cyanoacrylates and polyureas	Dr. Suresh K. Jewrajka, Senior Research Fellow, Dept. of Polymer Science, The Univ. of Akron, USA
30/03/2009	Observing and understanding nanostructure formation	Prof. Alon McCormick, Univ. of Minnesota, Minneapolis, USA

## Invited Talks / Lectures Delivered by NCL Scientists



## Dr. Ahmad, Absar

Date	Topic	Venue
10-Jan-2009	Fungus-mediated biosynthesis of oxide nanoparticles	Royal College, Mumbai
29-Jan-2009	Extracellular biosynthesis of metal sulfide nanoparticles using the fungus <i>Fusarium oxysporum</i>	University of Madras, Chennai
31-Jan-2009	Extracellular biosynthesis of CdS nanoparticles using the fungus <i>Fusarium</i> sp.	Bharti Vidyapeeth University, Pune
12-Feb-2009	Biological synthesis of inorganic nanoparticles	Saha Institute of Nuclear Physics, Kolkata
10-Feb-2009	Extracellular biosynthesis of inorganic nanoparticles using fungi	Marathwada Mitramandal Pharmacy College, Pune
05-Mar-2009	Extracellular biosynthesis of metal sulfide nanoparticles using the fungus <i>Fusarium</i> sp.	Fergusson College, Pune
06-Mar-2009	Fungus-mediated biosynthesis of oxide nanoparticles	S. P. College, Chandrapur,

## Dr. John, C. K

Date	Topic	Venue
16-Jul-2008	Biotechnologies for the conservation and sustainable utilization of medicinal plants	Netaji Subhashchandra Bose, Arts, Commerce and Science College, Nanded
17-Jan-2009	Plant Tissue Culture and Micropropagation	Changu Kana Thakur College, New Panavel

## Dr. Grover, G. S.

Date	Topic	Venue
30-Aug-2008	Safety practices in handling chemicals in the laboratory	University of Pune
10-Sep-2008	Safety orientation course for young chemical and mechanical engineers - Part 1: Chemical safety	Vishwakarma Institute of Technology, Pune

## Invited Talks / Lectures Delivered by NCL Scientists



Date	Topic	Venue
10-Sep-2008	Safety orientation course for young chemical and mechanical engineers - Part 2: Safety with machines	Vishwakarma Institute of Technology, Pune
10-Sep-2008	Safety orientation course for young chemical and mechanical engineers - Part 3: Fire safety	Vishwakarma Institute of Technology, Pune
19-Sep-2008	Case studies: Chemical fires	National Safety Council, Mumbai
19-Sep-2008	Case studies: Toxic release and exposure	National Safety Council, Mumbai
16-Nov-2008	MSDS for the hazardous, toxic and/or flammable chemicals	Central Pollution Control Board, Delhi
04-Dec-2008	Laboratory safety - Ground rules and guidelines	Central Glass and Ceramics Research Institute, Kolkata
04-Dec-2008	Fire safety training and emergency response in a chemical lab	Central Glass and Ceramics Research Institute, Kolkata
07-Feb-2009	Safety practices in handling laboratory chemicals	Modern College of Arts, Science and Commerce, Pune

**Dr. Sivaram, S.**

Date	Topic	Venue
April 4, 2008	Polymer Nano Composites : Unmet Challenges	National Institute of Technology, Calicut
April 7, 2008	Materials and Energy Derived from Renewable Resources: Opportunities and Challenges	Indian Chemical Industry, Mumbai The Business and Technology Challenges
June 25, 2008	Technology led Growth in Performance/Specialty Chemicals: Emerging Opportunities	Frost & Sullivan's Executive Summit on 'Accelerating Growth in Chemicals, Materials and Foods: A Frost & Sullivan Executive MindXchange', The Leela, Mumbai
June 30, 2008	'Leveraging Science and Technology for Promoting Competitiveness: The CSIR Experience'	The Special Symposium on Emerging Science and Technology at Hanyang University, Seoul Korea
September 6, 2008	"Green Polymers from Renewable Resources - Emerging Technologies"	The K.T. Acharya Memorial Lecture Series, Indian Institute of Chemical Technology, Hyderabad

## Invited Talks / Lectures Delivered by NCL Scientists



Date	Topic	Venue
October 2, 2008	Four Decades in Chemistry: The Journey From MCC and Beyond (A Reflection on my Personal and Professional Journey)	Frontiers in Chemistry A Conference to Commemorate the Birth Centenary of Prof. S.V. Anantkrishnan, Madras Christian College, Chennai
October 14, 2008	Industry-NCL Interactions: Evolution of New Models of Engagement	Dow-Corning, Pune
October 17, 2008	Should Research Institutions and Universities Co-exist?	NISTADS(CSIR)-German Research Foundation Deliberations on Research Policy, New Delhi
December 17, 2008	Reactivity of Some Early and Late Transition Metal Complexes in the Polymerization and Oligomerization of Ethylene	The Seminar on 'Advances in Chemistry', Department of Chemistry, M. S. University, Vadodara
December 29, 2008	Materials and Energy derived from Carbohydrates : Opportunities, Challenges and Sustainability Assessment	Indian Institute of Science, Education and Research, Mohali
January 29, 2009	Sinews of Excellence: The Evolution of a Scientific Institution	Rajmitra B.D. Amin Memorial Lecture, Indian Chemical Council, Vadodara
January 31, 2009	12th Convocation Address	Dr. Babasaheb Ambedkar Technological University, Lonere

**Dr. Varma, A. J.**

Date	Topic	Venue
18-Sep-2008	Valorization of bio-based polymeric materials	ICS-UNIDO, Trieste, Italy



## Conferences / Workshops / Symposia Organized



**10/07/2008 - 11/07/2008**

Workshop on computer-based drug design

**09/11/2008 - 14/11/2008**

An EMBO Conference - Recent Developments in Macromolecular Crystallography

**9/11/2008 - 15/11/2008**

International workshop on The Booroola fecundity (FecB) mutation: Science and Practice

**12/01/2009 - 13/01/2009**

Indo-Korean Symposium in Organic Chemistry

**18/01/2009 - 21/01/2009**

19th National Symposium on Catalysis (CATSYMP-19): Catalysis for Sustainable Energy and Chemicals

**22/01/2009**

Indo-Russian Joint Workshop on Catalysis for Bio-mass Conversion and Environmental Engineering

**05/02/2009 - 08/02/2009**

3rd CRSI - RSC Symposium & 11th CRSI National Symposium in Chemistry (NSC-11)

**16/02/2009 - 19/02/2009**

'The deMon Developers' 9th Annual Workshop on Density Functional Theory: Present and Future

**04/03/2009 - 05/03/2009**

Indo-German Workshop in Micro-reaction Technology



## Awards / Recognitions



Name	Awards / Recognitions
Dr. Sourav Pal	J C Bose Fellow
	CRSI Silver Medal
Shri P.P. Barve	VASVIK Award in Chemical Sciences and Technology
Dr. M. K. Dongare	Silver medal of FICCI-Lokheed Martin Indian Innovation growth programme* for Nitrobenzene process
Dr. Vidya Gupta	Fellow, Maharashtra Academy of Sciences
Dr. Pankaj Poddar	CSIR Young Scientist Award in Physical Sciences
Dr. S.P. Joshi	Advisory Council member of Naoroji Godrej Centre for Plant Research, Satara
Dr. C.S. Gopinath	CRSI Bronze Medal
Dr. Anil Kumar	Fellow, Indian National Science Academy, New Delhi
Dr. P. P. Wadgaonkar	Fellow, Maharashtra Academy of Sciences
Dr. Absar Ahmad	Fellow, Maharashtra Academy of Sciences
	Fellow and Vice-President, Mycological Society of India
	MRSI Medal
Dr. C. V. V. Satyanarayana	Fellow, Maharashtra Academy of Sciences
Dr. R. P. Singh	MRSI Distinguished Lecturership Award

## Member, Board of Directors, Industry

**Mr. S. N. Nene**

Chembond Chemicals

**Dr. Paul Ratnasamy**

Hindustan Organic Chemicals Ltd., Rasayani

**Dr. S. Sivaram**

Asian Paints Ltd., Mumbai

GMM Pfadler Ltd., Mumbai

Apcotex, Mumbai



## Editor / Editorial Board Members of Research Journals

**Dr. Absar Ahmad**

- + *Kavaka*, Mycological Society of India

**Dr. Anil Kumar**

- + *Indian Journal of Chemistry Section A*, NISCAIR (CSIR), New Delhi
- + Editor (Chemistry), *Proceedings of The National Academy of Sciences (India)*, Allahabad
- + *Journal of Solution Chemistry*, Springer, The Netherlands.

**Dr. V. R. Choudhary**

- + *Catalysis Communications*, Elsevier, The Netherlands

**Dr. M. V. Deshpande**

- + *Indian Journal of Mycology and Plant Pathology*, Indian Society of Mycology and Plant Pathology, Udaipur
- + *Indian Journal of Microbiology*, Springer

**Dr. (Mrs) Vidya Gupta**

- + Associate Editor, BMC, *Plant Biology*
- + *Plant Cell Biotechnology & Molecular Biology*, Society for Biology and Biotechnology, Salem
- + *The Open Evolution Journal*, Bentham Sciences Publishers Ltd.
- + *The Open Horticulture Journal*, Bentham Sciences Publishers Ltd.

**Dr. S. B. Halligudi**

- + *The Open Organic Chemistry Journal*, an open access journal published by Bentham Science Publishers Ltd.

**Dr. P. A. Joy**

- + Associate Editor of the *Journal of American Ceramic Society*.

**Dr. B. D. Kulkarni**

- + *Chemical Engineering Science*, Pergamon/Elsevier, UK
- + *Industrial and Engineering Chemical Research*, American Chemical Society, USA
- + *International Journal of Chemical Engineering*, Hindawi Publishing
- + *The Open Chemical Engineering Journal*, Bentham Open
- + *Research Letters in Chemical Engineering*, Hindawi Publishing
- + *International Journal of Chemical Reactor Engineering*, The Berkeley Electronic Press
- + *Engineering Applications of Artificial Intelligence*, Elsevier
- + *The Open Petroleum Engineering Journal*, Bentham Open

**Dr. I. S. Mulla**

- + Editorial Board Member, *Science of Advanced Materials*, American Scientific Publishers, USA.
- + Editorial Advisory Board, *Sensors & Transducers Journal*, International Frequency Sensor Association

**Dr. S. B. Ogale**

- + Editorial Advisory Board of Silicon

**Dr. Ganesh Pandey**

- + *Tetrahedron*, Elsevier, The Netherlands

**Dr. Sourav Pal**

- + Board of Advisors, Springboard, Inc. (Engineering education), USA
- + *International Journal of Molecular Sciences*, MDP International, Switzerland
- + *International Journal of Applied Chemistry*, Research India Publications, Delhi

## Editor / Editorial Board Members of Research Journals



+ *Journal of Chemical Sciences*, The Indian Academy of Sciences, Bangalore

+ *Proceedings of the Indian National Science Academy*, New Delhi

### Dr. V. V. Ranade

+ Associate Editor, *Asia-Pacific Journal of Chemical Engineering*, Wiley InterScience

### Dr. Paul Ratnasamy

+ *Applied Catalysis*, Elsevier, The Netherlands

+ *Catalysis Letters*, Kluwer, USA

+ *Catalysis Surveys from Asia*, Kluwer, USA

+ *CATTECH*, Kluwer/ Plenum, USA

+ *Journal of Catalysis*, Elsevier, The Netherlands

+ *Microporous and Mesoporous Materials*, Elsevier, The Netherlands

+ *Topics in Catalysis*, Kluwer, USA

### Dr. S. Sivaram

+ *Bulletin of Materials Science*, The Indian Academy of Sciences, Bangalore

+ *Designed Monomers and Polymers*, VSP International Science Publishers, The Netherlands

+ *Indian Journal of Chemical Technology*, NISCAIR (CSIR), New Delhi

+ *Journal of Scientific and Industrial Research*, NISCAIR (CSIR), New Delhi

+ *International Journal of Polymeric Materials*, Gordon and Breach Publishers, New York, USA

+ *Journal of Polymer Materials*, Oxford and IBH Publishers, New Delhi

+ *Journal of Chemical Sciences*, The Indian Academy of Sciences, Bangalore

+ Regional Editor for India, Polymer International, Society of Chemical Industry, UK

### Dr. D. Srinivas

+ *Catalysis Surveys from Asia*, Springer, Germany

+ *Bulletin of Catalysis Society India*, Chennai

### Dr. (Mrs) V. S. Tare

+ *Journal of Environmental Biology*, Triveni Publishers, Lucknow

### Dr. A. J. Varma

+ *Carbohydrate Polymers*, Elsevier, The Netherlands

+ Editorial Board, *Trends in Carbohydrate Research*, India

### Dr. K. Vijayamohan

+ *Bulletin of Materials Science*, Indian Academy of Sciences, Bangalore

+ *Journal of Chemical Sciences*, Indian Academy of Sciences, Bangalore

+ *Science of Advanced Materials*, American Scientific Publishers, USA.



### NCL RF Annual Awards - 2008

Name of award	Award	Award winner	Awarded for
NCL RF Scientist of the Year Award (Sponsored by Maneckji & Shirinbai Neterwala Foundation)	Rs.20,000/- each + Citation (Shared Jointly)	Dr. P. A. Joy	For significant contribution to the study of ferromagnetism and changes in the electronic structure in transition metal doped ZnO based diluted magnetic semiconductors and thereby validating that ferromagnetism is an extrinsic property and changes in the electronic properties are due to doping effects.
		Dr. C Ramesh	For significant contribution to the understanding of the crystalline transitions in nylons and syndiotactic polystyrene (SPS). During transitions, the nylon chains experience violent rotational and translational motions similar to those observed in polyethylene, which are exploited to make ultra high modulus fibers. In the case of SPS, he observed for the first time, that the transition temperature shows a linear relationship with the amount of solvent present in the clathrate and is independent of the nature of solvent.
NCL RF Scientist of the Year Award (Sponsored by Dr. R. A. Mashelkar Endowment Fund)	Rs.20,000/- +Citation (Shared Jointly)	Dr. G. J. Sanjayan	For significant contribution to the study of scaffolds with well-defined secondary structural preferences that could be used to create new types of tertiary structures, which, in turn, lead to the creation of macromolecules with functional properties akin to those of the compactly folded biopolymers, proteins and RNA.
		Dr. B. L. V Prasad	For synthesis and surface modifications of nanomaterials in aqueous media and thereby achieving derivatization of ligands, molecules and polymers that aid in synthesis as well as act as capping agents for the nanoparticles with potential biomedical and bio-diagnostic applications.
Highest Industrial Earning Award	Rotating Shield & Trophy	Catalysis Division	Highest per capita (net) industrial earning during 2007-08.



Name of award	Award	Award winner	Awarded for
Award for 'New Initiative taken by R&D Support System'	Rs.20,000/- + Certificate of Merit (Shared Jointly)	Shri. S. B. Katte Shri. R. R. Lokhande Shri. TAB. Mulla Shri. K. G. Kharat Shri. M. H. Kamble Shri. P. S. Jadhav Shri. A. S. Date (Business Development Division)	For planning, execution and coordination of public relations, publicity and events management of NCL leading to enhancement of the image of NCL amongst its stake holders.
	Rs.20,000/- + Certificate of Merit (Shared Jointly)	Shri. P. Chiranjeevi Shri. Sardarilal Shri. Tapan Sah Shri. Naveen Pavithran Mrs. M. M. Kenkare Shri. S. N. Date Shri. Sanjay H. Jadhav Shri. A. S. Vaidya Shri. N. K. Alone Shri. K. T. Chaturkar Shri. R. T. Pagare Mrs. Prema Ravindran Shri. M. V. Suryavanshi Mrs. Lalitha G. Nair Shri. S. P. Purandare Shri. S. S. Daware Shri. Sachin B. Gawali Shri. R. P. Naik Shri. J. D. John (Stores and Purchase Division)	For undertaking the massive activity of digitization of all assets of NCL, creating a system of bar coding which will significantly contribute to the ease of annual asset verification.
Director's Commendation Award	Rs. 5,000/- + Certificate of Commendation	Shri. Dipak Jori (Physical & Materials Chemistry)	For meticulously assisting the Student Academic Committee in all its activities, including admission of research fellows, and conduct of pre PhD course work.
	Rs. 5,000/- + Certificate of Commendation	Shri. P. D. Jadhav (Security)	For efficient and conscientious service rendered towards the security of the laboratory.
	Rs. 5,000/- + Certificate of Commendation	Shri G. M. Pardeshi (Administration)	For efficiently dealing with vigilance, legal and RTI matters of the laboratory.



Name of award	Award	Award winner	Awarded for
	Rs. 5,000/- + Certificate of Commendation	Mrs. Shiney John (Administration)	For her efficient handling of important activities related to reimbursement of medical bills and other administrative matters of importance to the staff of the laboratory.
Individual Merit Award	Rs.5,000/- + Certificate of Merit	Shri. Gopal Prasad (Civil Engineering)	For performing several duties such as cleaning, plumbing and for his help in the transportation of heavy construction materials at NCL.
	Rs.5,000/- + Certificate of Merit	Mrs. Padmakumari Nair (Administration)	For her dedicated work in processing the recruitments of scientific and technical staff, and for keeping meticulous and systematic records.
	Rs.5,000/- + Certificate of Merit	Mrs. Vinaya V. Kulkarni (Administration)	For efficient and conscientious service rendered towards management of performance appraisal record of staff and scientists of NCL leading to timely submission of information to CSIR.
	Rs.5,000/- + Certificate of Merit	Mr. M. B. Vadhere (Administration)	For exemplary efforts in e-filing of income tax on a quarterly basis using a modified software, and handling of the salary bills for the laboratory staff with efficiency.
	Rs.5,000/- + Certificate of Merit	Ms. Amruta Bhangе (Administration)	For efficiently working on different desks dealing with the personal files of students, RGIS matter and the retention in service.
	Rs.5,000/- + Certificate of Merit	Dr. (Mrs) S. S. Kulkarni (CEPD)	For her dedicated services to chemical analysis required for process development activities and research programmes.



Name of award	Award	Award winner	Awarded for
Merit Scholarship Award to the children of class IV employees of NCL	Rs. 4,000/- + Certificate of Merit	Master Rishikesh Kamathe	For standard IX Boys
	Rs. 1,750/- Each + Certificate of Merit (Shared Jointly)	Master Parag Jadhav Master Vaibhav Ranawade	
	Rs. 4,000/- + Certificate of Merit	Ms. Poonam Rathwadkar	For standard IX Girls
	Rs. 3,500/- + Certificate of Merit	Ms. Sayali Shukla	
	Rs. 4,000/- + Certificate of Merit	Master. Vishal Bhise	For standard X Boys
	Rs. 3,500/- + Certificate of Merit	Master. Ganesh Sevi	
	Rs. 4,000/- + Certificate of Merit	Ms. Amrin Punekar	For standard X Girls
	Rs. 3,500/- + Certificate of Merit	Ms. Pooja Magade	
	Rs. 4,000/- + Certificate of Merit	Master Prashant Pawar	For standard XI Boys
	Rs. 3,500/- + Certificate of Merit	Master Sanket Gurav	
	Rs. 4,000/- + Certificate of Merit	Ms. Deepa Srivastava	For standard XI Girls
	Rs. 3,500/- + Certificate of Merit	Ms. Sneha Magade	
	Rs. 4,000/- + Certificate of Merit	Master Vijay Kumar Valmiki	For standard XII Boys
	Rs. 2,400/- + Certificate of Merit (Shared Jointly with Master Kunal Sakpal and Master Abhijit Lande)	Master Prakash Giri	
		Rs. 4,000/- + Certificate of Merit	Ms. Yogita Dudhale





### Science Day Awards - 2008

#### Best Research Fellows 2008

Name of Award	Award	Award winner	Awarded for
Keerthi Sangoram Endowment Awards for 'Best Research Scholars' year 2008	Rs. 2,500/- each + Citation	Ms. Deepti S. Sidhaye and Mr. Rahul Kar (Shared Jointly)	Physical / Material Sciences
		Ms. Varsha C. Pardeshi and Mr. Sarvesh Kumar Soni (Shared Jointly)	Biological Sciences
		Mr. B. K. Vaidya	Engineering Sciences
		Ms. Shraeddha Tiwari and Mr. Amit Delori (Shared Jointly)	Chemical Sciences



## Best Research Papers with the highest Impact factor

Area	Award	Title / Journal	Award Winner
Nanai Natu Award for 'Best Publication' in Organic Chemistry with the highest impactfactor for Scientists.	Rs.2,500/- + Citation	Title: pKa-Directed Host-Guest Assemblies: Rational Analysis of Molecular Adducts of 2, 4-Diamino-6-methyl-1,3,5-triazine with Various Aliphatic Dicarboxylic Acids  Journal : <i>Chemistry-A European Journal</i> (Impact Factor: 5.33)	Dr. V. R. Pedireddi
Dr. Rajappa Award for 'Best Publication' in Organic Chemistry with the highest impact factor for Research Scholars	Rs.1,000/- + Citation	Title: pKa-Directed Host-Guest Assemblies: Rational Analysis of Molecular Adducts of 2,4-Diamino-6-methyl-1,3,5-triazine with Various Aliphatic Dicarboxylic Acids  Journal : <i>Chemistry-A European Journal</i> (Impact Factor: 5.33)	Mr. Amit Delori
Gupta - Pardeshi - Sainani Award for 'Best Research Papers in Biological Sciences'	1. Rs.2,500/- + Citation	Title: Characterization of smallest active monomeric penicillin V acylase from new source: A yeast, <i>Rhodotorula aurantiaca</i> (NCIM 3425)  Journal :Process Biochemistry Impact Factor: 2.336	Mr. Atul Kumar  For Highest Impact Factor in Biological Sciences
	2. Rs.2,000/- + Citation	Title: Steady State and Time-Resolved Fluorescence Studies of a Hemagglutinin from <i>Moringa oleifera</i>  Journal : J. Fluoresc Impact Factor: 2.101	Ms. Uma V. Katre  For Second Highest Impact Factor in Biological Sciences

## Venture Center

The Venture Center is a technology business incubator hosted by the NCL. The Venture Center specializes in incubating technology enterprises offering products and services exploiting scientific expertise in the areas of materials, chemicals and biological sciences and engineering. The Venture Center is an initiative of the NCL under the CSIR's scheme titled 'Scheme for setting up incubation centers in CSIR laboratories'. The Venture Center is approved and part-funded by the National Science and Technology Entrepreneurship Development Board of the Department of Science and Technology, Government of India (DST-NSTEDB). The Venture Center is incorporated as 'Entrepreneurship Development Center' under Section 25 of the Companies Act, 1956 (India) with following purpose:

- + Putting in place and implementing policies, systems and procedures for finance, accounts, company law and other compliance, hiring, human resource management, procurement, asset management and ICT systems,
- + Putting in place a competent Management Team as well as an Operations Team at Venture Center,
- + Meeting performance and expenditure targets of the DST-NSTEDB's TBI project,
- + Building the initial collection for the Venture Center Library and executing the DST-NSTEDB's VC Library project,
- + Mentoring NCL students, promoting student entrepreneurship and the guiding the NCL Technology and Entrepreneurship Club,
- + Driving infrastructure development - in particular, the Lab Block; Getting renovated areas into operation and putting in place maintenance systems for other infrastructure developed in the NCL Innovation Park which is relevant to Venture Center.

### Incubatees and Entrepreneurship Support Programmes

Tridiagonal Solutions Pvt Ltd (TSPL) – a start-up founded by the NCL alumni based on knowledge competencies of the Industrial Flow Modeling – used the address and hot-desking services during this year. The TSPL successfully grew its turnover beyond Rs. 1 crore and the company staff count exceeded 20. Towards the end of the year, TSPL successfully exited the incubator's hot-desking space and moved into larger commercial premises at NSG IT Park in Aundh. The TSPL is still using Venture Center's address service. The TSPL is expected to make a transition from a solutions/services company to a product company in FY 2009-2010.

During this year, Battelle began its India operations at the Venture Center and subscribed to the address and hot-desking services. Venture Center actively assisted Battelle India in identifying suitable human resources for their start-

up phase. Battelle India proposes to build a strong R&D and technology development team initially focused on materials and water technology emphasizing Indian markets and needs.

### Funding

- + This was the first year of DST-NSTEDB 5-year grant funding for the Technology Business Incubator (TBI) project. This first installment totaled Rs. 152.01 lakh (Rs. 131.01 lakh towards Capital Expenses and Rs. 21 lakh towards Recurring Expenses) and was the largest source of financing for the Venture Center.
- + The DST-NSTEDB also approved and released a one-time grant of Rs. 10 lakh for setting-up the VC Library.
- + The Ministry of Micro, Small & Medium Enterprises (MoMSME) has approved a funding scheme for micro and small enterprises to be operated by Venture Center. As per the scheme, Venture Center has to identify 10 technology entrepreneurs and support them to the extent of roughly Rs. 6.25 lakh each (on average). The Venture Center shall receive a grant of Rs. 3.78 lakh towards its expenses. The MoMSME is expected to start releasing funds under this scheme in FY 09-10.
- + During the year, the Venture Center submitted proposals for (1) TePP Outreach Centre, and (2) Technology Opportunity Fellowships to DSIR.

### Service Revenue

Venture Center earned Rs. 9.93 lakh for entrepreneurship, incubation and start-up support services offered to incubatees and other clients. The revenue-earning services during the year were hot-desking services, address services and training room services.

### Policies and Systems

- + Venture Center developed and implemented the following policies and systems during this fiscal year: (1) Human resources and employee policy systems/procedures,
- + (2) Procurement policy/systems/ procedures, asset and inventory recording systems,
- + (3) IT and web systems including intranet document sharing/management, intranet web portal, email systems, etc.
- + The in-house processes for accounting systems, tax compliance, financial management, company law and other government compliance etc were strengthened and systematized.
- + Venture Center set-up up and supervised new contracts for general maintenance in and around the Center.

## Venture Center



Lab Block progressing towards completion

### Infrastructure and Resource Centers

The Venture Center Library began stocking books in late 2008. It is an unique library catering to technology entrepreneurs, technologists and inventors, technology managers and IP professionals.

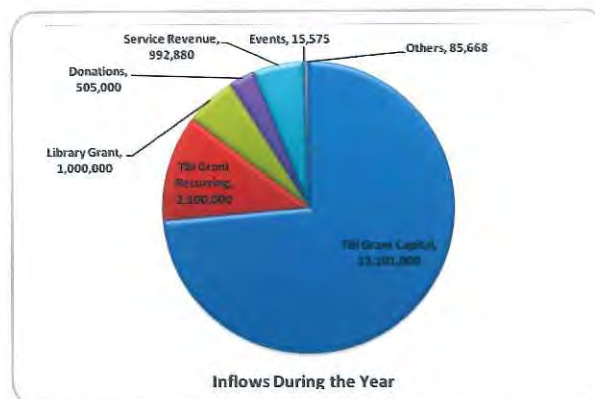
The Lab Block, under renovation and expected to come on-stream in May 2009, shall be one of the key resources of the Venture Center with dedicated labs for incubatees and shared plug-and-play labs with ready instruments for incubatees developing products/ services based on materials science and biotechnology.



### Finance

- ✦ The Total revenues earned during the year was Rs. 10.94 lakh. Most of the revenue (Rs. 9.93 lakh) was earned through the services provided to the incubatees.
- ✦ The Capital Grant (Rs. 131.01 lakh) received from DST-NSTEDB was fully committed towards equipment purchase of the Lab Block.
- ✦ Raised Rs. 5 lakh from Dr. K Gharda of Gharda Chemicals Limited in support of NCL Technology and Entrepreneurship Club (NCL-TEC).

The details of financial performance of Venture Center during the year is represented in the following pie diagram





## राजभाषा का कार्यान्वयन

राजभाषा विभाग, भारत सरकार की राजभाषा नीति सभी केन्द्रीय सरकारी कार्यालयों में लागू है। राष्ट्रीय रासायनिक प्रयोगशाला भारत सरकार के वैज्ञानिक एवं औद्योगिक अनुसंधान विभाग के अधीन एक अनुसंधान प्रयोगशाला है और इस प्रयोगशाला में भी राजभाषा के कार्यान्वयन हेतु हर स्तर पर सभी संभव प्रयास किए जाते हैं। यहाँ अधिकांश कार्य वैज्ञानिक अनुसंधान एवं तकनीकी स्वरूप का होता है जो अंग्रेजी में संपादित किया जाता है और शेष प्रशासनिक स्वरूप का कार्य हिन्दी में किया जाता है। प्रयोगशाला में राजभाषा के सुचारु रूप से कार्यान्वयन हेतु राजभाषा विभाग द्वारा समय-समय पर जारी किए गए सभी दिशानिर्देशों का अनुपालन किया जाता है। सभी रबड़ की मोहरें, पत्र-शीर्ष, फॉर्म तथा मानक मसौदे द्विभाषी बना लिए गए हैं। सभी साइनबोर्ड एवं नामपट्ट द्विभाषी बने हुए हैं। प्रयोगशाला के कम्प्यूटरों को यूनिकोड प्रणाली के माध्यम से द्विभाषी बना दिया गया है। राजभाषा अधिनियम की धारा 3 (3) के अन्तर्गत जारी होने वाले सभी दस्तावेज अनिवार्य रूप से हिन्दी तथा अंग्रेजी दोनों में साथ-साथ जारी किए जाते हैं। हिन्दी में प्राप्त पत्रों के उत्तर हिन्दी में ही दिए जाते हैं। प्रयोगशाला की राजभाषा कार्यान्वयन समिति की बैठकें प्रत्येक तिमाही में नियमित रूप से निदेशक की अध्यक्षता में आयोजित की जाती हैं एवं इन बैठकों में प्रयोगशाला में हिन्दी के प्रगामी प्रयोग की समीक्षा की जाती है।

प्रयोगशाला में राजभाषा के कार्यान्वयन को प्रभावी बनाने हेतु हरसंभव प्रयास किए जाते हैं। इसी क्रम में प्रयोगशाला के स्वागत कक्ष में ब्लैकबोर्ड पर प्रतिदिन एक सुविचार लिखा जाता है। इससे कर्मचारियों में हिन्दी के प्रति रुचि उत्पन्न होती है और वे हिन्दी में कार्य करने के लिए प्रेरित होते हैं। प्रयोगशाला के तीन अनुभाग अपना सारा सरकारी कार्य हिन्दी में ही करते हैं। वार्षिक कार्यक्रम में दिए गए निर्देशानुसार प्रयोगशाला के पुस्तकालय हेतु हिन्दी पुस्तकें प्रतिवर्ष खरीदी जाती हैं। निदेशक महोदय का स्टाफ को सम्बोधित पत्र प्रत्येक तिमाही में अंग्रेजी के साथ-साथ हिन्दी तथा मराठी में भी जारी किया जाता है। प्रयोगशाला से जारी होने वाली सभी निविदा सूचनाएँ हिन्दी में भी प्रकाशित की जाती हैं। प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानों एवं संगोष्ठियों की रिपोर्टें सीएसआईआर समाचार एवं सीएसआईआर न्यूज में प्रकाशनार्थ क्रमशः हिन्दी और अंग्रेजी दोनों में राष्ट्रीय विज्ञान संचार एवं सूचना स्रोत संस्थान (निस्केयर), नई दिल्ली को नियमित रूप से भेजी जाती हैं।

प्रयोगशाला के स्टाफ को हिन्दी में कार्य करने हेतु प्रोत्साहित किया जाता है। इस हेतु स्टाफ के लिए टिप्पण एवं आलेखन सम्बन्धी प्रोत्साहन योजना तथा अन्य प्रोत्साहन योजनाएँ भी लागू हैं। 'क' तथा 'ख' क्षेत्रों को जाने वाले अधिकांश पत्रों के लिफाफों पर पते हिन्दी में लिखे जाते हैं। हिन्दी का कार्यसाधक ज्ञान रखने वाले कर्मचारियों के लिए नियमानुसार हिन्दी कार्यशालाओं का आयोजन किया जाता है। कर्मचारियों की हिन्दी में लेखन एवं अभिव्यक्ति क्षमता को विकसित/प्रोत्साहित करने हेतु 'एनसीएल आलोक' नामक वार्षिक राजभाषा पत्रिका का प्रकाशन नियमित रूप से किया जाता है। प्रयोगशाला की शीर्ष स्तर की प्रबन्ध परिषद की बैठकों की कार्यसूची द्विभाषी रूप में तैयार की जाती है और इन बैठकों में हिन्दी में भी चर्चा होती है। भारत सरकार के जैवप्रौद्योगिकी विभाग के सौजन्य से प्रयोगशाला ने हिन्दी में 'वसुन्धरा का हरित परिधान' नामक एक वृत्त चित्र (डॉक्युमेंटरी फिल्म) का भी निर्माण किया है।

प्रयोगशाला में राजभाषा के नियमों का समुचित रूप से अनुपालन किया जाता है। इसी क्रम में प्रयोगशाला के लगभग 90 प्रतिशत कर्मचारियों को हिन्दी का प्रशिक्षण दिया जा चुका है। शेष कर्मचारियों को भी हिन्दी में प्रशिक्षित करने की प्रक्रिया जारी है। चूँकि प्रयोगशाला के 80 प्रतिशत कर्मचारियों को हिन्दी का कार्यसाधक ज्ञान प्राप्त है, अतः इसे राजभाषा नियम, 1976 के नियम 10 (4) के अधीन राजपत्र में अधिसूचित किया जा चुका है। प्रयोगशाला की वेबसाइट हिन्दी में भी तैयार की गई है। प्रयोगशाला में प्रतिवर्ष हिन्दी सप्ताह का भव्य आयोजन किया जाता है। इस अवसर पर स्टाफ के लिए विभिन्न प्रतियोगिताएँ एवं अन्य सांस्कृतिक कार्यक्रम आयोजित किए जाते हैं। इसके अतिरिक्त

प्रयोगशाला में अन्य समारोहों का आयोजन एवं संचालन भी हिन्दी माध्यम से किया जाता है। सीएसआईआर मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिन्तन लेखमाला आदि योजनाएँ प्रयोगशाला में लागू हैं। इन योजनाओं में प्रयोगशाला के वैज्ञानिक एवं कर्मचारी भाग लेते हैं।

इस प्रयोगशाला में विज्ञान की विभिन्न विधाओं में अनुसंधान किया जाता है, तथापि वैज्ञानिक अनुसंधान में भी यह प्रयोगशाला राजभाषा के कार्यान्वयन के प्रति पूर्णतः सजग है। यहाँ राजभाषा के प्रयोग को बढ़ावा देने के लिए समय-समय पर हिन्दी माध्यम से विज्ञान संगोष्ठियों एवं सम्मेलनों का आयोजन किया जाता है। यहाँ के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाले राष्ट्रीय विज्ञान सम्मेलनों/संगोष्ठियों में भाग लेकर हिन्दी में अपना शोधपत्र प्रस्तुत करते हैं।

इस प्रकार राष्ट्रीय रासायनिक प्रयोगशाला भारत सरकार की राजभाषा नीति के अनुसरण में वैज्ञानिक, तकनीकी एवं प्रशासनिक कार्यों में राजभाषा के अधिकाधिक प्रयोग एवं राजभाषा के कार्यान्वयन को गतिशील बनाए रखने हेतु सतत रूप से प्रयासरत है।

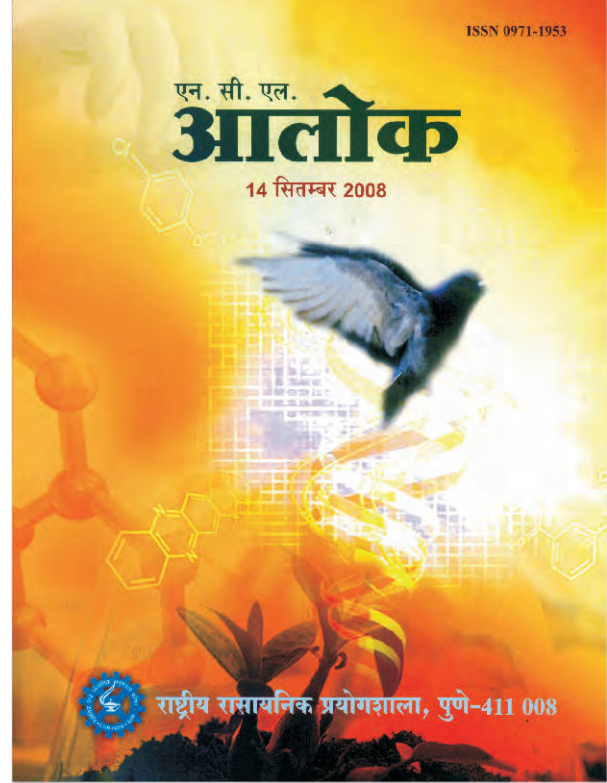
## एन.सी.एल. में हिन्दी सप्ताह का आयोजन



भारत सरकार की राजभाषा नीति के कार्यान्वयन के क्रम में राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में दिनांक : 15 सितम्बर से 22 सितम्बर, 2008 तक की अवधि में हिन्दी सप्ताह समारोह का आयोजन किया गया। हिन्दी दिवस, 14 सितम्बर को अवकाश होने के फलस्वरूप समारोह का प्रारंभ 15 सितम्बर, 2008 से हुआ। इस दिन प्रयोगशाला की वार्षिक राजभाषा पत्रिका, 'एनसीएल आलोक' का लोकार्पण किया गया। पत्रिका के विमोचन के अवसर पर मुख्य अतिथि के रूप में उपस्थित प्रो. (डॉ.) वी.एन. भालेराव, अध्यक्ष, हिन्दी विभाग, पुणे विश्वविद्यालय ने राष्ट्रीय और अन्तर्राष्ट्रीय स्तर पर हिन्दी का महत्त्व और उसकी प्रासंगिकता प्रतिपादित की। उन्होंने कहा कि यद्यपि हमारा देश बहुभाषी है फिर भी इसकी पहचान हिन्दी के द्वारा ही होती है। हिन्दी का अध्ययन-अध्यापन विश्व के लगभग 140 विश्वविद्यालयों में हो रहा है जो इसकी व्यापकता को सिद्ध करता है। प्रो. भालेराव ने आगे कहा कि प्रयोगशाला की इस राजभाषा पत्रिका का बहुआयामी स्वरूप है और इसमें प्रकाशित लेखों का स्तर काफी अच्छा है। इस समारोह की अध्यक्षता प्रयोगशाला के वैज्ञानिक 'जी' डॉ. एम.जी. कुलकर्णी ने की।

हिन्दी सप्ताह के दूसरे दिन 16 सितम्बर को निबन्ध प्रतियोगिता का आयोजन किया गया जिसमें 15 स्टाफ-सदस्यों ने भाग लिया। तदुपरान्त 17 सितम्बर को वाक् प्रतियोगिता तथा 18 सितम्बर को वाद-विवाद प्रतियोगिता आयोजित की गई। दिनांक : 19 सितम्बर को चतुर्थ श्रेणी कर्मचारियों के लिए हिन्दी शुद्धलेखन प्रतियोगिता आयोजित की गई जिसमें बड़ी संख्या में चतुर्थ श्रेणी कर्मचारियों ने उत्साहपूर्वक भाग लिया। हिन्दी सप्ताह का समापन समारोह दिनांक : 22 सितम्बर, 2008 को सम्पन्न हुआ जिसमें राष्ट्रीय प्राकृतिक चिकित्सा संस्थान, पुणे के निदेशक, डॉ. बाबू जोसफ मुख्य अतिथि के रूप में उपस्थित थे। इस समारोह में मुख्य अतिथि ने चारों प्रतियोगिताओं के विजेता स्टाफ-सदस्यों को नकद पुरस्कार एवं प्रमाणपत्र प्रदान किए। अपने संबोधन में उन्होंने कहा कि हिन्दी अपने देश की एक सशक्त भाषा है और मातृभाषा के बाद यह निश्चित रूप से दूसरे स्थान पर है। डॉ. बाबू जोसफ ने त्रिभाषा फॉर्मूला का समर्थन करते हुए कहा कि हर भारतीय को अपनी मातृभाषा के साथ हिन्दी और अँग्रेजी का ज्ञान अवश्य अर्जित करना चाहिए। समारोह की अध्यक्षता करते हुए प्रयोगशाला के निदेशक, डॉ. एस. शिवराम ने भी इस अवसर पर राजभाषा, राष्ट्रभाषा और सम्पर्क भाषा के रूप में हिन्दी की अपरिहार्यता को रेखांकित किया। उन्होंने प्रयोगशाला के वैज्ञानिकों से अपील की कि वे प्रयोगशाला में हो रहे कार्यकलापों को हिन्दी के माध्यम से आम जनता तक पहुँचाएँ। डॉ. शिवराम ने कहा कि यह हर भारतीय को जानने का अधिकार है कि प्रयोगशाला क्या कर रही है और यह कार्य हिन्दी के माध्यम से अच्छी तरह किया जा सकता है।

हिन्दी सप्ताह समापन समारोह के प्रारंभ में प्रयोगशाला के वरिष्ठ हिन्दी अधिकारी, डॉ. रमाशंकर व्यास ने सभी का स्वागत किया और अन्त में श्री बी.बी. कस्तुरे, प्रशासन अधिकारी ने धन्यवाद दिया। समारोह का संचालन श्री उमेश गुप्ता, हिन्दी अधिकारी ने किया।



## Dateline NCL

**June 06, 2008**

The Seventh Prof. K. Venkantaraman Memorial Lecture by Prof. S. V. Keskar, Professor Emeritus, Department of Chemistry and Centre of Advanced Studies in Chemistry Punjab University, Chandigarh on 'Activation of C-H Bonds by Heteroatom Lewis Acid Complexation: Application and Mechanism'

**June 18, 2008**

The Third NCLTEC lecture 'Commercializing New Science' by Prof. George M. Whitesides

**June 19, 2008**

The Fourth Dr. R.A. Mashelkar Endowment Lecture by Prof. Whitesides, University Professor of Chemistry at Woodward L. & Ann A. Flowers, Harvard University, USA on 'Complexity and Emergence'

**September 01 to September 02, 2008**

Orientation Course for newly joined Ph.D. students and scientists

**September 26, 2008**

CSIR Foundation Day Function and CSIR Foundation Day Lecture under the series 'Builders of CSIR' by Dr. T. Ramasami, Secretary to Government of India, Department of Science and Technology, New Delhi on 'CSIR in the Emerging, S&T Landscape of India: A Personal Cherished Dream'

**December 17 to December 18, 2008**

CPYLS Counselling Session for meritorious students of class X, and Keynote address by Dr. Pradeep Srivastava, Scientist, CDRI, Lucknow

**January 09, 2009**

NCL Foundation Day Function and Curtain raiser of NCL Diamond Jubilee Year 2009-10, and lecture by Professor Samir K. Brahmachari, DG-CSIR and Secretary, DSIR, Ministry of Science & Technology, New Delhi

**February 27, 2009**

National Science Day Function and National Science Day Lecture by Prof. N. Kumar, Homi Bhabha Distinguished Professor, Raman Research Institute, Bangalore on 'Viewing Raman Through His Effects'

## Outreach Programme

The NCL Science Outreach lecture series is aimed at conveying the excitement of science and technology to school students, and thereby, hopes to attract the brightest talent from the next generation towards careers in science and technology. The Outreach lectures are aimed at students in the 8th to 10th standard, viz. at the time when they will be making a decision on whether to stay in the science stream. The lecture series is also intended to communicate to the people of Pune, the research that we do in our laboratory and its impact on society.

In the first year of the Outreach programme, lectures were organized once a month, on Sunday mornings. The lectures are delivered by NCL scientists, and invitees from academia and industry, and are open to students and science teachers. Lectures are announced well in advance and the bio-sketch of the speaker is publicised through the dedicated yahoo groups, NCL Academy webpage and also through local press. School students and science teachers register for the lectures ahead of time, and are invited for the talks on a first-come-first-served basis. The lectures typically incorporate experimental demonstrations, exercises and demonstrations to bring the science alive and to kindle the students' curiosity. These lectures aim to expose students to the exciting world of research, and to give them a glimpse of exactly what goes on in a cutting edge laboratory. We have also used these lectures as a platform to inform students about the CSIR Innovation Competition and the National Science and Technology fairs. This has resulted in several submissions from Pune for these competitions.

The first NCL Outreach lecture was delivered in September 2008 by Dr. Chetan Gadgil, and his talk was entitled, " $P + C + M = B$ ", and discussed the interdisciplinary nature of modern scientific research. Subsequent talks by physicists (postdoctoral fellow, Dr. Chirag Kalelkar; Dr. Nilanjana Sengupta), chemists (Dr. Sayam Sengupta, Dr. Vanka Kumar) and chemical engineers (Dr. V. Premnath, Dr. Mugdha Gadgil, Dr. K. Guruswamy) focused on a variety of topics including chemistry in daily life, glassy phases of matter, computational chemistry, biomimetics and innovation. All lectures were held at the NCL Innovation Park, and have been supported by the Venture Center (help with logistics and setting up the talks) and by Battelle India (who have generously provided funding for these lectures).

The NCL Outreach lectures have resulted in raising the awareness of science, technology and research among students, and have increased participation from the city of Pune in national science and innovation competitions. The lectures have been acclaimed by the students and their parents, and by the local print media. NCL has been able to reach out to a large number of students via these lectures. Students from over 40 different schools, as far away as Baramati and Pimpri/Chinchwad regularly attend these lectures, and the Outreach mailing list has several hundred students registered with it. Recently, Forbes Marshall has been sponsoring the transportation costs for 5 children and a school teacher from an underprivileged school in Pimpri to attend the NCL Outreach lectures. There are ambitious plans to upscale the Outreach programme in the next year, including taking these Outreach lectures to local underprivileged schools, thereby greatly expanding their reach.

## Committees



Scientists, in addition to their research and development functions, also give their valuable time for effectively managing various activities in the laboratory. The committees are charged with the responsibility of effective utilization and management of available resources and to ensure wider participation of scientists and staff in decision making in the laboratory.

Statutory Committees	Chairperson
Building and Construction Committee	Shri Sanjay Nene
Canteen Management Committee	Dr. Anil Kumar
Colony Affairs Committee	Dr. Ganesh Pandey
Committee to safeguard the welfare of Women Employees	Dr. (Mrs.) Vidya Gupta
Compassionate Appointment Committee	Dr. B.D. Kulkarni
Grievance Redressal Committee	Dr. Ganesh Pandey
Information and Library Committee	Dr. M.G. Kulkarni
Investigation Team for Write-off	Dr. R.A. Joshi
Medical Services Committee	Dr. (Mrs.) Vidya Gupta
Normalisation Committee for Tech. Officers APAR gradings	Dr. B.D. Kulkarni
Official Language Implementation Committee	Dr. S. Sivaram
Patents Committee	Dr. M.G. Kulkarni
Staff Quarter Allotment Committee	Dr. B.D. Kulkarni
Standing Committee for Recommending Distribution of Income from Intellectual Property, Fee for contract R&D & S&T	Dr. B.D. Kulkarni
Standing Committee on Lab. Safety	Dr. S. Sivaram
Standing Purchase Committee - I	Shri B.B. Kasture
Standing Purchase Committee - II	Dr. A.J. Varma
Sub-committees of Standing Purchase Committee - II	Dr. Anil Kumar

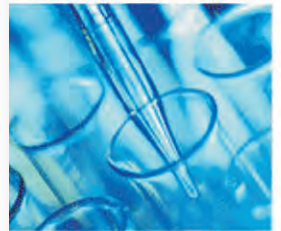
Institutional / Ad-hoc Committees	Chairperson
Major Equipment Purchase Committee	Dr. Anil Kumar
Coordinating Committee for Central NMR Facility	Dr. Ganesh Pandey
Monitoring Committee on Stores Management	Dr. M.G. Kulkarni
Students Academic Committee	Dr. Sourav Pal
Financial Assistance to Students to Participate in International Conferences	Dr. Sourav Pal
Student Accommodation on Campus Committee	Dr. S. Ponrathnam
Leadership Team Committee	Dr. S. Sivaram



# National Chemical Laboratory



## Admission to Postgraduate Research Programme in Engineering



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### Reports & Press Releases

- Symposium on Advances in Chemical Engineering and Process Technology
- National Symposium on Catalysis at NCL

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### NCL in News

- A reaction to chemistry's changing needs ( Indian Express, 25 Apr 2010)
- PM to attend annual NCL function on Thursday (Indian Express, 31 mar 2010)

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### Major Events

- NCL Foundation Day Lecture - "Adventures in Molecular Recognition: Dynamic Combinatorial Chemistry and Supramolecular Nanotubes " by Professor Jeremy K.M. Sanders, University of Cambridge, UK
- 50th Annual Conference of Association of Microbiologists of India on Third Golden Era of Microbiology

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राष्ट्रीय रासायनिक प्रयोगशाला

**National Chemical Laboratory**

(Council of Science & Industrial Research)

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