National Chemical Laboratory

राष्ट्रीय रासायनिक प्रयोगशाला

वार्षिक प्रतिवेदन 2009-10

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निदेशक की कलम से

मुझे राष्ट्रीय रासायनिक प्रयोगशाला का वर्ष 2009-2010 का वार्षिक प्रतिवेदन प्रस्तुत करते हुए अतीव प्रसन्नता हो रही है ।

राष्ट्रीय रासायनिक प्रयोगशाला ने अपनी स्थापना की स्मृति में यह सम्पूर्ण वर्ष हीरक जयन्ती वर्ष के रूप में मनाया। इस यशस्वी हीरक जयन्ती समारोह का समापन 1 अप्रैल, 2010 को भारत के प्रधानमंत्री के प्रयोगशाला में पदार्पण के साथ सम्पन्न हुआ। राष्ट्रीय रासायनिक प्रयोगशाला में हम सभी के लिए यह एक गौरवपूर्ण क्षण था। पं. जवाहरलाल नेहरू ने 3 जनवरी, 1950 को राष्ट्रीय रासायनिक प्रयोगशाला का उद्घाटन किया था। तब से लेकर वर्तमान समय तक हमें तीन प्रधानमंत्रियों को अपनी प्रयोगशाला में आमंत्रित करने का सौभाग्य प्राप्त हो चुका है। सन् 1975 में श्रीमती इन्दिरा गाँधी जी, सन् 2000 में श्री अटल बिहारी वाजपेयी जी और सन् 2010 में डॉ. मनमोहन सिंह जी का हमारी प्रयोगशाला में पदार्पण हुआ । यह सचमुच एक विलक्षण तथ्य है जो भारत की किसी अन्य वैज्ञानिक संस्था के लिए दुर्लभ है। भारत के प्रधानमंत्री की एनसीएल में उपस्थिति महज एक घटना नहीं है बल्कि यह एक अर्थपूर्ण और गहन महत्त्व का विषय है। यह एनसीएल की प्रतिष्ठा और ख्याति तथा भारत में वैज्ञानिक संस्थाओं के मध्य उसके एक महत्त्वपूर्ण स्थान का सूचक है।

एनसीएल का आधुनिक भारत के वैज्ञानिक पुनरोत्थान के इतिहास में एक विशिष्ट स्थान है जिसके कारण ही क्रमिक रूप से प्रधानमंत्रियों का इस प्रयोगशाला में आगमन संभव हुआ और वे हमारे इतिहास के यशस्वी क्षणों के सहभागी बन सके।

इस वार्षिक प्रतिवेदन में एक विशेष खण्ड है जिसके अन्तर्गत इस ऐतिहासिक अवसर का वर्णन किया गया है । मेरा निवेदन है कि आप इन पृष्ठों को पढ़ें और इस विशेष दिवस के आनन्द में हमारे सहभागी बनें ।

अब जब कि एनसीएल अपने साठ वर्ष पूरा करके अमृत महोत्सव की ओर अपनी यात्रा प्रारंभ कर रही है, मैने सोचा, यह समीचीन होगा कि मैं इस प्रतिवेदन में वर्ष 2025 में प्रतिबिम्बित होने वाले एनसीएल के स्वरूप और भविष्य के बारे में अपने विचार प्रकट करूँ ।

राष्ट्रीय रासानिक प्रयोगशाला जो वैज्ञानिक एवं औद्योगिक अनुसंधान परिषद की एक संघटक इकाई है, की स्थापना वर्ष 1950 में पं. जवाहरलाल नेहरू के असाधारण स्वप्न और दूरदृष्टि को साकार करने के लिए की गई थी । विज्ञान के बारे में पं. नेहरू की दूरदृष्टि अनन्त सीमा को समेटे हुई थी । उनका यह विश्वास परिपूर्ण था कि विज्ञान और प्रौद्योगिकी ही भारत के विकास का साधन है । विज्ञान के विकास और संवर्धन के प्रति उनकी प्रतिबद्धता उत्कट थी । पं.नेहरू ने कहा था, " एकमात्र विज्ञान ही भूख तथा निर्धनता, बर्बाद हो रहे व्यापक संसाधनों एवं निर्धन लोगों से बसे हुए एक समृद्ध देश की समस्याओं का समाधान कर सकता है।"

बीसवीं शताब्दी में भारत में वैज्ञानिक अनुसंधान की विकसित हो रही परम्पराओं में सीएसआईआर - एनसीएल की स्थापना एक महत्त्वपूर्ण मील का पत्थर थी । एनसीएल वैज्ञानिक अनुसंधान में सर्वश्रेष्ठ बनी हुई है और इसने गत छह दशकों में मूलभूत और अनुप्रयुक्त विज्ञान एवं प्रौद्योगिकी दोनों में वैज्ञानिक उत्कृष्टता के उच्चतम मानकों को परिश्रमपूर्वक बनाए रखा है ।

एक संस्था के इतिहास में साठ वर्षों का समय एक महत्त्वपूर्ण मील का पत्थर है । इस अवधि में एनसीएल में नेतृत्व की एक ऐसी सुप्रतिष्ठित परम्परा रही है जिसने इतिहास के विभिन्न मोड़ों पर इसके भाग्य को सँवारा और निर्देशित किया है । इस नेतृत्व ने भारत के सर्वोत्तम विज्ञान-अध्येताओं और वैज्ञानिकों का पोषण किया है । यह नई चुनौतियों का सामना करने के लिए प्रत्येक दशक के अन्त में स्वयं को रूपान्तरित और पुनर्गठित करती रही है । एनसीएल के क्रमिक नेतृत्व ने श्रेष्ठता के सतत लक्ष्य को प्रोत्साहित किया है ।

एनसीएल ने भारत में रासायनिक उद्योग के विकास और अभिवृद्धि की दिशा में महत्त्वपूर्ण योगदान दिया है । इसने विश्व की कुछ महानतम कम्पनियों के साथ भागीदारी स्थापित करके अनुसंधान कार्य किया है । अनेक प्रक्रियाओं और उत्पादों जिन पर एनसीएल ने अनुसंधान कार्य किया है, का उद्योग जगत ने घरेलू उपभोग तथा निर्यात हेतु सफलतापूर्वक व्यवसायीकरण किया है । एनसीएल/सीएसआईआर ने कृषि-रसायन, औषध, सूक्ष्म रसायन, बहुलक या उत्प्रेरकीय प्रक्रियाओं जैसे भारतीय रासायनिक उद्योग के विकास में महत्त्वपूर्ण भूमिका निभाई है । भारतीय उद्योग अपने भावी प्रौद्योगिकीय लक्ष्यों की प्राप्ति में आज भी एनसीएल/सीएसआईआर की सहायता और मार्गदर्शन प्राप्त कर रहा है। एनसीएल/सीएसआईआर के निदेशकगण शैक्षणिक और औद्योगिक अनुसंधान दोनों में एक सन्तुलन बनाए रहे हैं । उद्योग जगत विज्ञान, प्रौद्योगिकी और नवोन्मेष के पहलुओं पर चर्चा करने के लिए अनेक औद्योगिक मंचों पर एनसीएल/सीएसआईआर के नेतृत्व को आमंत्रित करते

हैं । उद्योग जगत के मुख्य कार्यकारी अधिकारी भी हमारी अनुसंधान परिषद की बैठकों में तथा प्रौद्योगिकी विकास को लक्ष्य में रखकर बनाए गए हमारे अनेक अनुसंधान कार्यक्रमों में भाग लेते हैं । एनसीएल ने रसायन विज्ञान तथा उससे सम्बन्धित विज्ञान की अन्य विधाओं एवं अभियांत्रिकी के क्षेत्र में शिक्षा जगत और उद्योग जगत दोनों को ही उच्च गुणवत्ता युक्त मानव संसाधन उपलब्ध कराया है । एनसीएल से पीएच.डी. किए हुए 1700 से अधिक लोग उद्योगों, शिक्षण संस्थानों और सरकारी प्रतिष्ठानों में उच्च एवं प्रतिष्ठित पदों पर कार्यरत हैं ।

यद्यपि एनसीएल की भूतकाल की उपलब्धियाँ, असाधारण और प्रशंसनीय रही हैं तथापि इसे अब भविष्य के बारे में सोचना और ध्यान देना है । पिछले 60 वर्षों के दौरान भारत में विज्ञान एवं प्रौद्योगिकी परिपक्व हो चुकी है और नवोन्मेष हेतु हमारी क्षमताओं और सामर्थ्य को देखते हुए हमारी गिनती विश्व के अग्रणी देशों में की जाती है । भारतीय उद्योग द्रुत गति से आकार तथा भौगोलिक दोनों दृष्टि से परिपक्व और विकसित हो रहा है। भारतीय तथा विश्व की कम्पनियाँ अभिनव आविष्कारों और नवोन्मेष हेतु भारत की ओर देखती हैं ।

एक देश के रूप में भारत वास्तव में अत्यन्त भयंकर चुनौतियों का सामना कर रहा है। प्रत्येक क्षेत्र में चाहे वह स्वास्थ्य, पर्यावरण, जल, ऊर्जा, परिवहन या उत्पादन का क्षेत्र हो, भारत को पर्याप्त नवोन्मेष की आवश्यकता है ताकि मूल्य और निष्पादन के व्यापक आधार पर विविध समस्याओं का समाधान प्रस्तुत किया जा सके । यदि इन समाधानों को उचित समय-सीमा में प्राप्त करना है तो विज्ञान एवं प्रौद्योगिकी पर और अधिक ध्यान केन्द्रित करना होगा ताकि उससे उत्पाद एवं प्रक्रियाएँ विकसित की जा सकें । इन उत्पादों और प्रक्रियाओं को प्रयोगशाला से बाहर निकल कर बाजार तक पहुँचना होगा जिससे ग्राहक उन्हें अपना सकें । अनुसंधान और प्रौद्योगिकी की सफलता का बस एक ही प्रमाण है- जन स्वीकृति । जब आम आदमी किसी नवोन्मेष को अपनाता है तो उसके लिए सहर्ष पैसा देता है।

अतः एनसीएल के लिए यह आवश्यक है कि वह इस ऐतिहासिक अवसर पर पुनः अपने को समर्पित करे। एनसीएल के वैज्ञानिकों और वैज्ञानिकों के ग्रूपों का अनुसंधान कार्य राष्ट्रीय आवश्यकताओं और अपेक्षाओं के अनुरूप होना चाहिए ।

एनसीएल अपनी रुचि के सारभूत विज्ञान की विधाओं पर अपना विशेष ध्यान केन्द्रित रखेगी । यह एक आवश्यक प्राथमिक अपेक्षा है । विज्ञान के अग्रणी क्षेत्रों में कार्य किए बिना समाज को विज्ञान के लाभ नहीं मिल सकते हैं । अतः रसायन विज्ञान तथा सम्बद्ध विज्ञान की विधाओं में सारभूत विज्ञान और प्रौद्योगिकी एनसीएल का आधार बने रहेंगे । मैं इसे प्रथम स्तर कहता हूँ ।

तथापि केवल आधार अकेले भवन का निर्माण नहीं कर सकता है । इस आधार पर हमें विषय - वस्तु सम्बन्धित कार्यक्रमों का आन्तर्विधात्मक नेटवर्क तैयार करना चाहिए । एनसीएल के लिए प्रासंगिक विषय हैं - प्रगत एवं कार्यात्मक पदार्थ, संकर पदार्थ, जैव-प्रेरित पदार्थ, संश्लिष्ट जीवविज्ञान, जैव-संसाधन प्रौद्योगिकी, जैव-रूपान्तरण, जैवसक्रिय अणु, उत्प्रेरकीय प्रकियाएँ तथा बहुविध लम्बाई और समय के पैमाने में वैज्ञानिक कम्प्यूटिंग । इसे दूसरा स्तर कहा जा सकता है । इन विषयों पर कार्य करने के लिए अधिक आन्तर्विधात्मक अनुसंधान की जरूरत होगी जिसके फलस्वरूप रसायन विज्ञान, जीवविज्ञान, पदार्थ विज्ञान और अभियांत्रिकी के क्षेत्र में परस्पर बड़े पैमाने पर समन्वयन स्थापित होगा । हाल ही के वर्षों में एनसीएल ने इन कुछ क्षेत्रों में विषय-वस्तु सम्बन्धी श्रेष्ठता केन्द्र स्थापित किए हैं ताकि विभिन्न विभागों में कार्यरत वैज्ञानिक एवं इंजीनियर एक मंच पर आ सकें और एक समान लक्ष्य और दृष्टिकोण से कार्य कर सकें ।

इस तरह के दोनों औपचारिक और अनौपचारिक आन्तर्विधात्मक नेटवर्क से केन्द्रीकृत प्रयासों को बल मिलेगा जिसके फलस्वरूप स्वच्छ एवं सस्ते ऊर्जा संसाधन, रोगों की बेहतर समझ, सस्ती चिकित्सा सुविधाएँ, स्वच्छ जल, अधिक सक्षम तथा स्वच्छ प्रक्रमण प्रौद्योगिकी, पदार्थों हेतु सुदृढ़ बिल्डिंग ब्लॉक तथा अपशिष्ट द्रव्यों से धनार्जन आदि जैसे मुद्दों का समाधान हो सकेगा । यह तीसरा स्तर है । इस तीसरे स्तर के प्रयासों से ही समाज और जनहित पर पड़ने वाले प्रभाव दिखाई देंगे । हम आज लाभाकांक्षी और उपयोगितावादी विश्व में रह रहे हैं । हमारे साझेदार विज्ञान और प्रौद्योगिकी से उत्तरोत्तर यह अपेक्षा करेंगे कि वह समाज को आर्थिक रूप से समृद्ध बनाए । तथापि तीसरे स्तर को प्रभावी बनाने के लिए दूसरे स्तर में ठोस क्षमताएँ और सामर्थ्य विकसित करना और प्रथम स्तर में सुदृढ़ आधार तैयार करना अत्यावश्यक है ।

हाल के वर्षों में एनसीएल की यह कार्य योजना रही है कि प्रथम स्तर पर अनुसंधान की विविधता तैयार करके दूसरे स्तर पर क्षमताओं और योग्यताओं को विकसित किया जाए । ऐसा विश्वास है कि इन प्रयत्नों से एनसीएल हमारे समाज की आवश्यकताओं को पूरा करने की दिशा में बेहतर ढंग से तैयार हो सकेगी । अपनी सामूहिक क्षमता और सामर्थ्य को प्रदर्शित करने के लिए एनसीएल एक मिशन के तौर पर कुछ कार्यक्रमों को परिभाषित और कार्यान्वित करने की योजना बना रही है ।

इस दृष्टिकोण को ध्यान में रख कर एनसीएल ने पिछले कुछ वर्षों में ऊर्जा (हाइड्रोजन एवं सौर ऊर्जा) कृषि के अपशिष्टों तथा जैवसंसाधनों से मूल्य प्रवर्धित रसायन और पदार्थ, रसायनों हेतु स्वच्छ प्रौद्योगिकी तथा अभिनव उत्प्रेरकों एवं रासायनिक अभियांत्रिकी के सिद्धान्तों पर आधारित सूक्ष्म रसायनों हेतु अधिक सक्षम प्रक्रियाओं के क्षेत्र में नए अनुसंधान कार्य प्रारंभ किए हैं ।

विज्ञान एवं प्रौद्योगिकी अब अधिक सहयोगी हो रहे हैं । विज्ञान की विधाओं के अन्तरापृष्ठों पर विघटनकारी नवोन्मेषों की मात्रा बढ़ रही है । सिद्धान्त, अनुप्रयोग तथा मापन विज्ञान नई अन्तर्दृष्टि और ज्ञानार्जन के लिए एकीकृत हो रहे हैं। प्रयोगशाला के एक कोने में बैठ कर कार्य करने वाले और नई धारणा एवं संकल्पना को प्रस्तुत करने वाले एक अकेले वैज्ञानिक का स्वप्न अब विज्ञान के इतिहास का एक भाग है । यद्यपि विज्ञान में वैयक्तिक श्रेष्ठता पूर्व शर्त है तथापि चुनौतीपूर्ण भावी वैज्ञानिक समस्याओं के समाधान के लिए यह अकेले पर्याप्त नहीं है । विज्ञान की सभी विधाओं में परस्पर भागीदारी और सहयोग आवश्यक है तभी वह समाज के लिए मूल्यवान और उपयोगी बन सकेगा । वर्तमान युग के वैज्ञानिकों को मिलजुल कर कार्य करते हुए परस्पर सहयोग की संस्कृति सीखनी चाहिए और उसे कार्यान्वित करना चाहिए । विज्ञान की अन्तर्विधाओं के परस्पर समन्वयन से एक अनुकूल और सुविधाजनक वातावरण बनता है । ऐसी स्थिति में विचारों और अभिव्यक्ति

निदेशक की कलम से

की स्वतंत्रता होती है । पदानुक्रम में वरिष्ठ पदाधिकारियों के साथ स्वस्थ सम्बन्ध बनते हैं तथा प्रभागों एवं विभागों के अधिकार शिथिल होने से स्वामीभक्ति तथा संकीर्ण सोच समाप्त हो जाती है । संगठन के शक्तिशाली मुख्य कार्यकारी अधिकारी के अधीन कार्यरत स्टाफ और अनुयायियों की जो परम्परा है उसके स्थान पर स्वतः अनुशासित प्रबुद्ध वैज्ञानिकों का दल होना चाहिए जो एक स्वस्थ मनोवृत्ति के साथ मिल-जुल कर कार्य करें तथा उपलब्ध संसाधनों का परस्पर उपयोग करते हुए प्रशासनिक व्यवस्था को सुचारु रूप से चलाने में भागीदार बनें ।

एनसीएल को उस संस्कृति एवं मूल्यों को दृढ़तापूर्वक बनाए रखना चाहिए जो अबाधित ज्ञान के प्रवाह, आन्तर्विधात्मक कार्यों, सुविधाओं के परस्पर उपयोग, रचनात्मकता, मौलिक संकल्पना तथा कार्यकलापों की उच्च पारदर्शिता के लिए सहायक एवं अनुकूल हैं ।

एनसीएल को युवा वैज्ञानिकों तथा पीएच.डी. डिग्री हेतु अनुसंधान करने के लिए आने वाले छात्रों के लिए एक प्रतियोगी और आकर्षक केन्द्र के रूप में भी बने रहने की आवश्यकता है । एनसीएल का एक यह भी दायित्व है कि वह विशेष रूप से अभिनव प्रौद्योगिकी से सम्बन्धित आन्तर्विधात्मक क्षेत्रों में अगली पीढ़ी की वैज्ञानिक प्रतिभाओं को प्रशिक्षित करे। एनसीएल के वैज्ञानिक विज्ञान तथा अभियांत्रिकी के प्रगत पाठक्रमों को भी पढ़ा रहे हैं । आगामी वर्षों में अनुसंधान एवं अध्यापन कार्य और अधिक एक दूसरे के नजदीक आ जाएँगे ।

समाज में धन का अर्जन करने हेतु एनसीएल की उद्योग जगत तथा सरकारी संस्थाओं के साथ भागीदारी आवश्यक है । एनसीएल को पहले से ही भारतीय उद्योगों और विश्व के उद्योगों के साथ अनुसंधान भागीदार होने का गौरव प्राप्त है । इसी सार्वजनिक-निजी भागीदारी के फलस्वरूप ही उसे प्रौद्योगिकी हस्तान्तरण में हाल ही में अनेक सफलताएँ मिली हैं । एनसीएल को अनुसंधान एवं विकास से सम्बन्धित उद्योगों के साथ समर्पित संयुक्त अनुसंधान केन्द्रों की स्थापना के माध्यम से अपनी भागीदारी को और अधिक मजबूत करना चाहिए । एनसीएल ने जीनोमिकी एवं समवेत जीवविज्ञान संस्थान (आईजीआईबी), नई दिल्ली, इन्दिरा गाँधी परमाणु ऊर्जा अनुसंधान केन्द्र (आईजीसीएआर), कल्पक्कम तथा भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान (आईआईएसईआर), पुणे के साथ भी अनुसंधान भागीदारी स्थापित की है । ऐसी सार्वजनिक - निजी भागीदारी से मौलिक विज्ञान में प्रथम स्तर की क्षमता एवं योग्यता सुदृढ़ होती है तथा वैज्ञानिकों एवं छात्रों दोनों के लिए ज्ञानार्जन के नए अनुभव होते हैं ।

किसी वैज्ञानिक उद्यम का सारभूत प्रयोजन ज्ञान से धनार्जन करना है । एनसीएल/सीएसआईआर अन्य शैक्षणिक अनुसंधान प्रयोगशालाओं से इस मामले में भिन्न है कि यह ज्ञान को अनुप्रयोग से जोड़ने के लिए सक्रियता से कार्य करती है। मेरा मानना है कि सरकारी सहायता प्राप्त अनुसंधान संस्थाओं को विज्ञान के माध्यम से धनार्जन करने तथा इस प्रकार समाज को लाभ पहुँचाने की दिशा में अवश्य ध्यान केन्द्रित करना चाहिए । यद्यपि ज्ञान का अर्जन महत्त्वपूर्ण और आवश्यक है, तथापि उस ज्ञान की उपयोगिता का सृजन करने के लिए भी सतत रूप से ध्यान केन्द्रित करना चाहिए । एनसीएल/सीएसआईआर को केवल समस्या का समाधान प्रस्तुत करने तक ही सीमित न रह कर सम्बन्धित समाज या उद्योग को दिए जाने वाले समाधान से धनार्जन करने को भी सोचना चाहिए ।

प्रौद्योगिकी सम्बन्धित अधिक खतरों और बाजार की अनिश्चितताओं के कारण प्रथम चरण की खोजों या नवोन्मेषों का व्यापारीकरण करना बहुत कठिन है । ज्ञान को धन में रूपान्तरित करने के लिए विघटनकारी नवोन्मेषों को पूरी तरह से दूसरा भिन्न रूप देना होगा। इस प्रक्रमण को कार्यान्वित करने के लिए एनसीएल प्रवर्तन पार्क नामक एक नया परिसर बनाया गया है । यह परिसर सीएसआईआर की सार्वजनिक-निजी भागीदारी कार्यक्रमों का घरेलू स्थल बनेगा । इस स्थल पर उद्यमिता विकास केन्द्र (वेंचर सेण्टर) नामक एक धारा 25 की गैर-लाभ कम्पनी भी स्थापित है ।

वेंचर सेण्टर एक प्रौद्योगिकी व्यवसाय संवर्धन केन्द्र है जो विज्ञान तथा प्रौद्योगिकी विभाग तथा सीएसआईआर के आर्थिक सहयोग और सुविधाओं से स्थापित किया गया है । इसका उद्देय विज्ञान एवं प्रौद्योगिकी अभिमुख उद्यमिता को बढ़ावा देना है । सीएसआईआर वर्तमान में एनसीएल परिसर में एक नवोन्मेष कॉम्प्लेक्स स्थापित करने की प्रक्रिया में है जो एक विश्वस्तरीय नवोन्मेष परिस्थिति की तंत्र के रूप में होगा । इसे सार्वजनिक और निजी भागीदारी के आधार पर बनाया जाएगा । यह सीएसआईआर की क्षमता और सहयोग से विकसित होकर नई प्रौद्योगिकियों को बाजारोन्मुखी बनाएगा ।

नवोन्मेषों को महत्त्वपूर्ण बनाने के लिए यह आवश्यक है कि एनसीएल के वैज्ञानिक एवं इंजीनियर यह नहीं सोचें कि उनका कार्य केवल अच्छे विज्ञान तक ही सीमित है और उनके विज्ञान से धनार्जन करने का कार्य किसी दूसरे व्यक्ति का है। हमें उन्हीं को मान्यता प्रदान करनी चाहिए जो विज्ञान के अनुप्रयोग बाजार एवं समाज तक ले जाते हैं । ऐसे कार्यों को बाजार तथा समाज की स्वीकृति मिलनी चाहिए ।

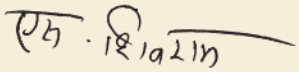
युवा विज्ञान अध्येताओं को यह बताया जाना चाहिए कि मात्र पीएच.डी. डिग्री के बाद बाहर किसी दूसरे देा में विज्ञान के क्षेत्र में डॉक्टरोत्तर अनुसंधान कार्य करके आजीवन किसी बड़े औद्योगिक या सरकारी संस्था में कार्य करने के अलावा उनके भविष्य (कैरिअर) हेतु और भी विकल्प हैं । युवाओं को वैज्ञानिक उद्यमिता के अवसरों को प्राप्त करने के लिए प्रयत्नशील रहना चाहिए। उन्हें यह सोचना चाहिए कि इस प्रकार से वे दूसरे को भी रोजगार प्रदान करने की स्थिति में हो सकते हैं । उद्यमिता के मानदण्डों का स्तर

थोड़ा कम करने की जरूरत है । इससे युवाओं को इस क्षेत्र में प्रवेश हेतु प्रोत्साहन मिलेगा जिससे समाज को बड़ा लाभ होगा।

एनसीएल के अन्दर और आसपास का क्षेत्र एक विशाल नवोन्मेष समुदाय केन्द्र के रूप में उभर रहा है । इसमें अनुसंधान एवं प्रौद्योगिकी के अनेक पेशेवर तथा युवा छात्र कार्य करेंगे । मैं सीएसआईआर-एनसीएल को एक ऐसी संस्था के रूप में देख रहा हूँ जो श्रेष्ठतम मूल्यों से ओतप्रोत है। ये सर्वोत्तम मूल्य अधिग्रहण (अनुसंधान), संप्रेषण (अध्यापन) तथा ज्ञान का प्रयोग और कार्यान्वयन (प्रौद्योगिकी) के लिए समर्पित हैं ।

इस शानदार संस्था के निदेशक के रूप में मेरा यह अन्तिम प्रतिवेदन है । मुझे इस पद पर कार्य करने में खुशी हुई है और एनसीएल को एक सुदृढ़ संगठन बनाने में मैनें सर्वोत्तम प्रयास किए हैं । जैसा कि मैने 1 जुलाई, 2002 को एनसीएल के स्टाफ और वैज्ञानिकों को सम्बोधित करते हुए कहा था, कि इस महान संस्था का नेतृत्व न्यासिता के समान है जो भाग्यवश मुझे प्राप्त हुई थी । मैने इसे बड़ी सावधानी के साथ रखा और अपनी पूरी योग्यता एवं क्षमता के साथ इसका पोषण किया । अब मैं इसे दूसरे व्यक्ति को हस्तान्तरित करने के लिए तैयार हूँ जो सौभाग्य से इस प्रयोगशाला को नेतृत्व प्रदान करेगा।

मैं अपनी प्रयोगशाला के प्रत्येक वैज्ञानिक एवं अन्य स्टाफ द्वारा दिए योगदानों के लिए अपना विनम्र आभार प्रकट करता हूँ । इन सभी ने मिल कर इस प्रयोगशाला को एक ऐसा आनन्ददायक और रचनात्मक स्थान बनाया है जहाँ हम सभी सुविधापूर्वक काम कर सकें। अपने कर्तव्यों एवं जिम्मेदारियों का निर्वहन करने में मुझे इस प्रयोगशाला की अनुसंधान परिषद एवं प्रबन्ध परिषद से आचर्यजनक सहयोग मिला है जिसका यहाँ उल्लेख करना मैं अपना कर्तव्य समझता हूँ । मैं एनसीएल को दिए गए अबाधित और अनवरत सहयोग के लिए सीएसआईआर के महानिदेशक और स्टाफ को भी धन्यवाद देता हूँ ।



(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 2009-10.

NCL commemorated the Diamond Jubilee Year of its inception all through the year with a fitting finale on April 1, 2010, when once again yet another Prime Minister of India set foot in the hallowed portals of this Laboratory to bring the curtain down on this glorious anniversary. It was a proud moment for all of us at NCL. Since the inauguration of NCL on January 3, 1950 by Pandit Jawaharlal Nehru, we have had the privilege of hosting Madam Indira Gandhi in 1975, Shri Atal Behari Vajpayee in 2000 and Dr Manmohan Singh in 2010. This is truly an exceptional record unequalled by any other scientific institution in India.

The presence of a Prime Minister of India in NCL is not a mere event. It is pregnant with deep significance. It is indicative of the prestige and reputation of NCL and its place in the pantheon of scientific institutions in India. NCL occupies a special place in the history of modern India's scientific resurgence which has made it worthwhile for successive Prime Ministers to come to this Laboratory and share in the proud moments of our history.

There is a special section in this Annual report that records this historic occasion. I welcome you to browse these pages and share with us the happiness of this Day.

As NCL completes its sixtieth year and begins its journey towards the Platinum, I thought it is only fitting that I share in this Report my own visions of what NCL should be in the year 2025.

The National Chemical Laboratory (NCL) of the Council of Scientific and Industrial Research (CSIR) came into existence in the year 1950, giving shape to the extraordinary vision of Pandit Jawaharlal Nehru. Nehru's vision of science as a truly endless frontier was all encompassing; his belief that science and technology was a tool for the development of India was total; and his commitment to the growth of science was passionate. Pandit Nehru said, "It is science alone that can solve the problems of hunger and poverty; of vast resources running to waste; of a rich country inhabited by poor people."

Establishment of CSIR- NCL was an important milestone in the expanding traditions of scientific research in India in the twentieth century. NCL continues to be an enduring symbol of the very best in scientific research and has assiduously maintained over the past six decades the highest standards of scientific excellence, both, in basic and applied sciences and technology.

Sixty years is a significant milestone in the history of an institution. NCL has had a distinguished lineage of leadership who has guided its destiny at various turns of history. It has nurtured the best minds of India. It has continuously transformed and reinvented itself to meet new challenges at the turns of every decade. Successive leadership of NCL has encouraged a culture of sustained pursuit of excellence.

NCL has contributed significantly to the growth and development of the Chemical industry in India. It has partnered research with some of the largest companies of the world. Many of the processes and products that have come out of NCL have been successfully commercialized by industry, both, for domestic consumption and exports. NCL/CSIR played a critical role in the development of the Indian chemical industry, may it be, agro-chemicals, pharmaceuticals, fine chemicals, polymers or catalytic processes.

The Indian industry continues to seek the association of NCL/CSIR in addressing their future technology goals. The Directors of NCL/CSIR have had, interestingly a balanced appreciation of both, academic as well as industrial research.

Industries seek actively the participation of the leadership of NCL/CSIR in many of the industry forum to discuss aspects of science, technology and innovation. Industry leaders actively participate in our Research Council (RC) as well as in many of our research programmers aimed at technology development.

NCL is a rich provider of high quality human resources in chemical and related sciences and engineering to both academia and industry. Its alumni, in excess of 1700 PhDs, occupy positions of eminence in industry, academia and the government.

While past accomplishments of NCL have been exceptional and praise worthy it must, however, now look into the future. Over the past sixty years science and technology in India has matured and we are now counted amongst the front ranking nations of the world in terms of our capacities and potentials for innovation. Indian industry is fast maturing and growing in, both, size and geographies. India is being increasingly looked at as a crucible for creating new innovations by both Indian and global companies.

The challenges faced by India as a nation is indeed very daunting. In every area, whether it is health, environment, water, energy, transportation or manufacturing India needs substantial innovation to provide solutions to multiple stakeholders across a wide matrix of price and performance. If these solutions have to be found within reasonable time frame, science and technology must become more focused and eventually result in products or processes. Products and processes must move out of the laboratory and reach the market gaining wide customer acceptance. The only proof of success in research and technology is when a consumer is ready and willing to pay for an innovation.

It is, therefore, important for NCL to once again rededicate itself on this historic occasion. The research agenda of the scientists and the scientific groups of NCL must align itself more intimately with the national agenda.

NCL will continue to sharpen its focus on core science in the disciplines of its interest. This is an essential pre-requisite. Without scientists capable of working in the frontiers of science, no benefits from science can flow to the society. So core science and engineering in chemical and related sciences shall remain as its foundation. I call this Level 1.

However, a mere foundation does not make an edifice. On this foundation we must build an inter-disciplinary network of thematic programmes. Themes that are relevant to NCL are advanced and functional materials, hybrid mateials, bio-inspired materials, synthetic biology, bio-resource technologies, bio-transformation, bioactive molecules, catalytic processes, scientific computing across multiple length and time scales, etc. These can be termed as Level 2. These themes will demand more interdisciplinary research with larger interface between chemistry, biology, material science and engineering.

NCL has created thematic Centres of Excellence (CoE) in recent years around some of these areas to bring together scientists and engineers working across departments and provide them a common vision.

Such interdisciplinary networks, both formal and informal, will lead to focused efforts to address issues such as clean and affordable energy resources, better understanding of diseases, lower cost therapeutics, clean water, more efficient and clean processing technologies, sustainable building block for materials, converting waste to wealth, etc. This is Level 3. Impact on society and public good can be realized only from Level 3 efforts. We live today in a utilitarian world. Our stakeholders will increasingly expect S&T to create value in society. However for Level 3 to be effective in delivery, one must build solid competencies in Level 2 and a robust foundation in Level 1.

NCL's strategy in recent years is to consciously build research diversity in Level 1 and create Level 2 competencies. It is believed that with these efforts, NCL will be better prepared to make an impact on the needs of our society. NCL hopes to define and execute a few programmes in a mission mode with a view to demonstrate its collective strength.

With this perspective in view NCL has over the past few years commenced building new research platforms in the area of energy (hydrogen and solar), value added chemicals and materials from agricultural wastes and bio-resources, cleaner technologies for chemicals and more efficient processes for fine chemicals based on novel catalysts and chemical engineering principles.

Science and technology is becoming more collaborative. Disruptive innovations are increasingly occurring at the interfaces of discipline. Theory, experiments and measurement sciences are becoming seamlessly integrated to create new insights and knowledge. The vision of a lone scientist labouring in a corner of a laboratory and coming up with new ideas is now part of the history of science. Whereas, individual excellence in science is a prerequisite, this alone

From the DIRECTOR'S DESK

is not sufficient to solve the challenging scientific problems of the future. Partnership and collaboration across disciplines is essential if science has to create value to society. Ability to work in teams and collaborate is a culture that present day scientists must learn and practice. Breaking down barriers and walls between scientific disciplines require a facilitative environment, namely, freedom of thought and expression, a healthy disrespect for hierarchy and loosening the power of divisions and departments which often tend to promote loyalty and parochial thinking.

The traditional pyramidal organizational structure of a strong leader with many followers must be replaced by self managed teams of scientists with many thought leaders working in a flat organizational structure with a healthy attitude towards sharing of resources and a participative style of governance.

NCL, must steadfastly hold on to the culture and values that promote seamless learning environment, a high degree of cross functional and inter-disciplinary interactions, a culture of sharing facilities, an ambience which stimulates creativity and encourages original thinking and a high level of transparency of activities and functions.

NCL also needs to remain competitive as well as be an attractive destination for a large number of scientific professionals who want to make science as a career and to a large number of young students who wish to pursue their Ph.D. degree. NCL has a distinct obligation to train the next generation of scientific talent, especially, in interdisciplinary areas related to innovative technologies. Scientists of NCL are also increasingly engaging themselves in teaching advanced courses in science and engineering. Research and teaching will become even more closely entwined in the years to come.

Partnerships, both with industry as well as public institutions, are essential for NCL to create wealth in the society. NCL already has a high reputation of being a credible research partner with both Indian and global industry. Many of its recent successes in technology transfer have been a consequence of public-private partnerships. NCL should strengthen such partnerships through creation of dedicated joint centres or ventures of research with industries around key R&D platforms. NCL has also set up focused research partnerships with Institute of Genomics and Integrative Biology, New Delhi (IGIB), Indira Gandhi Center for Atomic Energy Research, Kalpakkam (IGCAR) and Indian Institute of Science Education and Research, Pune. (IISER). Such public-public partnerships strengthen Level 1 competency in basic science and open up new learning experiences for both scientists and students.

The core purpose of any scientific enterprise is to create wealth out of the knowledge. NCL/CSIR distinguishes itself from academic research laboratories by the fact that it aggressively attempts to link knowledge to applications. I believe that publicly funded research institutions must have a clear focus on creating value through its science and benefiting society at large. Whereas knowledge generation is important and necessary there has to be continuing attention to create utility out of the knowledge an institution generates. NCL/CSIR should be focused not merely on solving a problem, but selling the solution to the relevant stakeholder be it either the society or industry.

However early stage discoveries or innovation are the most difficult to commercialize in view of large technology risks and market uncertainties. Disruptive innovations will require a completely different translational model to convert knowledge to wealth. To facilitate this process a new campus, called, NCL innovation Park has been created. This campus will become home to public-private-partnership initiatives of CSIR. This campus is also home to a Section 25 Not for Profit Company, called Entrepreneurship Development Center (Venture Center).

Venture Center is a Technology Business Incubator created with seed funds and facilities provided by Department of Science and Technology and CSIR with the avowed purpose of facilitating spin offs and promoting S&T driven entrepreneurship. CSIR is also currently in the process of conceiving an Innovation Complex at NCL Campus which is intended as a world-class innovation eco-system. This is proposed to be built using a PPP model that will leverage CSIR strengths to develop and efficiently take new technologies to the market.

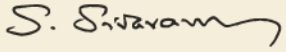
For innovation to assume importance scientists and engineers in NCL must abandon the thinking that their job is to merely create good science and it is somebody else's responsibility to create value out of their science. Our

peer recognition system must equally reward those who create applications of science which is accepted by the market. Young people must be taught that there is an alternative career path than merely doing a PhD, pursuing a post doctoral research in some country abroad and then seek lifelong employment in a large industrial or government institution. Young people must be exposed to opportunities in scientific entrepreneurship and to the thought that they can create employment for others. There is a need to lower the barrier to entrepreneurship and encourage young people to a higher risk career opportunity with a larger pay off to society.

The area in and around NCL is thus emerging as a powerful innovation cluster and will be home to a large number of research and technology professionals as well as young students. I envision CSIR-NCL as an institution with enduring values of excellence devoted to acquisition (research), transmission (teaching) as well as application and exploitation of knowledge (technology).

This will be my last Report as a Director of this magnificent institution. I have enjoyed my stay in this position and have done my best to leave NCL a stronger organization. As I said on July 1, 2002, when I addressed the staff and scientists of NCL, the leadership of this great institution is a trusteeship, which I have been fortunate to receive. I have held it with great care and embellished it with whatever I could. I am now ready to pass this legacy on to the next person who will have the good fortune of leading this laboratory.

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, MISSION, and GUIDING PRINCIPLES & Values

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 programs 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 PRINCIPLE & VALUES

GUIDING PRINCIPLE & VALUES

To be deeply committed to the success of our stakeholders

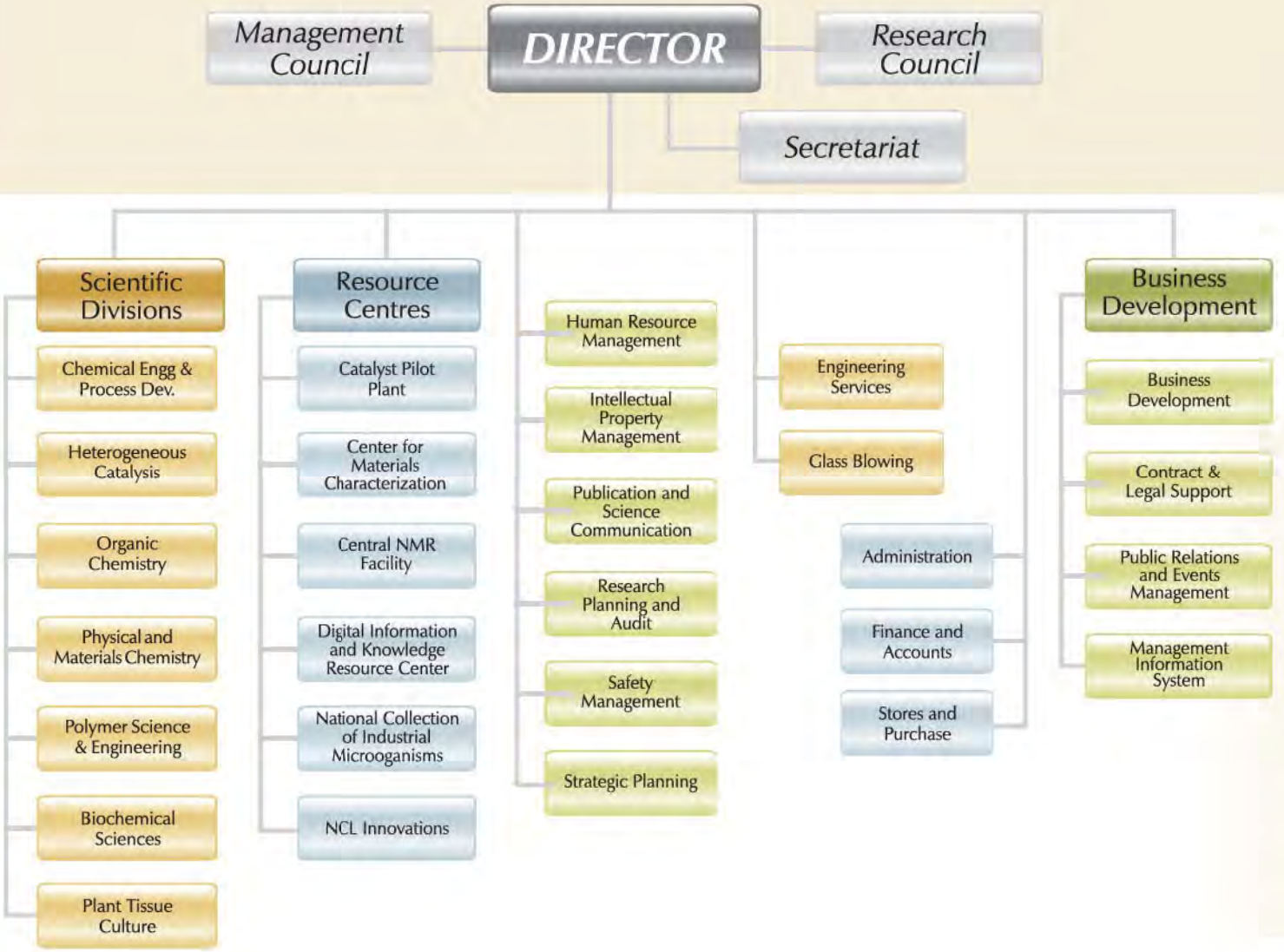
To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency

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

Organization CHART



Research AREAS

Catalysis

- Heterogeneous catalysis
- Homogeneous catalysis

Biochemical Sciences

- Enzymology and microbiology
- Plant molecular biology
- Plant tissue culture

Organic Chemistry

- Synthetic methodologies
- Asymmetric synthesis and organometallics
- Carbohydrate chemistry
- Supramolecular chemistry
- Chemical biology
- Photochemistry

Polymer Science and Engineering

- Polymer chemistry
- Polymer physics
- Complex fluids and polymer engineering

Physical and Materials Chemistry

- Nanomaterials science and technology
- Materials chemistry
- Theory and computational science

Chemical Engineering Science

- Reaction engineering
- Catalysis, Reactors and Separation
- Process simulation and modeling
- Biochemical engineering
- Industrial flow modeling
- Process design and Process development

Knowledge Competencies

- Chemical Biology and Bio-organic Chemistry
- Chemical Engineering Science
- Complex Fluids and Polymer Engineering
- Enzymology and Microbiology
- Heterogeneous Catalysis
- Homogeneous Catalysis
- Industrial Flow Modeling
- Materials Chemistry
- Nanomaterials : Science and Technology
- Organic Chemistry
- Plant Molecular Biology
- Plant Tissue Culture
- Polymer Chemistry and Materials
- Process Design, Development and Engineering
- Theory and Computational Science

Research COUNCIL

Chairman

Prof. D. Balasubramanian

Research Director

L.V. Prasad Eye Institute
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Hyderabad - 500 034.

Members

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Indian Institute of Science
Bangalore - 560 012.

Prof. Dipankar Chatterji
Molecular Biophysics Unit
Indian Institute of Science
Bangalore - 560 012.

Prof. S. K. Sopory
Group Leader
Plant Molecular Biology
International Centre for Genetic
Engineering & Biotechnology
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Dr. Amit Biswas
Senior Vice President (R&T)
Reliance Industries Limited
Swastik Mill Compound
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Dr. Javed Iqbal
Director
Institute of Life Sciences
University of Hyderabad
Gachibowli
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Prof. Rajesh S. Gokhale
(DG's nominee)
Director
Institute of Genomics and Integrative Biology
University Campus
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Delhi - 110 007.

Dr. Naresh Kumar
(Permanent invitee, CSIR)
Head
R&D Planning Division (CSIR)
Anusandhan Bhavan, Rafi Marg
New Delhi - 110 001.

Dr. R. Brakaspathy
(Agency representative, from June 2009)
Sc. G, SERC 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, Pune

Members

- **Dr. B. D. Kulkarni**, Deputy Director, NCL
- **Dr. B. M. Khan**, Scientist, NCL
- **Dr. (Ms.) V. A. Kumar**, Scientist, NCL
- **Mr. G. Prabhakaran**, Scientist, NCL
- **Dr. S. Ponrathnam**, Scientist, NCL
- **Dr. B.L.V. Prasad**, Scientist, NCL
- **Mr. R. P. Purandare**, Technical Officer, NCL
- **Mrs. Mariamma John**, F&AO, NCL

Members

(with effect from 01.01.2010)

- **Dr. Sourav Pal**, Scientist, NCL
- **Dr. Darbha Srinivas**, Scientist, NCL
- **Dr. S. K. Asha**, Scientist, NCL
- **Dr. Nayana Vaval**, Scientist, NCL
- **Dr. Satish Shetye**, Director, NIO, Goa
- **Mr. G. Prabhakaran**, Scientist, NCL
- **Mr D. B. Pradhan**, Technical Officer, NCL

Member Secretary

Mr. B. B. Kasture
Administrative Officer
NCL

The Diamond Jubilee OF National Chemical Laboratory

COMMEMORATION OF NCL *Diamond Jubilee*

National Chemical Laboratory (NCL), Pune, a constituent laboratory of Council of Scientific and Industrial Research (CSIR), New Delhi commemorated its Diamond Jubilee on April 1, 2010 by Dr. Manmohan Singh, Prime Minister of India and the President, CSIR unveiling of the NCL Diamond Jubilee Plaque and by inaugurating and dedicating to the Nation Diamond Jubilee Polymers and Advanced Materials Research Laboratory.

Dr Manmohan Singh also unveiled the Foundation Stone of Indian Institute of Science Education and Research (IISER), Pune. Shri K. Sankaranarayanan, Governor of Maharashtra presided over the function.

Coinciding with the commemoration of Diamond Jubilee of NCL a CSIR exhibition on 'Touching Lives in a Million Forms' was organised on April 2 and 3, 2010. The exhibition which was open to general public was Inaugurated by Prof. Samir Brahmachari, DG - CSIR on the afternoon of April 1, 2010. About one hundred exhibits from NCL, NCL-Innovations, URDIP as well as other CSIR labs, including CSIR HQ were arranged in a pavilion of about 3000 sq ft area at NCL Innovation Park.

The exhibits covered historic perspectives and the journey of sixty years of NCL, its current activities as well as major contributions to basic science, industry and society by CSIR labs, in general, and NCL, in particular. Posters, models, and products were displayed depicting the CSIR achievements in the area of affordable health, affordable housing, provisioning potable water, sustainable energy, empowering farmers, empowering industry, waste to wealth, lead programmes such as CSIR-OSDD, CSIR 800, TKDL, Soleckshaw tricycle, human resource, intellectual property rights, etc. About 3000 visitors including students, teachers, and faculties from various colleges and Universities visited the exhibition.

The curtain raiser of Diamond Jubilee was held on January 3, 2009, when Prof S. K. Brahmachari, DG CSIR addressed the staff and scientists of NCL. During the year 2009-10, NCL was privileged to welcome many distinguished scientists from India and overseas and as well as large number of students as CSIR-NCL organized several workshops seminars and conferences. It was felt that the best way to celebrate sixty years of CSIR-NCL was to enable as many professionals as possible to come to NCL, to share ideas and thoughts and form deep bonds of friendship.

Address by

PANDIT JAWAHARLAL NEHRU

The Honourable Prime Minister

on 3 January 1950

Pandit Jawaharlal Nehru delivering the address.

I was thinking that the Government, over which I have the honour to preside, has done something, I suppose, during the last two, three years or more. It has left undone many things for the cynics who point out our sins of omission and commission, but they have to admit with some justification that in the matter of scientific research the Government has done something. The record might have been greater, but it is substantial. Of course, during the period what has been done is largely to lay the foundation of future work.

The conception of eleven national laboratories all over India, and the National Chemical Laboratory is the seventh in a chain of eleven laboratories, had been planned not by the Government of India but by their predecessors. I think it is rather an exciting conception to see large numbers of young men and women coming into these laboratories and research institutes in India and working with zeal and enthusiasm for the advancement of science in India, and through science, the advancement of the Indian People.

I have wandered about a great deal in this country of ours and I have met innumerable persons. I have seen young people. I think. I am fairly conscious of their feelings. I came to the conclusion long ago that generally speaking, the material that India possesses, the human material, is of the most excellent quality, provided, and there are many provisos and 'buts' about it,-- but I will not go into these at the present moment. But in particular in regard to scientific research, I think there is good material in India, provided they have a chance to advance.

They have not had their chance in the past. Some of our brightest students, who normally ought to have gone into scientific research, have preferred secondary positions in the executive services of Government. Probably they gave them a higher status in the warrant of precedence. So science in the past has certainly not been encouraged, in the sense that neither the man who was able had the chance to do his work properly nor men if he did it, did he get encouragement when it was due. But in practice, I think, I am right in saying that the opportunities have been strictly limited.

Dr. Bhatnagar mentioned the names of industrial leaders of this country who had encouraged science, and he rightly honoured them. While the names of industrial leaders who had encouraged science have been honoured, I think it might be more appropriate to mention the names of industrial leaders who constitute a majority who have discouraged science and not taken any interest in it. I am surprised at the amazing ignorance of some industrial leaders who seemed not to realise the importance of science to industries. They are so extremely narrow-minded that they did not see where the country was going and what would happen to it if they did not shake themselves up and do something about it.

There is talent in our country. But the question is how to tap that talent and give opportunities to the young men and women of India, who had the requisite ability. Somehow the doors seemed to be barred against them, and when it did open it opened only in a limited way and to a limited number of people. So the problem before us, for any kind of progress, is how to tap this vast reservoir of talent and material. For material, money is necessary. So if we have the human beings in this country and if we have the resources and the material, the problem is how to join these two together.

I hope that so far as these laboratories are concerned they would help to some extent at least in opening the doors to large numbers of young men and women and give them opportunities to do good work for the country in the cause of science and in application of science for the public good. Now, I am not at all against the conception of scientists strictly confining themselves to pure research.

It is essential to have their freedom. But in the present day world when we have to face tremendous problems, it is the function of a scientist to a large extent, keeping these problems in view - the major problems - to try to help directly and indirectly by creating an atmosphere of objective and dispassionate consideration of these problems. These problems if not solved will swallow us. I think that the conception of a large number of research institutes and laboratories and the like will help not only to the cause of science but will also help in creating an atmosphere which is perhaps more important for considering the vital problems.

I came to see the National Chemical Laboratory three months ago. I am to some extent guilty together with Dr. Bhatnagar in having rather hurried the process of building the Laboratory.

Many people said it would not be ready so quickly. While certainly I have this in mind that this is a good occasion to have its opening ceremony I have also something else in mind. In a long time past, as well as today, we think a great deal about the bricks and mortar than of human beings. More money is spent when bricks and mortar are put together.

I would like our public buildings stoutly built and be enduring monuments and not to be ugly and not good enough. Nevertheless, I think it is more important that money should be spent on human beings and not on mortar. We should work in temporary sheds instead of waiting for huge stone structures to grow up.
We cannot afford to wait. We must create psychology for work, whatever the disabilities attached to it. We should be able to work with disabilities. This laboratory started functioning as quickly as possible even with disabilities. We must have that psychology and the sense of urgency of work as soon as the slightest opportunity is available.

I should like to express my gratitude not to everybody that has been mentioned by

The Opening of The National Chemical Laboratory

Address by

Dr. MANMOHAN SINGH

The Honourable Prime Minister

on 1 April 2010

I am indeed very happy to be here today to participate in the Diamond Jubilee Celebrations of the pioneering National Chemical Laboratory. Let me begin by extending my greetings and best wishes to the scientists, students and other members of staff of the Laboratory and to all others who have been associated with this premier institution of the Council for Scientific and Industrial Research.

Ladies and Gentlemen, The National Chemical Laboratory is one of the first research laboratories conceived by the Council for Scientific and Industrial Research. It was born of a dream of a nascent nation, awakening to freedom and aspiring to harness the immense potential of science and technology for the benefit of its people. This institution owes its existence to the vision of Pandit Jawaharlal Nehru, who believed that India would need advanced centres of research where the best Indian minds could pursue their passion for science and contribute to building our nation.

Sixty years is a significant milestone in the lifespan of any institution. The National Chemical Laboratory has had a lineage of distinguished leaders who have guided its destiny with great distinction. With this tradition of excellence in scientific research, this laboratory has nurtured some of the best minds in India. Several scientists of this institution have been elected to distinguished academies of sciences, both in India and overseas. The Laboratory made a seminal contribution to the emergence of Indian pesticides industry which was critical to the success of the Green Revolution in our country. Post-1970, the research conducted at the National Chemical Laboratory gave birth to the Indian generic drug industry, a forerunner to the vibrant Indian pharmaceutical industry of today.

More recently, this Laboratory has contributed to the growth of the petrochemicals, polymers and fine chemicals industry. With its world class facilities, it is my hope that the National Chemical Laboratory will sustain this culture of excellence and continue to explore the boundaries of frontier science.

Our country looks up to its premier scientific institutions like the National Chemical Laboratory for finding pragmatic solutions to some of the most vexing problems that confront our society and our development efforts. Our scientific laboratories have to align their priorities even more closely to the national needs. They must contribute to the creation of wealth in our society. They must seek and deliver appropriate solutions which would change the lives of the most vulnerable sections of our people.

It is our scientific capabilities that will determine our ability to overcome challenges which lie ahead in areas such as climate change, clean energy, environment friendly technologies, sound water management, affordable healthcare, food security, and biotechnology.

Our Government has declared 2010-2020 as the "Decade of Innovations". We need to instil the spirit of innovation in our young minds so that they can find solutions in a variety of areas to achieve the goal of inclusive and sustainable development. Innovators must be challenged to produce solutions our society needs.

The solutions must be found in a timely manner, and must then move out of the laboratory quickly and gain wider acceptance. I am happy to learn that an ambitious proposal to establish a CSIR Innovation Complex in this historic campus in a public-private partnership mode is under active consideration.

I am also delighted to participate in the Foundation Stone laying ceremony of the new campus of the Indian Institute of Science Education and Research (IISER), Pune. The charter of this Institute is to create world class institutions for

undergraduate as well as postgraduate education in science with an intellectually alive atmosphere for research. In these institutions, education will be totally integrated with the state-of-the art research. The project is also a reflection of the good coordination between Education and Science & Technology Ministries.

I understand that the IISER Pune has already progressed well in the above dimensions since its inception in the year 2006, with more than 300 undergraduate and Ph.D. students and a young and enthusiastic faculty.

I share the concerns that our bright young men and young women are not taking up science in sufficient numbers after the 10+2 stage. It is important to bring them into the fold of exciting and stimulating research environment of colleges and universities devoted to science education. Our government has undertaken significant expansion of the education system, including science education, at various levels. But, we need to do more.

We need to improve the quality of teaching of science in our schools, focus on faculty development, increase our expenditure on science and technology from the current low level of about 1 % of our GDP, and further strengthen academia-industry interface. Our competitive advantage in the R & D sector maybe lost unless we ensure that the country produces, on a continuing basis an adequate number of competent and motivated young people who could lead our national laboratories, science agencies and knowledge based industries.

The power and status of a nation in the world of today is determined to a large extent by its achievements and capabilities in the field of science and technology. Our scientific laboratories and institutions must assume a leadership role, and take on the challenge to build a new and resurgent India which will be the envy of the world at large.
I hope both the National Chemical Laboratory and the Indian Institute of Science Education and Research will live up to the expectations the people of our country have from them and other such institutions.

Ladies and Gentlemen, Let me end by wishing both the institutions and all those associated with them every success in the years to come. May your path be blessed.

Prime Minister Dr Manmohan Singh unveiling of the NCL Diamond Jubilee Plaque

Prime Minister Dr Manmohan Singh inaugurating and dedicating the Diamond Jubilee Polymers and Advanced Materials Research Laboratory via remote

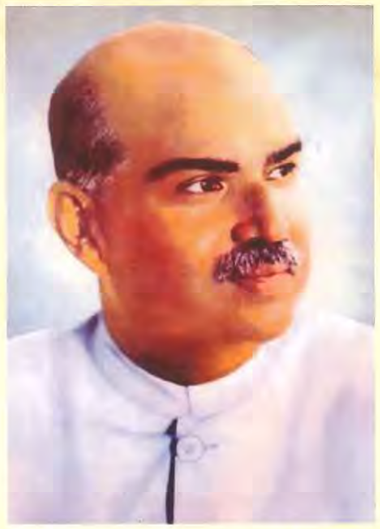
I urge the Indian scientific community to come forward and make the Indian Institute of Science Education Research system a unique brand of academic excellence and help in realizing our dream of making our beloved country the knowledge hub of the world.

Speech by

Dr. S. P. MOOKERJEE

The Hon'ble Minister for Industry and Supply

on 3 January 1950



The formation of the National Chemical Laboratory at Poona is the natural outcome of the two-fold policy followed by the Council of Scientific and Industrial Research. One part of this policy has been to utilise the existing institutions of research for scientific study of problems affecting industrial development. A large number of research schemes has been worked out by selected scholars in different Universities and specialised institutes out of funds made available to them by the Council.

It was nevertheless realised from the inception of the Council that the facilities offered by existing research institutes and Universities, valuable as they are, could not meet the ever-growing needs of a country like India. The other strand of the Council's policy, which was followed simultaneously with the first, was therefore to establish a chain of national laboratories, which, with their resources and equipments, would be able to tackle the vast and growing problems of industrial research. Such national laboratories in other countries have played a unique part in achieving scientific advance and industrial regeneration. The National Chemical Laboratory at Poona is the first of these laboratories to be formally opened in India.

There is enough evidence to show that a high degree of chemical knowledge was acquired by Indians more than 1500 years ago. Ancient India recorded remarkable growth of chemical and medical science in India. While there was a decline in the knowledge of arts and science in India during the middle ages, with the introduction of English education in India, India had again a renaissance of learning. Chemistry has been one of the various subjects in which Indian Universities have made considerable progress.

We recall today with gratitude the unique services rendered in this connection by the late Acharyya Profulla Chandra Ray. Apart from his own personal contributions, he succeeded in creating an Indian School of Chemistry, of which India may well feel proud. He was no visionary, but was essentially a practical man, and it was left to him to inspire the establishment of the first big chemical works in India. Today there over 300 factories scattered throughout India, employing about 60,000 men successfully producing a variety of articles, such as chemicals, drugs, medicines. There are, however, still many gaps in our industrial production which need to he immediately filled both for defence purposes and for the progressive welfare of the people.

The National Chemical Laboratory will thus occupy a definite place in the future development of chemical industries in the country. The main purposes of such a laboratory have been emphasised by experts associated with similar institutions abroad. We have to organise research leading to fundamental reference data of general value. The importance of such data cannot be over-emphasised. We have to develop new methods and techniques of chemistry on which expert groups must remain constantly engaged.

We have to deal with the problems of utilisation and conservation of raw materials, especially those which are indigenous and with concentration of low grade substances. The importance of this aspect of our work in building up our national economy cannot be minimised. There need therefore be no fear of overlapping of activities between our national laboratories on the one hand and Universities and research institutes on the other.

The success of our efforts will depend on our ability to secure the services of competent research workers who will carry on their duties under the guidance and inspiration of senior officers attached to the laboratory. Here, our policy must naturally be to attract the best type of Indians and if necessary, to get them trained by sending them abroad. Where, however, in the interests of efficiency is necessary for us

to recruit foreign experts, we should not hesitate to do so for such limited periods as may be required. Our anxiety is to build up these laboratories in such a manner that we may be able to maintain the highest possible standard, making it unnecessary for our youths to go abroad except for very special purposes. We are fortunate in having as our first Director a scholar and administrator of the eminence of Professor McBain who has already evinced keen enthusiasm in the discharge of his heavy responsibilities. I am sure that under his leadership workers of all grades will be able to give to this institution the best that they can and thus help in creating traditions of service which may be worthily emulated in other institutions.

The establishment of national laboratories of such dimension entails a huge expenditure which is not easy to provide. No Government can, however, ever spend too much on scientific research provided it is well-planned and well coordinated. Government which have been compelled to adopt economy measures in various directions recently have decided to go ahead with its existing schemes for the establishment of national laboratories in different parts of India. Such laboratories, however, must receive generous support from industries themselves, as also from private benefactors. Here is a field of voluntary investment which, although it may not bring an immediate monetary return, is bound to reduce cost of production, develop new processes and ultimately maintain high industrial efficiency.

Our national laboratories will not be run as a Department of Government. They will be given sufficient autonomy and flexibility of administration, so that their activities may not be hampered in any way. I shall be failing in my duty if I do not pay my tribute of admiration for the pioneer work done by Dr. Bhatnagar, our Director, but for whose indefatigable energy and spirit of idealism these laboratories would not have come into existence within such a short period of time.

I can only hope that as our national laboratories come into existence one by one dealing, as they will, with such important departments of activity as Chemistry, Physics, Metallurgy, Fuel Technology, Glass and Ceramics, Leather, they will be able to play a coordinated role in securing that industrial development of our country on which our future progress and prosperity so largely depend.

Speech by

Shri PRITHVIRAJ CHAVAN

Minister of State for S&T (IC)

on 1 April 2010

I am extremely happy to welcome Honorable Prime Minister at the Diamond Jubilee Celebrations of one of our most prestigious public research facilities. NCL, as an oldest and the first constituent lab of the CSIR family, has been a fore-runner in India's scientific march. It has the proven record of leadership in terms of all indicators, quality of science produced, number of publications, number of Ph.D. students, industry interaction, and in technologies successfully transferred to industry.

NCL's history is intimately tied to the history of independence in India. CSIR NCL came into existence in the year 1947, giving shape to the dream of Pandit Jawaharlal Nehru and his belief that science and technology was an important tool for national development. NCL has had unique distinction of having the Prime Ministers of India to grace each of the significant landmarks. And your visit today Sir, is a continuation of that tradition.

Successive leaders of NCL have encouraged a culture of sustained pursuit of excellence in science. NCL Scientists have won several laurels and peer recognition. One of its distinguished former Directors, Dr. Mashelkar has been elected Fellow of the Royal Society and is a foreign member of the US National Academy of Sciences, exclusively based on work done here at NCL.

As many as six individual scientists have been honoured with Padma Awards, twenty five scientists have been elected to the prestigious Indian National Science Academy and fourteen scientists have won Bhatnagar prize. NCL has an excellent record of close co-operation with industry, and it has been responsible for birth of several industries such as pesticides, generic drugs, catalytic processes, plant tissue culture and bio-technology.

Soon after the amendment of Indian Patent Act in 1970, NCL launched the generic pharma industry in India. It is but natural that NCL is held in high esteem by the Indian chemical industry. Alumni from NCL today occupy positions of influence in the Indian chemical industry, many other products and processes that have come out of these labs, have been successfully commercialized by Indian industry, both for domestic consumption and exports.

NCL was the first lab to have recognized the challenges and opportunities of globalization.

Over the years, NCL has successfully transformed and re-invented itself to meet these challenges. Recognizing that the India is sure to become a hub for global R & D and innovation, NCL put in place an IP policy and began partnership with global companies. As a consequence, many global companies have established their own R & D Centres in India, notable among them being GE in Bangalore, Du Pont in Hyderabad and Dow in Pune.

NCL's use of Public Private Partnership model in process and product development during the past decade has resulted in formation of several new industries. NCL's record in technology transfer to industries, is unmatched by any other institution in the country.

The Innovation Park created by NCL in its campus, to support new ideas, joint R & D Centres with industry and a Business Incubator, will promote science and technology based entrepreneurship. NCL has set up a Section 25 company called Venture Centre, as a vehicle to promote an innovation eco-system in and around NCL. NCL also expects to participate in a few mega-projects in the area of solar energy materials, solid state lighting systems, alternate energy resources, clean coal technologies, thereby contributing to finding solutions to some of the complex problems facing in the country today.

CSIR's decision to co-locate the new IISER, within the campus of NCL, by donating hundred acres of land will prove to be a historic decision which will create a world-class science cluster. By the year 2012-13, NCL and IISER together will have together 400 scientists with Ph.D. degrees in Chemistry, Physics, Biology, Mathematics and Chemical Engineering and will have over 1000 students perusing Ph.D. programs. Sir, IISER will remain your great legacy to the nation.

The Prime Minister has given a clarient call to make the decade of 2010-2020 a decade of innovation. NCL and CSIR whom you preside as President, is allied with the fact that publicly funded research organisations must re-invent themselves with changing times. Under the dynamic leadership of Dr. Sivaram, NCL today renewed its commitment to innovation, to focus on delivery, to leapfrog the technology generations and to become a true catalyst for excellence. Your presence here today Sir, will be inspirational for the scientists not only here in Pune, but in the entire CSIR family across the country. And I assure you that the NCL and CSIR will fulfill the expectations that you have set for all of us.

Speech by

Dr. S. S. BHATNAGAR

Director, Council of Scientific and Industrial Research

on 3 January 1950

Your Excellency, Respected Panditji, Ladies and Gentlemen! I am happy and proud that I have today the privilege of speaking to you before our beloved Prime Minister declares open the National Chemical Laboratory of India. The interest which he has evinced in Science is well-known. Here as in other things he sees far horizons and his scientific mind desires that our Country should be equipped to meet the demands of the modern world. His message of inspiration has been that there is no development without effort and effort means work. This is a message which has often inspired me to greater speed of action even when the flesh was unwilling.

When in 1940 I was asked by the then Viceroy, Lord Linlithgow, to take up the post of Scientific Adviser and Director, Scientific and Industrial Research, I was hesitant to leave the peaceful cloisters of learning in my University for the maddening hurry and strife of government work. The request from the Viceroy was, however, a command and the Chancellor of my University told me that no patriotic individual could refuse the call for help in the War effort; as I was expected to make good by the aid of science the shortages of supplies in India and the Middle East resulting from the War.

I was still wondering as to what to do when Sir Ramaswamy Mudaliar cornered me in my den in the Punjab University and urged me to accept this office. He assured me that this temporary activity might ultimately result in big developments for scientific research in this country. His statement convinced me that I must leave the university for a larger field to help in building up India's scientific research, training her young scientists and inspiring her young men to take up research as a career not for monetary gain but for the sake of research itself. In that hour when I decided to take up office, I dreamt of a chain of National Laboratories, of large teams of scientists working for the development of India and the creation of a scientific outlook on life among India's masses. Those who consider that India's ills can he cured by increasing productivity must realise that this can be achieved only by the application of science to its agriculture.

I have struggled through the years to fulfil that dream and it seems that it may now come true. Of the eleven National Laboratories we have been planning, equipping and executing, seven will be opened this year. The remaining four will soon materialise. It is a day of real thanksgiving for me and I feel I must pay my homage of thanks to all those who have helped me to realise my dream.

My thoughts turn to Sir Ramaswamy Mudaliar, the first President of the Board and the Council of Scientific and Industrial Research and to those eminent men who succeeded him. I particularly recall the names of Sir Ardeshir Dalal and Sir Akbar Hydari, now unfortunately no longer with us, our Governor-General, Shri Chakravarty Rajagopalachari, Doctor Syama Prasad Mookerjee and our Nations' Hero, Pandit Jawaharlal Nehru. These great men and their distinguished colleagues, the Members of the Council of Scientific and Industrial Research have given a great deal of their time and thought to these activities. Without their help and guidance I could have accomplished nothing.

The Premier of Bombay, Shri B. G. Kher who zealously espoused my cause when Your Excellency's predecessor took the view that a Chemical Laboratory could not be allowed near the Government House in the salubrious climate of Poona, will be gratefully remembered by the present and future generations of young chemists in India. Nor can I forget Dr.

John Matthai who was Chairman of Planning Committee of the National Chemical Laboratory in its early stages. His modest acquiescence to my caustic remark that there would be no more stinks from the well designed Chemical Laboratory than from the kitchens and sewage system of His Excellency's staff quarters gave me courage and ultimate success in securing this beautiful site. Nor must I forget to mention the help given by Mr. H. M, Patil and the Army Officers in Poona. Without their bulldozers we could not have held this ceremony today.

Industrial development in the United States and in the United Kingdom is largely the result of close co-operation between government, science, technology and industry. The Council of Scientific and Industrial Research is an excellent example of this collaboration. We have a proud record of work. Forty five processes have been evolved and given to industry for development. Some of the processes have produced more wealth than all the money spent on all scientific research in India and will continue to bring prosperity to the country for a long time to come.

The present tension which seems to exist between government and big business men can at best be a passing phase. Such a tension has existed at one time or the other in every country. A well-known quotation from the writings of William H. Vanderbilt about business men in America indicates the struggle that was going on there. "You can't keep business men down. They are very shrewd men. I don't believe that by any legislative enactment or anything else, through any of the States or all the States, you can keep such men down. You can't do it! They will be on top all the time. You see if they are not."

Those interested in Industrial Development would do well to study carefully this great writer. On the other hand our rich business men should remember that a ruthless new technique of making them act has been developed at least in one region which will gain momentum if they do not wake up. It is only the spirit and genius of Mahatma Gandhi and the present Government of India which has so far checked the application of that technique here. When I was in the U. S. A. a few months ago, a big business man asked me as to why the Indian Government is so hard on Indian industrialists. "Let them enjoy themselves as long as they live, he said. You may fleece them when they die by imposing heavy death-duties.

" I replied that I would recommend this proposal provided that the American questioner guaranteed that the capitalists would not refuse to die if the death-duties were exorbitant. Before we resort to anything else Indian industrialists should be allowed all that they require to help in India's development but they should realise the world trends and difficulties which face the government. Applied scientists want industries to flourish as without industrial problems to solve they feel frustrated.

One of the most important functions of the National Chemical Laboratory will be to bridge the gulf between science and its application. It will be the link between the universities and other scientific institutes in the country and industry. It will work out ways and means for the application of scientific knowledge to practical problems of human welfare.

The road from a scientific discovery to its successful industrial application is long and difficult. Developmental work involves work by team of scientists of high quality and originality and requires expenditure of money which at the outset may seem unproductive. National Chemical Laboratories are being equipped and organized to meet the need for such developmental work.

The laboratory will try to improve old processes in the light of new scientific knowledge and to discover new processes. The development of new processes will be carried to the pilot plant stage in the laboratory. This is what we have not had in India with the result that many processes have gone by the way, for it is only when a process has been taken to the pilot plant stage that industry gets interested in adopting it for large scale production.

After a successful process has been passed on to industry, the National Chemical Laboratory will continue to keep in touch with the industry, and difficulties or problems that may arise in the large scale manufacture of the product will be studied and solved in the laboratory. In addition to the processes developed in the National Chemical Laboratories, other problems of industry which fall within the scope of the laboratory will be taken up. The scientists of the laboratory will on their own initiative investigate India's raw materials and technological processes to help industrialization. In short the National Laboratory will be a living and vital link with the universities, scientific institutes and industry.

The problems of industry are seldom such as to fall within the narrow groove represented by a particular branch of chemistry. Usually for the successful solution of problems the co-operation of experts from different fields of Science is necessary.

The National Chemical Laboratory will, therefore, embrace not only chemistry, but also physics, mineralogy, engineering and biology in so far as they relate to chemical problems and chemical utilization of national resources. Without provision for such a wide scope, the laboratory might become sterile.

The scope of industrial applications of chemistry is vast. There is hardly any industrial product, raw material or process in which chemistry does not play a part. The National Chemical Laboratory with a view to equipping itself for its work will have seven divisions:

- Division of Inorganic Chemistry including Analytical Chemistry
- Division of Physical Chemistry including Electro-chemistry
- Division of Chemistry of Plastics and High Polymers
- Division of Organic Chemistry
- Division of Bio-chemistry including Biological Evaluation
- Division of Chemical Engineering
- Division of Survey and Information

Another principal object of this laboratory will be to undertake fundamental research. This research will be undertaken for its own sake to extend the frontiers of knowledge in directions likely to prove useful to human progress. Fundamental research has always had a stimulating influence upon research workers and has attracted to the laboratory men who work for ideals and whose motto is "It is better to have wisdom than gold."

To carry out research it is necessary to have suitable buildings for laboratories, up-to-date equipment and a good team of scientists. It is too much to hope that atomic weights could now be determined accurately with the aid of apothecaries balances or in shaky and dusty buildings. Modern research requires modem buildings.

The building is 640 ft. long and 200 ft. wide and has over 150 rooms. It has a basement, a ground, a first and a possible second floor with an auditorium, library, seminars and sectional laboratories. It also has rooms for laboratories for applied processes. The seven sections which I had mentioned earlier will all be fitted into the places which have been specially built for them. The structure of the building is such that the size of the rooms can be altered at will.

A feature of interest is that the basement is a dug out tunnel from which the service mains for water, gas, electricity and steam have been worked up vertically. This provides an efficient distribution of services with the minimum of expenditure. The basement which is dug out from the rock is a boon to workers in physical chemistry and it has many other uses which the distinguished Director of the laboratory wishes fully to make use of. The necessary equipment required for the various sections is being acquired and some of the sections have already started work.

A laboratory can only work well if it has a Director who is a leader in thought and action. We have been fortunate in securing as the first Director of the National Chemical Laboratory, Prof. James William McBain, F.R.S., who is well known the world over as a distinguished physical chemist. He has been Vice-President of the Faraday Society, Chairman of Colloid Division, American Chemical Society and was elected Fellow of the Royal Society in 1923. No description of him will he complete without a mention of Mrs. McBain. As Miss Mary Laing she distinguished herself in chemical research.

We have secured in appointing Dr. McBain two distinguished chemists for one salary. Dr. McBain and I selected Dr. Truttwin, a distinguished Swedish Chemical Engineer for help in giving a real push to this important but much neglected subject. He has already joined us. Two more foreigners will assist the Director in his task. We have appointed a large number of our countrymen who have distinguished themselves in chemistry.

We arc hoping to secure the services of an eminent Indian Chemist for Organic Chemistry. We have on the staff Dr. S. Siddiqui and Dr. M. Damodran who are internationally known in chemical circles. A General and his officers make an army. A Director and his colleagues make a laboratory. This team of workers at the National Chemical Laboratory is a strong one and I am sure that it will do its best to help our industries and train our chemists in research.

In planning and execution of the construction work I had the assistance of a Local Planning Committee whose hard work deserves special mention. Principal D. G. Karve, Chairman of this Committee, has helped us greatly. Dr. B. D. Laroia has done good work in building up this laboratory. But for his help and able assistance we could not have had this building ready so early. I must not omit to mention Dr. Bashir Ahmad who originally assisted me in the planning of the laboratory.

The Architects, Messrs. Master, Sathe and Bhuta of Bombay have rendered great help in planning the beautiful and useful buildings and so have the two young architects of the Council of Scientific and Industrial Research, Messrs. Kanvinde and Shaukat Rai, Messrs. Gannon Dunkerley and Co., Ltd. of Bombay and their staff, particularly Mr. Engineer, have rendered great assistance in constructing the laboratories.

There was a time we had trouble with them over the speed of work - there is trouble in the best of families but with good-will on both sides these troubles were overcome and during the past few months, the contractors and the staff have been working willingly night and day to get the buildings ready. As soon as the work of construction is completed and it may take three to four months now, the Council of Scientific and Industrial Research should appreciate their services in a more tangible way. I must not forget to thank the Dorabji Tata Trust for their munificent donation of Rs. 8.3 Lakhs for the establishment of the National Chemical Laboratory and with this I must connect the names of Mr. J. R. D. Tata and the late Sir Ardeshir Dalal. I hope that other industrialists will follow this lead and give generous donations for our National Laboratories. Sir Ardeshir Dalal's untimely demise is a great sorrow to me for he would otherwise have been here today to see the opening of the laboratory with which he was so closely associated. He was present when the foundation-stone of the laboratory was laid and I know how happy his soul in heaven would be today to see this ceremony performed by the Prime Minister.

We owe a debt of gratitude to Dr. Jivraj Mehta for the help he has rendered. It was through him that we were able to obtain quickly the electricity required for the laboratory and have the road joining the laboratory with Ganeshkhind Road built.

The question of having the Opening Ceremony of the National Chemical Laboratory was discussed by the Minister- in-Charge of the Council of Scientific and Industrial Research: both Dr McBain and I felt that if the ceremony as postponed for a few months, we would give the public a display and spit and polish which ostentation desires. Panditji, however, felt and he is right that since some of the sections of the laboratory had already started work, it would be appropriate to have the Opening Ceremony when the Indian Science Congress was in session and the cream of Indian and Foreign scientists as well as all our young university men are available without any extra expenditure.

The ceremony has indeed been fixed on an auspicious day for we have on this day amongst us the greatest Indian and Foreign scientists to give us their blessings and good wishes. ceremony has indeed been fixed on an auspicious day for we have on this day amongst us the greatest Indian and Foreign scientists to give us their blessings and good wishes.

We are fortunate to have in our midst today the greatest living chemist of the world, Sir Robert Robinson, who is now the President of the Royal Society. He is accompanied by his wife, Lady Robinson, who is also a very distinguished chemist, it is said that whichever laboratory Sir Robert Robinson has visited has become a seat of productive chemistry. As this honour is going to be shared by the National Chemical Laboratory of India in company of Lady Robinson, may I venture to say that this laboratory so honoured will become a veritable home of chemistry!!

There are also with us great scientists from abroad well-known to all of us Prof. Desmond Bernal, Prof. and Madame Curie-Joliot, Prof. Herman Mark, Dr. E. W. Condon, of the Bureau of Standards, U.S.A., Prof. P. Auger of UNESCO, Chancellor Arthur Holly Compton, celebrated for his work on X-rays and nuclear physics and Mrs. Compton, Prof. O. E. H. Rydbeck, Dr. S. Trone, the well-known planner, and his distinguished wife Mrs. Trone who plans the planner.

I would ask of all the scientists gathered today both my own Indian colleagues and my foreign brothers their blessings for the new created National Chemical Laboratory of India. I would request the Governor of Bombay and our beloved Prime Minister to give it their blessings and I would ask all the young scientists and workers who are gathered here today to help the laboratory in their work in whatever manner they can. I am sure that with the blessings of our elders and the efforts of our younger generation of scientists, the National Chemical Laboratory will be able to perform the work for which it is being built and to help in the rapid development of our industries and to train research workers in specialized fields of chemistry and technology.

Speech by

Prof. S. K. BRAHMACHARI

Director General, Council of Scientific and Industrial Research

on 1 April 2010

Today on the occasion of Diamond Jubilee Celebrations of National Chemical Laboratory, Sir, we are honoured to have you amongst us. It is my singular privilege to welcome you to this iconic laboratory of CSIR- the place of many a path-breaking scientific accomplishments. Dr. Shanti Swarup Bhatnagar - the Founder Director of CSIR, and Dr. J.W. McBain, the first Director of NCL would have been proud of what NCL has achieved and symbolizes today.

I have always been struck by the vision of Pandit Jawaharlal Nehru, who, even in the early days of India's Independence, put his faith in national development using scientific and technological route and it was this faith that led to the inauguration of NCL at his hands in 1950.
It is testimony to the expectations of - the then, a new nation and also to its commitment with respect to Science and Technology. Today, while celebrating 60 glorious years of NCL, I am reminded of what Pandit Nehru once said. "Time is not measured by passing of years but by what one does, what one feels, and what one achieves". Sixty years down the road, I feel proud, as DG-CSIR, to say that NCL has more than fulfilled our nation's expectations.

NCL's milestones of progress stand out brightly. The decades spanning the 50s to the 70s were dedicated to Self-Reliance. NCL technologies laid the foundation of the Pesticide Industry; formed the backbone of the Bulk Chemicals Industry and laid the base of the Polymer Industry in India.

Sir, Government policy is ingrained in enabling Scientists to deliver for the nation. In the 70s, the government took a decision that allowed process patent over products patents for drugs in India. CSIR Institutes led by NCL, Indian Institute of Chemical Technology and Central Drug Research Institute wrote luminous chapters in the history of generic drug development.

Today India is globally recognized for generic drugs which deliver affordable health to all.

This step not only laid a new paradigm of working on innovative, efficient and economic manufacturing technologies but gave our country a leadership position. I am tempted to say, to quote Sir William Bragg, "The important thing in science is not so much to obtain new facts or procedures or products as to discover new ways of thinking or working about them." It was this approach that enabled NCL to break that glass ceiling and consequentially the monopoly of multi-national cartels in catalysts production and supply.

NCL of today has envious leadership position. It enjoys enormous credibility and goodwill. It is the nation's knowledge storehouse in clean-coal technology, agrochemicals, specialty chemicals, organic synthesis and polymer chemistry & membranes. For NCL, excellence is not a skill, but an attitude, and we in CSIR are proud of that attitude.

In keeping with CSIR's tradition of anticipating the future and preparing for it, in December 2006, Dr. Sivaram and I, as Director, IGIB designed the futuristic NCL-IGIB Joint Research Initiative; interfacing Chemistry with Biology with the support of the then DG, CSIR, Dr. R. A. Mashelkar. Today, it is a model programme in the CSIR system. NCL has also embarked on the development of fuel cell technology and is a key player in CSIR's Solar Mission Project.

Under the proactive leadership of our Hon'ble Minister and your astute guidance Sir, CSIR is taking giant strides towards fulfilling your vision. We are putting in our best efforts to deliver a new CSIR. NCL has already become the first CSIR laboratory to have spin-off companies in this new CSIR venture.
On the occasion of the Diamond Jubilee of NCL, I wish NCL the every best to undertake its journey towards its Platinum Jubilee and to put India in a leadership position in Green Chemistry, Solar Energy research and at the interface of Chemistry and Biology.

While concluding, I am privileged to quote from one of your speeches, wherein you have said, I quote, "My top most priority is to deal with India's massive social and economic problems, so that chronic poverty, ignorance and disease can be conquered in a reasonably short period of time." 'Unquote'. Sir, CSIR of today knows that route to solve these problems is through appropriate applications of science and technology - and we in CSIR are fully committed to live with and deliver your expectations.
Hon'ble Prime Minister, Sir, I thank you once again, for being present here today. Your presence symbolizes the government's commitment towards Science. We are proud to have you as President of CSIR.

Speech by

Prof. JAMES W. McBAIN

Director, NCL

on 3 January 1950

On this important and auspicious occasion we are gathered here to dedicate the National Chemical Laboratory of India. The Prime Minister himself, who is President of the Council of Scientific and Industrial Research and the Minister for Industry and Supply, who is Vice President, and the Director of Scientific and Industrial Research, with His Excellency the Governor of Bombay have each taken part in this official opening ceremony. Scientists, industrialists and students of civilization throughout the world are interested in this event and its significance.

The National Chemical Laboratory, like the others of the chain of laboratories sponsored by the Council of Scientific and Industrial Research, owes its existence to the vision of Sir Shanti Swarup Bhatnagar and the unfailing support of our beloved Prime Minister, President of the Council, the Hon'ble S. P. Mookerjee. Vice President of the Council and especially of Dr. Bhatnagar himself. At Poona. Dr. B. D. Laroia has given untiring and devoted services to the construction of the Laboratory.

The present years are a turning point in history, when India is undergoing a conscious revolution or evolution, and is about to resume, after long centuries, her ancient place of influence in the affairs of mankind.

The other distinguished speakers present have addressed themselves eloquently and impressively to the Dedication of this your National Laboratory which is designed to play a key role in the development of the Nation. However, I, as the Director of the Laboratory must avail myself of this ceremonial occasion to dedicate myself to your service, not only myself, but the whole personnel that is to have the privilege of serving in this great institution. Your Laboratory can only achieve its purpose through the quality and devotion of its personnel. Equally important is your co-operation. Without your sympathetic and active Co-operation. some of the main purposes of the laboratory cannot be fulfilled.

We need the close co-operation of industry, the understanding support of the public, and the constant inspiration to be derived from close contact with the Universities, with the research institutes, and with the many other Government Laboratories. We have in the creation of this Laboratory, tangible evidence of the far seeing aims and hopes of India, that have gone into the careful planning and building of these splendid laboratories. The House of Tatas demonstrated their keen interest in this laboratory by the munificent donation which they made towards its inception.

India is using her newly won freedom to turn to science for the amelioration of the conditions of life of her people, and to participate in the progress of Western civilization. Here I would at once emphasize that science and applied science need introduce no conflict with the highest spiritual and ethical traditions of humanity, but must be integrated with them.

We shall examine what science has to offer, and stress the qualities of character and ideals that must be maintained if science itself is to succeed in its own field. Righteousness exalteth a nation; and science is very exacting of its disciples. Recently, Dr. Condon, one of the many distinguished foreign guests here present, wrote, "Society is at this moment at the threshold of an undreamed mastery of our natural environment, for science, which provides that mastery, is in its golden age."

No nation dare neglect to avail itself of this power of modifying and controlling its environment and material well being. However, one must be on guard to prevent its abuse for unworthy or narrowly selfish aims.

Science must be directed to the common good. Likewise its distinctive ideals must be accepted and adopted and become a part of the national consciousness.
Applied science can and does produce unparalleled wealth, but the fact must be faced that modern scientific research is costly and requires a big investment, although it repays that investment many fold. During 1948 the industrial corporations in the United States alone spent three quarters of a billion dollars for research, approximately 375 crores for that one year alone, and yet it pays. The investment is great but the rewards are far greater.

The most prosperous corporations in the United States are the chemical industries, and I desire especially to see in India a great and profitable chemical industry, with many firms supplying and utilizing basic chemicals, fine chemicals, synthetic chemicals of all kinds, and in particular, those directly useful in medicine, public health and agriculture. These afford the basis of almost all other industrial enterprises.

It is of great pertinent interest to note that several of the foremost chemical corporations of the present time began, within the present generation, with almost no capital. This can be done here. The opportunity, and the need, are both here with us today.

Science is the most creative new development of the modern world. Its potentialities are great, provided that man is rational and activated by good will. Science offers material comforts for all; adequate and well balanced food for every living being; proper shelter and clothing for every man, woman, and child in the world; and the abolition of most diseases although all these gains would merely supply the material foundation for a civilization.

These are tremendous objectives; and what can anyone of us do to achieve them? At the very least each scientist is like a coral insect, contributing some small permanent residue, which goes to make up the coral reef, and finally a large island. During World War I, there was created at Shawinigan Falls in Canada. a collosal plant utilizing enormous water power comparable with that which is obtained from Niagara Falls. From coal and lime-stone they managed to produce on a vast scale, substances like acetone, acetic acid, and alcohol, valuable for innumerable other products and uses. Their proud boast was that these great achievements were entirely the co-operative work of a group of men who were just ordinary chemists. Thus, trained men of science can accomplish these great results. However, the flashes of genius and inspiration have to come from the individual. Even so, it is rare for any discovery to be entirely the work of any one individual. Most great advances are co-operative, usually there are international; and without free international exchange of ideas, progress is limited.

In Science there is room for the most varied types of men, provided that they are devoted to the service of truth. This devotion to truth is the essential of science. It must not be deflected by any other consideration A scientist must have the character to recognize truth no matter how unwelcome it may be to his theories or preconceptions or emotions or self interest. He must always be ready to put ideas to actual critical test, and be ready to learn from the result. We must take to heart the candid and pregnant words of Faraday, who was one of the most successful experimenters and profound thinkers whom Chemistry and Physics has known:

"The world little knows how many of the thoughts and theories that have passed through the mind of a scientific investigator have been crushed into silence and secrecy by his own severe criticism and adverse examination, that in the most successful instances not one tenth of the suggestions, the hopes, the wishes, the preliminary conclusions, have been realized."
Kettering, the outstanding inventor of General Motors Corporation has publicly confessed that in 99 out of 100 cases he has found himself wrong. Kenneth Mees, the great research Director of the Eastman Kodak Company acknowledges that most of the highly successful and lucrative operations of that big corporation arose from ideas in his research group that he did not think were practical.

Science for the most part is so incredibly new; - it is within the memory of older men now living, and of men they knew in their youth, that nearly all advances in medicine and surgery of the last two thousand years were actually accomplished: for example, anesthetics, antiseptics, and all the rest. Of course, a minor portion of science, according to Bernal, another of the distinguished foreign scientists here present, that comprises about one third of our known techniques, is not new at all, but for the most part antedates history, such as the arts and crafts of weaving, dyeing, clay working, and other basic operations. However, the systematic pursuit of science is new, and each of these techniques is now in rapid development.

One of the requirements of modern science, equal in importance to that of co-operation, is the use of refined measurements. Their value is so great that I should like to stress what has been pointed out before; that the laboratory that buys a refined scientific instruments is purchasing the thought and skill of all the preceding investigators who made the instrument possible, and of the mechanics that brought it into being; thus involving and bringing to hear a great quantity and variety of skill and labour. Such weapons are clearly essential in scientific laboratories; it is obvious that they will always be expensive, and that there will never be finality in the ease of any single instrument; each will be

improved as knowledge advances. This is an added argument for liberal endowments for equipment and materials.

It seems clear to me that there must be in this country somewhere at least one of each of the most advanced scientific instruments, together with scientists trained in its use; and furthermore, scientists who are willing to use it not only for their own purposes, but equally for the projects of others. Again, you will note one of the ethical principles inculcated by science; namely, loyalty to truth and willingness to sacrifice everything to its discovery. Is this not one aspect of Mahatma Gandhi's satyagraha? For success in co-operative science and in applied science, loyalty is a requisite; loyalty to the pursuit and unswerving recognition of truth, loyalty to the complete honesty of work, loyalty to one's group loyalty to one's firm or company, loyalty to one's country, and above all, loyalty to humanity which transcends the lesser loyalties.

These loyalties must be mutual, from the leader towards his group, and from the industrialist towards the community of his operators. These are the great objectives of science and the inspiring thought is that they are capable of attainment. Now in practice one begins with patient labour in the laboratory, recognizing that there is no such thing as an insignificant fact, every actual fact having its importance. In the study and library one must bring to bear the boldest flights of creative imagination, always turning to the touchstone of truth and experimental verification and discovery. Thus, slowly there is built up a process of substantial value. All sorts of difficulties have to be overcome in the pilot plant stage. This takes time and much effort, resource and perseverance. Then a result on the industrial scale can be established.

Fortunately, besides these long range enterprises there are many short range ones where a worthwhile goal may be quickly attained; a process may be cheapened, or improved, or a more valuable product may be made.
Any one individual can do only so much, but the results are cumulative, and the achievement of the group can be impressive. The individual can take comfort in the thought that even if his actual contribution is soon forgotten, any service, however small, is eternal in the mind of God.
The most nearly permanent monument any man can erect, is to have influenced directly or indirectly the growth of improved ideas and traditions among the men in the street, in the factory, or on the farm.

Turning now to this actual Laboratory and to the laboratories in Delhi which it succeeds, these incomplete buildings have been in actual use for 8 months and the whole division of Biochemistry has been operating under the able guidance of Dr. M. Damodaran and getting results in spite of obvious handicaps. Side by side valuable results have been obtained in securing improved varnishes and other coatings from the natural products and vegetable oils of India.

In the Council laboratories in Delhi during the last decade, under the direction of Dr. S. S. Bhatnagar and Dr. Siddiqui, there are many substantial achievements to record such as the highly lucrative improvements in lubricating oils using vegetable blends, jettison tanks and unburstible containers, a new anti-gas cloth, jute containers, uses for Bhilawan oil in plastics and enamels, antioxidants for and from vegetable products and recently a very successful printing ink. Dr. J. S. Aggarwal is responsible for the study of Indian resources in vegetable oils.

A few months ago, the American Secretary of the interior, Krug stated 'Each nation or at best each region of the world is and probably will continue to be dependent upon its own resources for basic foods, fuels and energy. World trade in most instances can merely supplement local supplies and economics are always weighted against materials and goods which must be imported'. Therefore, the National Chemical Laboratory must not only apply existing knowledge to the utilization and benefication of Indian natural resources but it must also produce its own share of pure fundamental science.

India must not only copy and adapt what is known elsewhere but it must make fundamental advances of its own in order to take its proper place amongst the nations.

You and we, have this day dedicated a National Laboratory and its Staff, and its Sponsors, with the assurance that its work will grow and serve this country and the world and continue for the generations to come.

It is with these high hopes that we have dedicated the National Chemical Laboratory of India.

Speech by

Dr. S. Sivaram

Director, NCL

on 1 April 2010

Dr Manmohan Singh, Honourable Prime Minister of India, His Excellency the Governor of Maharashtra, Shri Sankaranarayanan, Shri Prithviraj Chavan, Union Minister of State (Independent Charge), Ministry of Science and Technology, Smt Purandeswari, Union Minister of State for Human Resource Development, Professor S.K.Brahmachari, Secretary to the Government of India and Director General CSIR, Professor Ganesh, Director, IISER, honoured invitees, staff and students of NCL and IISER, Ladies and Gentlemen:

It is my unique honour and privilege to welcome our Prime Minister and the dignitaries on the dais to NCL at this historic auditorium. Sir , you are the fourth Prime Minister of India to step into the hallowed portals of this institution and the third Prime Minister to address the staff and students of NCL from this very auditorium. Every major anniversary of NCL has been marked by the visit of the Prime Minister. Our Silver Jubilee was graced by Mrs Indira Gandhi and the Golden Jubilee by Shri Atal Bihari Vajpayee. By your presence here, we have continued this great tradition. We are immensely grateful to you beyond words!

CSIR- NCL was born out of the enduring vision of Pandit Jawaharlal Nehru, the architect of modern India and was an expression to his extraordinary foresight. This magnificent building dedicated to the nation by Pandit Nehru on January 3, 1950 is the earliest edifice of science and technology in independent India that our Founding Fathers felt necessary to take our country into the league of advanced nations.

As our Republic celebrates its sixtieth anniversary, so are we. The history and growth of NCL has been inextricably linked to the growth and progress of our nation. We are proud of our legacy, the culture of scientific excellence that pervades every corner of this Laboratory through successive generations of many men and women who have toiled here for the good of the people.

As we rejoice in our past, we are conscious of the great expectations that this country has from us. On this solemn occasion we rededicate ourselves to the task of building India of the future. We once again redeem the pledge that was taken in this very building sixty years ago; which is aptly captured in the words of the founder of our Republic at the midnight hour on August 15, 1947 and I quote, "the future is not one of ease or resting, but of incessant striving, so that we might fulfill the pledges that we have so often taken and the one we shall take today.

The service of India means the service to the millions who suffer. It means the ending of poverty and ignorance and disease and inequality of opportunity".

Conferences/ Workshops/ Symposia Organized

Symposium on Advances in Chemical Engineering and Process Technology

The symposium, aimed at exploring recent developments and trends in chemical engineering science and process technology was held on June 4-6, 2009. About 150 participants attended the symposium.

The symposium was inaugurated with the key note address by Prof James Katzer of the University of Iowa, Ames, USA.

There was a special session on "Directions in Chemical Engineering, Education and Research and Industry" highlighting the need for reforms in chemical engineering education and research to meet the challenges of the evolving role of chemical engineering in technologies of future. Eminent researchers from within the country and abroad delivered lectures spanning over 15 scientific sessions spread over three days.

Workshop on Nanotechnology and Advanced Functional Materials

The International Workshop on Nanotechnology and Advanced Functional

Materials was inaugurated at the hands of Prof. C. N. R. Rao, Director, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, Scientific Advisor to the Prime Minister and Chairman Nano Mission, DST, New Delhi.

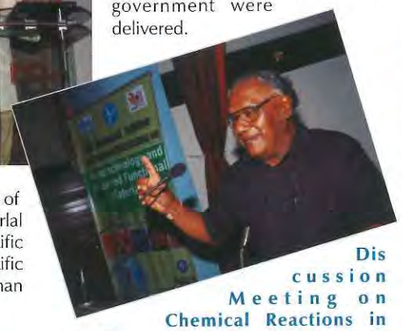
The workshop, held from 9-11 July 2009, highlighted the areas of nanotechnology and functional materials. The lectures covered a broad range of multidisciplinary activities encompassing a range of size, shape and functionalities from nano to macro scale. The workshop was attended by more than 350 participants including ten from industries, five each from USA and S. Korea, one each from Singapore and Australia, and about forty students from NCL.

The workshop was organised jointly with Materials Research Society of India (MRSI, Pune Chapter), and the Indian Institute of Science and Education Research (IISER, Pune). Prof. Paul Weiss, Pennsylvania State University, Prof. Anupam Madhukar, University of Southern California, Prof. Ajay Sood, IISc, Bangalore, Prof. Nitin Padture, Ohio State University, Prof. Haiwon Lee and Prof. Han of Hanyang University, Korea, Dr. Supratik Guha, Head Photovoltaics Division, IBM, USA, Prof. DD Sarma, IISc, Bangalore, Dr. Rajeswaran of Moser Bear, New Delhi, etc. delivered the plenary talks. There were 15 oral presentations and about 200 poster presentations in two sessions.

Symposium on Leveraging Digital Information for Research Productivity

A one-day symposium was organized on 26 August 2009 to deliberate the current status of digital information and its relevance to research.

It attended by more than 125 people. Plenary talks on libraries in digital era and e-governance in government were delivered.



Discussion Meeting on Chemical Reactions in Unusual Media

A discussion meeting was organized on 8-9 October 2009 with an aim to create a platform for exchanging ideas and fostering interdisciplinary collaborations dealing with chemical processes in unusual solvent media.

The main areas of focus for the discussion meeting were: modelling studies for water and aqueous solutions as reaction media, stimulation studies and applications of ionic liquids and their binary mixtures, and development and optimization of supercritical media.

A total number of Sixty five participants attended the meeting. The session began with a keynote talk on chemical reactions in supercritical fluids by Prof. Giridhar Madras, IISc, Bangalore.

NCL - University of Gottingen, Germany Workshop on Catalysis

A two-day Indo-German joint workshop on the Emerging Areas of the Catalysis was held during November 16 - 17, 2009. The University of Göttingen team comprising five members was lead by Prof. Ulf Diederichsen. About twenty five participants attended the workshop.

INSA Platinum Jubilee Symposium on Research in Molecular Medicine Based on Natural Resources and Traditional Knowledge

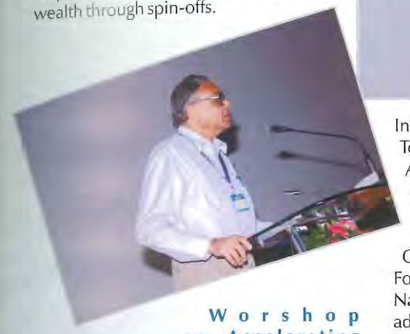
The INSA Platinum Jubilee meeting was organized on November 21-23, 2009. About 225 participants attended the symposium. Key speakers included: Prof. M. Vijayan, President, Indian National Science, Dr. R. A. Mashelkar, CSIR Bhatnagar Fellow, Dr. Samir Bhattacharya, Visva-Bharati University, Prof. John Yu, Academia Sinica, Taipei, Taiwan, and Prof. Asis Datta, NIPGR, New Delhi

RSC-CSIR Chemical Sciences Innovation Symposium

The symposium was organized on 30 November 2009 with the objective showcasing the best practices from UK and India in commercializing scientific

research, supporting academia-industry links and promoting innovation in the chemical sciences.

Prof Graham Richards, Dept of Chemistry, Oxford University gave an illuminating lecture on the experience of the Oxford University Chemistry Department in converting science into wealth through spin-offs.



Workshop on Accelerating Innovation Strategies for Collaboration and Commercia-lization by University of Toronto and NCL

A Joint Indo-Canadian workshop on Accelerating Innovation Strategies for Collaboration and Commercialization was held on December 10, 2009.

The Canadian team comprising eight members was lead by Dr. Lorna Jean Edmonds, Assistant Vice President, International Relations, University of Toronto participated.

About thirty participants attended the workshop. Prof. Cynthia Goh, Professor, Department of Chemistry and Associate Director, Institute for Optical Sciences, UoT and Co-Founder of Alexa Inc. and Vive Nano Inc. delivered the keynote address on "Creating innovators in science: Techno-preneurship" :

50th Annual Conference of Association of Microbiologists of India

The Annual Conference of Association of Microbiologists of India was hosted by NCL from December 15-18, 2009. The theme of this year's conference was Third Golden Era of Microbiology. Prof. Samir Brahmachari, Director General of Council of Scientific and Industrial Research and Secretary, Department of Scientific and Industrial Research gave an inaugural keynote talk "Looking at microbes for thirty years through the eyes of a physical chemist".

The scientific programme of the conference spread over three days addressed important problems such as microbial drug resistance, pollution, energy crisis, bioterrorism, etc. through five special sessions and nine parallel sessions.

Various aspects of basic and applied microbiology were discussed besides special sessions as frontiers of microbiology, space microbiology, molecular biology and microbial ecology.

An industry-academia interactive discussion forum was also organised.

The meeting was attended by more than 1000 delegates from all over India and also from countries such as UK, USA, Sweden and Germany.

Special Lectures Organized

22 May 2009
Prof. B.D.Tilak Memorial Lecture on 'Energy R&D For Rural Development' by Dr. Anil K. Rajvanshi, Director, Nimbkar Agricultural Research Institute (NARI), Phaltan

4 June 2009
Prof. L.K. Doraiswamy Lecture in Chemical Engineering on 'Liquid Transportation Fuel Options' by Dr. James R. Katzer, Department of Chemical and Biological Engineering, Iowa State University, USA

9 July 2009
Prof. J. W. McBain Memorial Lecture on 'Designing, Measuring and Controlling Molecular and Supramolecular Scale Properties for Molecular Devices' by Prof. Paul S. Weiss, Distinguished Professor of Chemistry and Physics, The Pennsylvania State University, USA

24 July 2009
NCL Diamond Jubilee Lecture on 'Science and Technology of Fast Breeder Reactor Programme in India Challenges and Achievements' by Dr. Baldev Raj, Director, Indira Gandhi Centre for Atomic Research, Kalpakkam

13 Aug 2009
Prof. K. Venkataraman Memorial Lecture on "A challenge for Total Synthesis Atom Economy" by Prof. Barry M. Trost, Job and Gertrud Tamaki Professor of Chemistry, Stanford University, USA

26 Aug 2009
NCL Diamond Jubilee Lecture on 'Research and Higher Education - Indian Challenges' by Prof. P. Balaram, Director, Indian Institute of Science, Bangalore

25 Sept 2009
CSIR Foundation Day Lecture 2009 on 'The Greatest Puzzle of Classical Physics The continuing challenge of turbulent flows' by Prof. R. Narasimha, Chairman, Engineering Mechanics Unit, JNCASR, Bangalore

4 Jan 2010
NCL Foundation Day Lecture on 'Adventures in Molecular Recognition Dynamic Combinatorial Chemistry and Supramolecular Nanotubes' by Prof. Jeremy Vice Chancellor and Head, School of Physical Sciences, University of Cambridge, UK

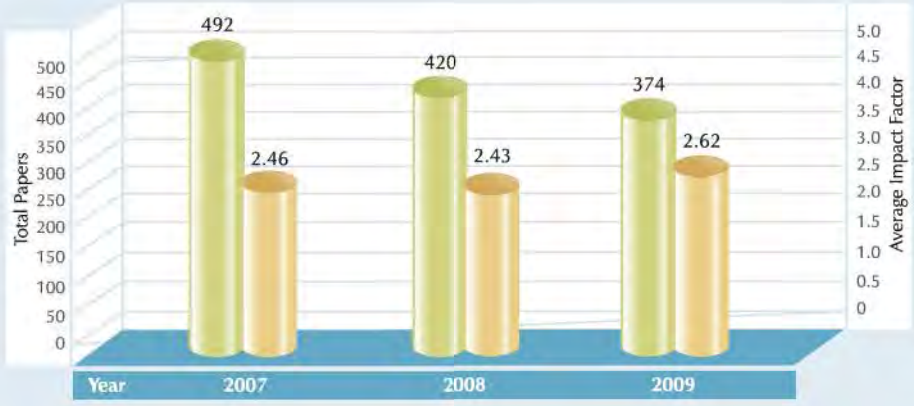
8 Feb 2010
NCL Diamond Jubilee Lecture on 'From Matter to Life Chemistry? Chemistry!' by Prof. Jean-Marie Lehn - Noble Laureate Nobel Laureate in Chemistry 1987, Universite de Strasbourg and College de France, Paris, France

27 Feb 2010
National Science Day lecture on 'Drugs and Drug Targets Against the Malarial Parasites' by Prof. G. Padmanaban, Honorary Professor, Indian Institute of Science, Bangalore

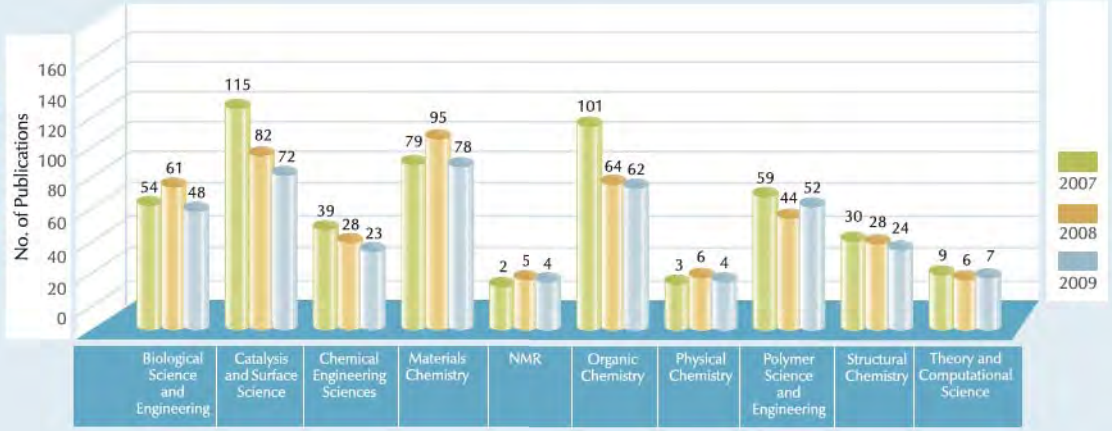
Performance Indicators

Science PERFORMANCE Indicators

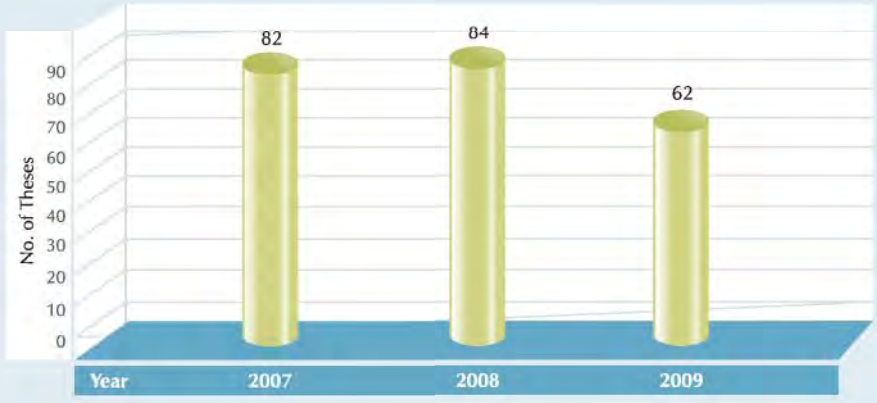
Research Output : Publications



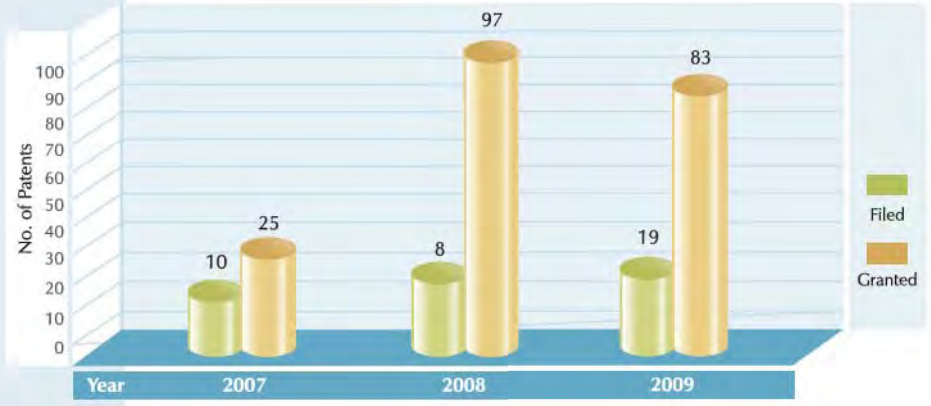
Areawise Publications



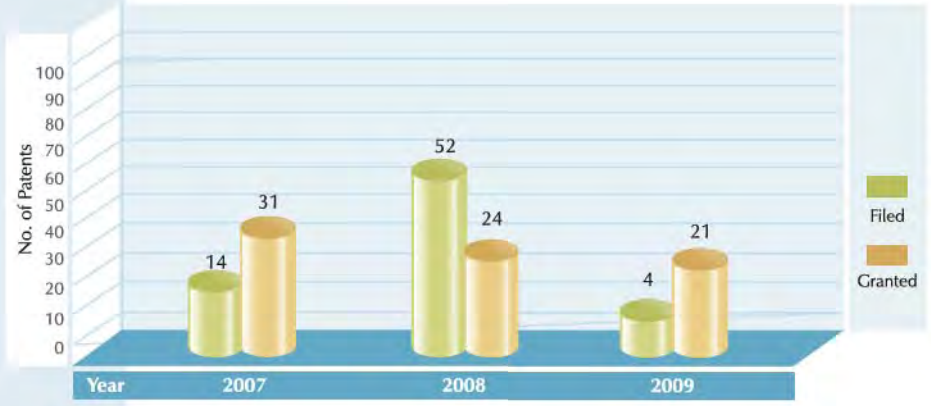
PhD Awarded



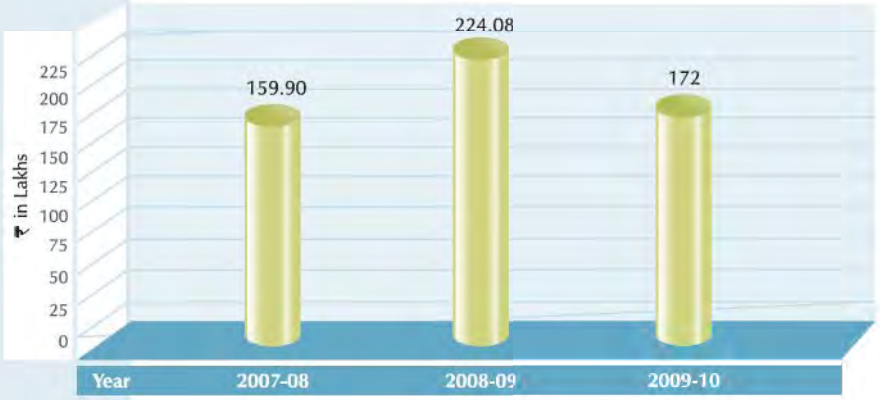
Technology PERFORMANCE Indicators



Indian Patents : Filed and Granted



Foreign Patents: Filed and Granted

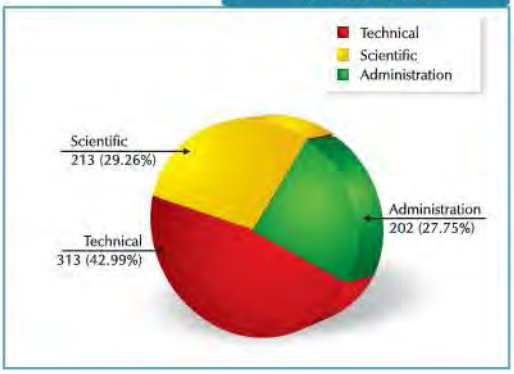


Premia/ Royalty Earnings

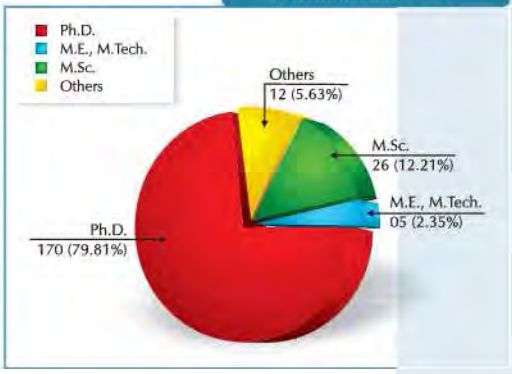
Human RESOURCE Indicators

(as on 31 March 2010)

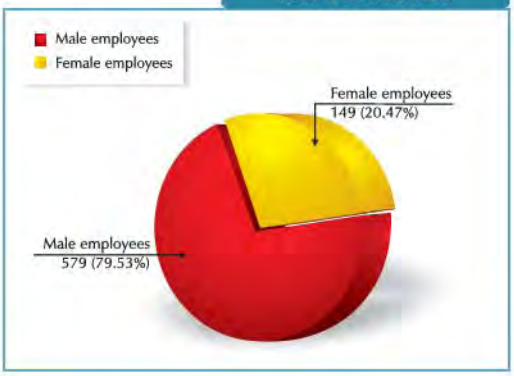
Total Staff : 728



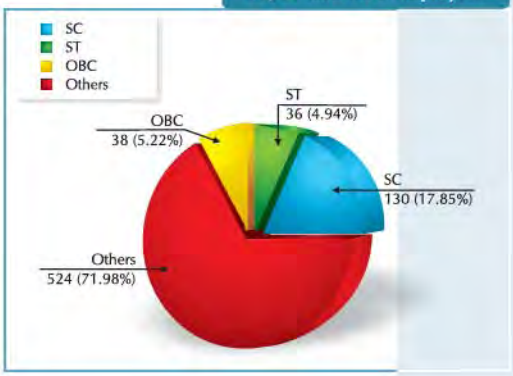
Scientific Staff : 239



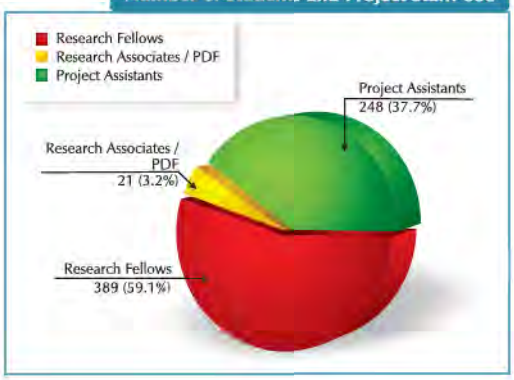
Male : Female ratio



SC, ST and OBC employees



Number of Students and Project Staff: 686



We WELCOME

Dr. Dattatraya H. Dethe
(30 July 2009)

Total Synthesis of Bioactive Natural Products

- Senior Research Scientist, Albany Molecular Research Inc., Singapore (July 2008 - July 2009)
- Post-doctoral research fellowship, Institute of Chemical and Engineering Sciences, Biopolis, Singapore (July 2005 - July 2008)
- PhD, Indian Institute of Science, Bangalore (Aug. 1999 - June 2005)

Dr. Nitin Shukla Tewari
(12 Oct. 2009)

Intellectual Property Management

- Patent Scientist at Lex Orbis, New Delhi (May 2008-Oct. 2009)
- PhD (Biomed Research), King George's Medical University, Lucknow 2008

Dr. K. Krishnamoorthy
(4 Nov. 2009)

Material Science and Device Physics

- Research Professor, University of Massachusetts - Amherst, USA (Jan. 2008 - Oct. 2009)
- Postdoctoral Research Associate, University of Massachusetts - Amherst, USA (Nov. 2005 - Jan. 2008)
- Postdoctoral Research Associate, Georgia State University and New Mexico State University, USA (Oct. 2004 - Oct. 2005)
- PhD, IIT-Bombay, Mumbai (June 2000 - June 2004)

Dr. Anu Raghunathan
(11 Nov. 2009)

Metabolic Engineering, Systems Biology, Molecular Evolution, Fermentation and Computational Biology

- Research Consultant, Mount Sinai School of Medicine, New York, USA (Jan. - Oct. 2009)
- Research Faculty, Mount Sinai School of Medicine, New York, USA (Jan. - Dec. 2008)
- Post Doctoral Research Associate, Department of Bioengineering, University of California at San Diego, La Jolla, USA (July 2002- Dec. 2005)
- Post Doctoral Researcher, Univ. Florida, Gainesville, USA (May 2000 - June 2002)
- Guest Researcher, Dept. of Chemical Engineering, University of Lund, Sweden (Nov. 1999- March 2000)
- PhD, IIT Bombay, (July 1995 - May 2000)

Dr. Pankaj Doshi
(11 Nov. 2009)

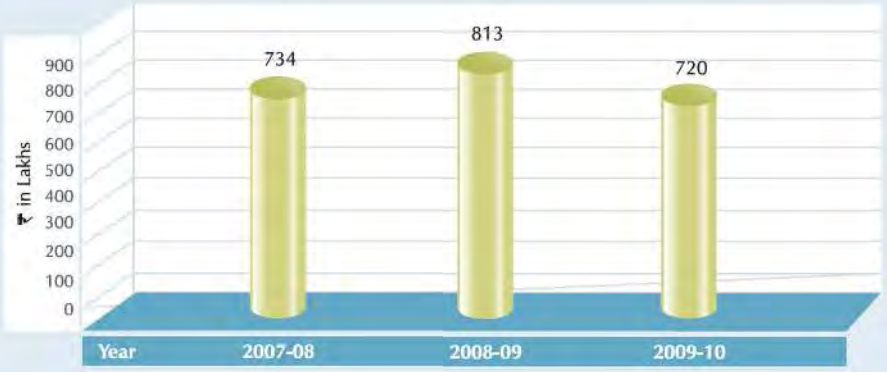
Computational Fluid Dynamics, Powder Flow and Mathematical Modeling of Pharmaceutical Processes

- Principal Scientist, Pfizer Inc, USA (Mar. 2008 - Oct. 2009)
- Investigator and member of Scientific Computing and Mathematical Modeling group, GlaxoSmithKline, USA (June 2005 - Mar. 2008)
- Postdoctoral Research, MIT, Cambridge, USA (March 2003 - May 2005)
- PhD, Purdue University, USA (Aug. 1997 - Jan. 2003)

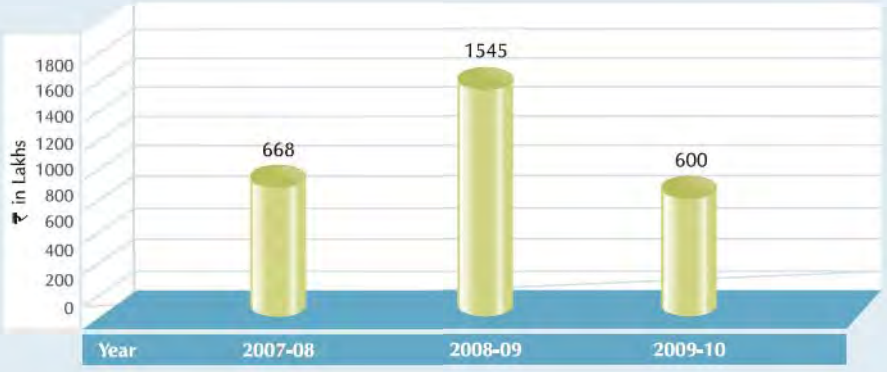
Financial PERFORMANCE Indicators

CSIR Budget

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)
2009-10 (CSIR Budget : 93.05 + Network Project : 19.47 + NMITLI Projects : 0.87)



Laboratory reserve: Receipts

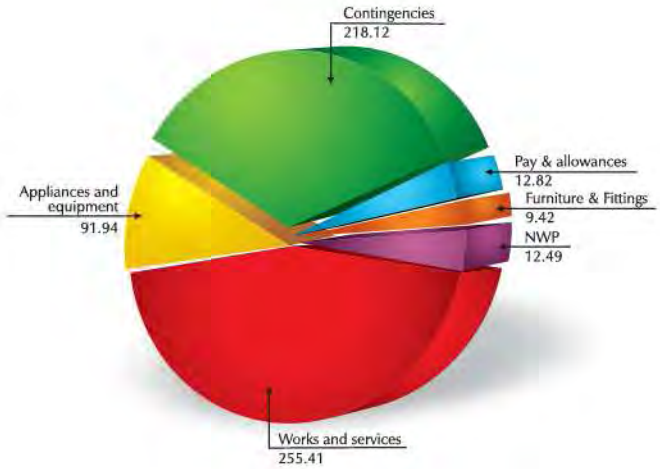


Laboratory reserve: Expenditure

Financial PERFORMANCE Indicators

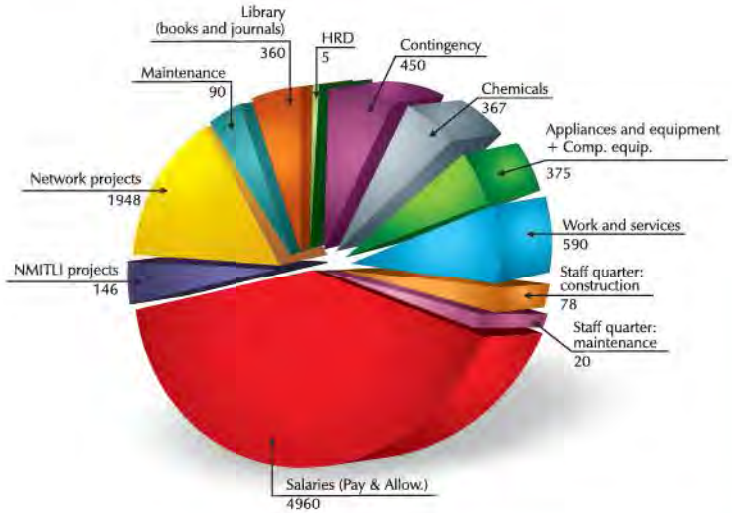
Expenditure: Laboratory reserve 2009-10 (Rs. Lakhs)

Appliances and equipment	91.94
Contingencies	218.12
Pay & allowances	12.82
Furniture & Fittings	9.42
NWP	12.49
Works and services	255.41



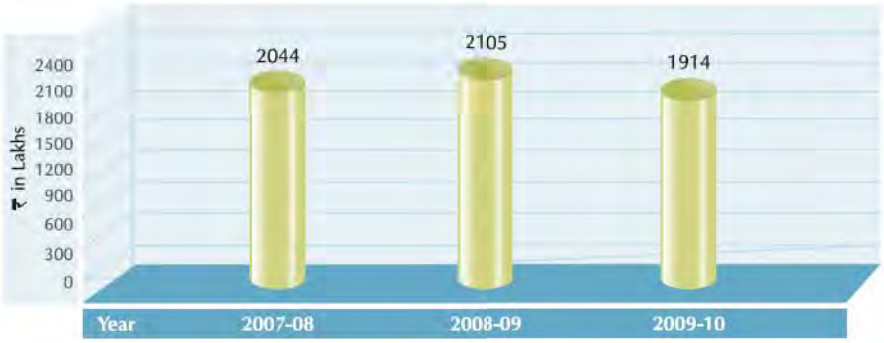
Expenditure: CSIR and Network Projects 2009-10 (Rs. Lakhs)

Appliances and equipment+ Comp. equip.	375
Chemicals	367
Contingency	450
HRD	5
Library (books and journals)	360
Maintenance	90
Network projects	1948
NMITLI projects	146
Salaries (Pay & Allow.)	4960
Staff quarter: construction	78
Staff quarter: maintenance	20
Work and services	590



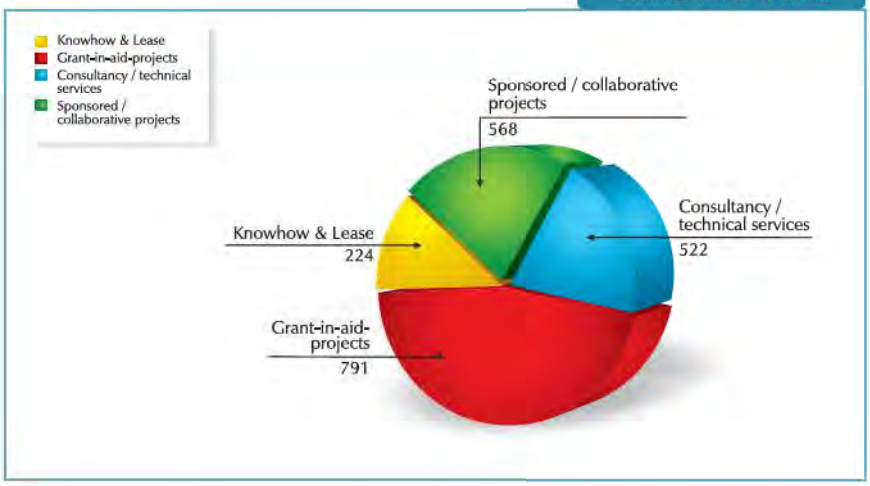
Financial PERFORMANCE Indicators

External Income

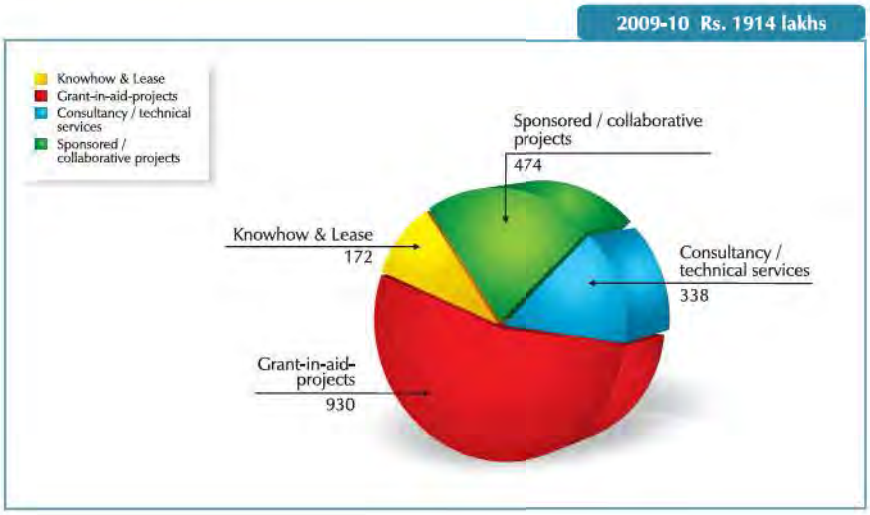


ECF by Source

2008-09 Rs. 2105 lakhs

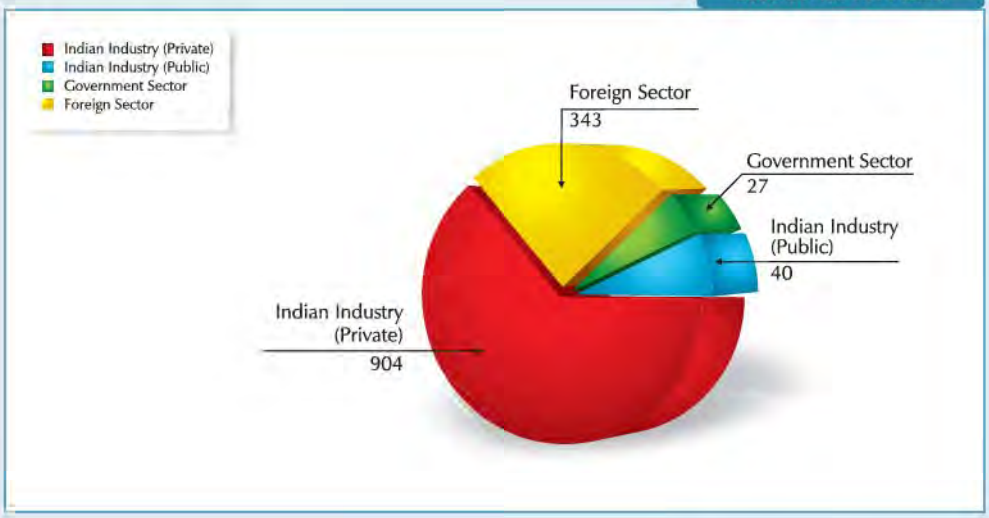


2009-10 Rs. 1914 lakhs

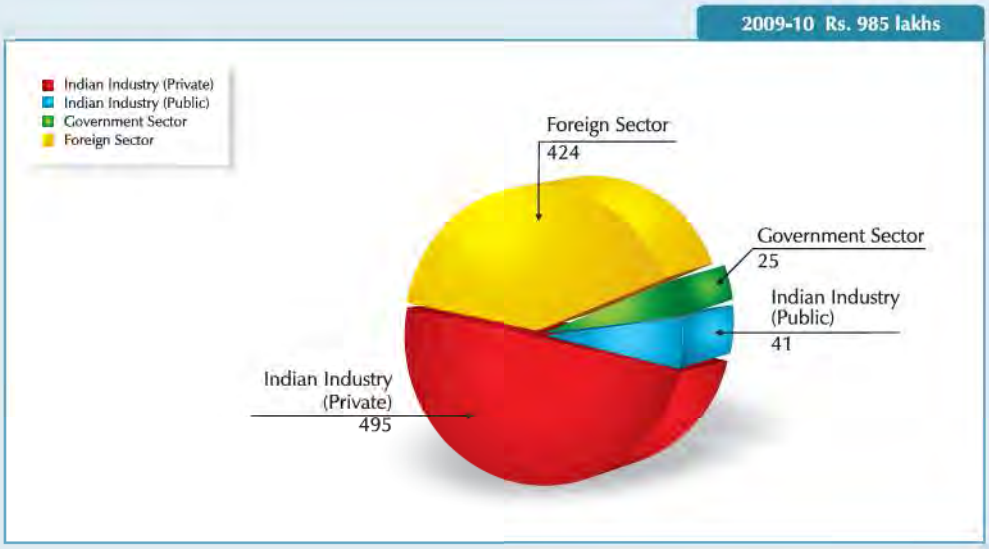


ECF for Industry

2008-09 Rs. 1314 lakhs



2009-10 Rs. 985 lakhs



Financial PERFORMANCE Indicators

Capital and Recurring Expenditure on R&D (2008 - 2010)

Source	Capital		Recurring	
	2008-09	2009-10	2008-09	2009-10
CSIR	711	1411	535	5892
Lab Reserve	86	357	45	231
Projects	335	377	1199	1194
Network Projects	1173	1216	720	732
NMITLI Projects	88	44	145	102
Total	2393	3405	2644	8151
Percentage %	48 %	29%	52 %	71%

Ongoing Publicly Funded Mission Mode and Internal Projects (2009-10)

Sr. No.	Description	Rs. In Lakhs
1	CSIR NMITLI	146
2	Major publicly funded projects (DST, DBT, NPSM, SDC, McNIGHT etc.)	930
3	Network projects	1948
4	Internal projects *	275
	Grand Total	**3299**

* - Funded from Lab Reserve of NCL

Capital and Recurring Expenditure on R&D (2008 - 2010)

Funding Source			Rs. in Lakhs
	Recurring	Capital	Total
CSIR	5893	1411	7304
LR	231	357	588
Total	6124	1768	7892

Outputs and OUTCOMES

Category of benefits	Benefit	Indicators	2007-08	2008-09	2009-10
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published in foreign journals/ publications (Calendar year)	470	394	364
		Number of papers published in Indian journals(Calendar year)	22	26	10
		Average Impact Factor	2.46	2.43	2.62
		Number of invention disclosure (Calendar year)	31	47	39
		Number of patents filed in India (Calendar year)	10	8	19
		Number of patents filed outside India (Calendar year)	14	50	4
		Number of patents licensed / assigned	6	2	1
		Number of major national/ regional collections, compilations, databases	3	3	3
	Highly trained man-power	Number of PhDs produced (Calendar year)	82	84	65
		Number of NET/GATE qualified students joined (including DBT JRF)	39	43	110
	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	10	9	9
	Pride and standing among nations; National image	Number of international awards won	-	-	1
		Memberships of major international academies and learned societies	7	7	10
		Memberships of editorial boards of international peer-reviewed journals (Cumulative membership years)	33	54	51
		Number of papers in foreign journals	470	394	364
		Number of IF research papers	451	384	360
		Number of foreign patents granted (Calendar year)	31	25	21
	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

Outputs and OUTCOMES

Category of benefits	Benefit	Indicators	2007-08	2008-09	2009-10
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)	13.56	13.14	9.85
	Continuing education	Total earnings from continuing education/ training programs (Rs. in Crore)	-	-	0.51
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (Rs. in Crore)	1.60	2.24	1.72
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)	3.43	4.88	0.87
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (Rs. in Crore)	6.87	7.91	9.30
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	Number of papers in foreign peer-reviewed journals	470	394	364
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	17	19	20
		Number of PhDs granted where lab scientists were research guides	82	84	65
		Number of staff who are members of National academies (Cumulative)	29	30	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)	13.56	13.14	9.85

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

1 Crore = 10 Million

Research & Development Reports

Advanced MATERIALS

T. G. Ajithkumar
tg.ajithkumar@ncl.res.in

Hybrid Materials

Member
- Bindhu Baby, JRF

Collaborator
- Dr. P. A. Joy, NCL

Publications
- *Solid State Comm*, **2010**, 150, 262
- *J Phys Chem C.*, **2009**, 113, 8556, 21114

Anchoring sites in spinel oxide nanoparticles : Solid-state NMR studies

Background

In the recent years, the synthesis and study of nanometer-sized oxide spinel particles have been the focus of intense fundamental and applied research with special emphasis on their size-dependent properties and applications. Decreasing size of the materials to nanometer size will change the surface area to volume ratio and this will strongly influence the properties of these materials. Normally, the degree of the distribution of the different ions in the tetrahedral and octahedral sites of the spinel lattice cannot be predicted in the case of the nanoparticles. Therefore, studying and understanding the coordination and distribution behavior of the different metal ions in the spinel oxide nanoparticles are very important. However, it is very difficult to get these information from the usual structural characterization techniques. Solid-state NMR is a powerful technique to obtain information on local structural variations. In our recent study, high resolution ^{27}Al Solid State MAS-NMR has revealed that the coordinatively unsaturated Al^{3+} centers (i.e., pentacoordinated Al^{3+}) on the surface of $MgAl_2O_4$ nanoparticles are anchoring sites for Pt. This suggest the possibility of getting information on the surface coordination behavior and activities of catalysts loaded on the surface of nanoparticles using solid state NMR techniques.

Work done and discussion

We have synthesized nanoparticles of the spinel-type compounds $MgAl_2O_4$ and the resulting powders were annealed at different temperatures to obtain particles of different sizes. ^{27}Al MAS and MQMAS NMR studies were carried out on these nanoparticles to understand the co-ordination behavior as a function of the particle size. We found the presence of a five-coordinated site in the nanoparticles apart from the usual tetrahedral and the octahedral Al coordinated sites and this contribution decreases with increasing particle size. In larger particles, five coordinated sites are totally absent (Figure 1). This indicates that the normal spinel structure is attained with an increase in the particle size. The nano-sized $MgAl_2O_4$ particles were loaded with 10% Pt and the resulting sample was studied using ^{27}Al MAS NMR which showed a reduction in the five-coordinated aluminium sites which suggests that Pt has loaded on the surface of the particles (Figure 2).

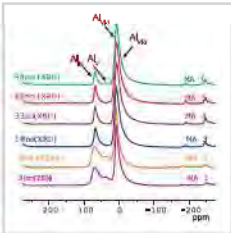
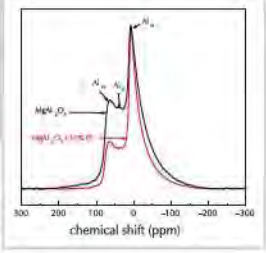


Fig. 1: The ^{27}Al Solid-state NMR spectrum of $MgAl_2O_4$ nanoparticles of various sizes that is indicated in the figure. The particles of sizes less than 10nm show a five-coordinated aluminium apart from the six-coordinated and the four-

Fig. 2 : The ^{27}Al Solid-state NMR spectrum of $MgAl_2O_4$ sample and Pt-loaded $MgAl_2O_4$.



Conclusion

Interesting changes in the local coordination behavior have been observed in nanoparticles of the spinel type compound $MgAl_2O_4$ by ^{27}Al solid-state NMR. The five-coordinated site is likely to be present on the surface of the particles due to changes in the coordination and bonding behaviour on the surface of the particles when their sizes are reduced to nanodimensions. A large percentage of the penta coordinated sites on the surface of the $MgAl_2O_4$ nanoparticles were found to have converted in to hexa coordinate sites on loading them with Pt as evidenced from the solid state NMR spectra. Simultaneously, there is an increase in the number of six coordinated sites.

S. Ganapathy
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Hybrid Materials

New solid state NMR methods and studies in diverse materials

Member
- K. Padma Prasad, SRF

Collaborators
- Prof. P. K. Madhu, TIFR, Mumbai
- Prof. S. Ramasamy, Univ of Madras, Chennai
- Prof. Niels C. Nielson, Univ. of Arhus, Denmark

Publications
- *Chem. Phys. Letts.*, **2009**, 478, 287
- *J. Phys. Chem.*, **2010**, B

Background

The main endeavour in this project has been to advance new high resolution solid state NMR methods and approaches and apply them effectively in a wider context to undertake studies pertaining to the structural and dynamical characterization of advanced materials, such as polymers and catalysts. Keeping this in view, we have undertaken following research initiatives.

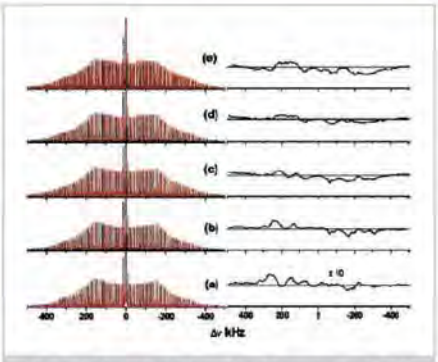

Fig. 2: Grain and grain boundary determination for 28 nm α-alumina from ^{27}Al satellite transition magic angle spinning (STMAS) spectra. Experimental spectra are shown on the left and the difference between experimental and computer simulated ^{27}Al STMAS spectra are shown on the right. (a) 50:50; (b) 40:60; (c) 30:70; (d) 25:75; (e) 20:80 grain to grain boundary ratio.

Sensitivity enhanced solid state NMR method for disordered materials

Materials such as polymers and catalysts are often disordered due to lack of long range order. X-ray diffraction techniques therefore become restrictive in the structural characterization of these materials. However, since these materials exhibit short range order, local structural characterization can be provided by employing solid state NMR methods.

The solid state NMR characterization effort in these materials is often beset with problems of NMR detection sensitivity. This may be due to the following factors: 1) the concentration of the species we wish to detect are small and often lie below the NMR threshold; 2) the NMR-active nuclei that we wish to employ has low natural abundance and/or has a low magnetogyric ratio (e.g., ^{15}N, ^{29}Si).

These invariably require a prohibitively long signal accumulation which can extend to several days. In many of the practical application of the above type of materials that we would like to characterize in this project, sensitivity limitation needs to be addressed and overcome before the desired NMR approaches are implemented. By far, a majority of NMR experiments are performed using cross-polarization (CP) for the signal enhancement. Even with CP enhancement, the signal accumulation times can become prohibitively long. In such cases, new strategies need to be introduced for enhancing the signal-to-noise ratio (S/N).

We have enhanced the sensitivity of ^{29}Si dipolar recoupled double quantum magic angle spinning experiment four-fold by implementation of CPMG acquisition in the dipolar recoupling symmetry sequences POST-C7 and Sr26$_4$. Preliminary experiments using natural abundance ^{29}Si show that in molecular sieves, the double quantum recoupling efficiency at shorter mixing times is higher with POST-C7 and is favourable for further CPMG implementation to

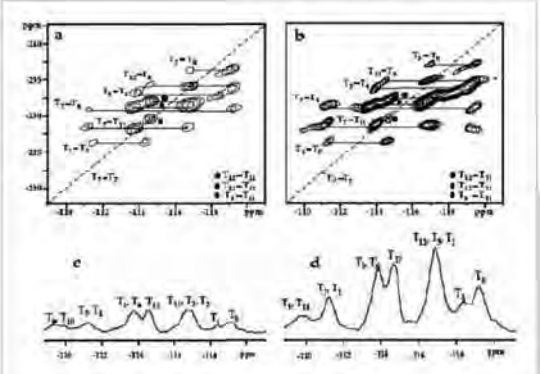

Fig. 1: Demonstration of the developed method on the molecular sieve ZSM-5 and its utility in signal assignments (a) 2D spectrum with normal POST C7 and (b) POST C7 CPMG. (c) SQ projection (F_2) from 2D POST C7, and (d) 2D POST C7 CPMG.

provide optimum sensitivity for the two dimensional double quantum correlation experiment. The application of POST-C7-CPMG for framework characterization has been fully demonstrated in the disordered and catalytically important ZSM-5 molecular sieve (Fig. 1).

Solid state NMR applications to nano-materials

Many of the analytical techniques used for nanomaterials characterization are surface techniques. Although grain and grain boundary structures can be identified, they do not provide in depth characterization at the molecular level. In this regard, solid state NMR provides new opportunities because the probe nucleus can be judiciously chosen for the particular type of nanomaterial that is being studied and, furthermore, the grain and grain boundary components can be inspected at atomic resolution.

If the probe nucleus is quadrupolar, the grain boundary behavior will be considerably amplified due to the large dynamic range brought into the NMR experiment by the quadrupolar interaction. Severe perturbations to electric field gradients would occur especially at the grain boundaries and these can be inferred from solid state NMR experiments. Since first-order and second-order quadrupolar interactions manifest in the NMR spectra, the quadrupolar spectra patterns can be analyzed and quantified.

^{27}Al solid-state NMR studies of nanocrystalline α-Al_2O_3 (52-12 nm) were undertaken by employing triple quantum (3_Q), satellite transition (ST), and central transition (CT) MAS techniques on Bruker AV-300 NMR spectrometer.

The effects of the grain size on the ^{27}Al electric field gradient tensor have been delineated through the experimentally determined ^{27}Al quadrupole interaction parameters (C_Q, η_Q) and isotropic chemical shifts (δ_{iso}) for the aluminum sites existing within the grains and grain boundaries.

3Q-MAS and STMAS experimental data of nano α-alumina were analyzed through extensive spectral simulations to probe ^{27}Al electric field gradients of aluminum in the grains and grain boundaries. By invoking the Gaussian isotropic model, in which the (C_Q, η_Q) parameter space is discretely sampled by the Czjzek distribution, grain and grain boundary components were quantitative determined from computer simulations of ^{27}Al STMAS spectra of nanocrystalline α-alumina (Fig. 2).

Jyoti Jog
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Hybrid Materials

Members
- Chetan Hanmal, SRF
- Prashant Patil, SRF
- Dhanalaxmi, SRF
- Lily Mandal, JRF
- Meenal Deo, JRF
- Dipti Dhakras, PA-II
- Raunak Naphade, PA-II

Collaborators
- Dr. Satish Ogale, NCL
- Dr. Ashish Lele, NCL

Functional polymer nanocomposites

Polymer nanocomposites represent a new class of materials based on reinforcement of polymeric materials using nanofillers. These nanocomposites show remarkable property improvements at low filler loadings compared to virgin polymer or conventional microcomposites. These property improvements include improvement in various physical properties including mechanical properties, which involve an increase in the modulus, strength, dimensional stability, and a decrease in the thermal expansion coefficient.

Since their discovery polymer nanocomposites based on carbon nano-tubes (CNT) have attracted much academic and industrial interest as researchers strive to enhance the polymeric material properties via nanosacle reinforcement. These nanocomposites have the obvious potential as lightweight technological materials having unprecedented mechanical, thermal and electronic properties.

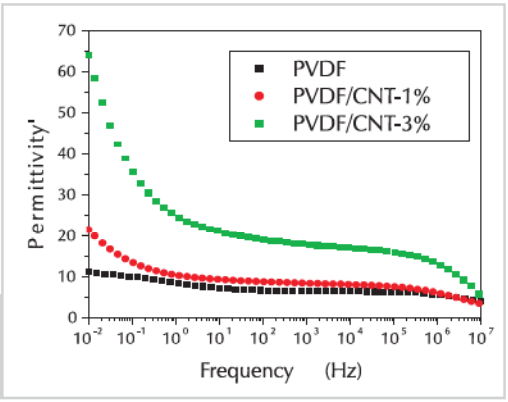

Fig. 1: Dielectric response of PVDF/MWCNT nanocomposites

Here we focus on functional polymer nanocomposites for various applications. The functionality is achieved by using functional nanofillers suh as MWCNT, semiconducting oxides etc.

PVDF nanocomposites

Electroactive polymers play an important role in many fields like micro-electronicmechanical systems (MEMs), gate dielectric material, embedded capacitor application and actuators. For such applications, a high electric energy storage density is necessary which can be achieved by increasing the dielectric permittivity of material.

Recently, polymer based nanocomposite materials with high dielectric permittivity were been explored as a potential candidate for such applications. Attempts have been made in the past to improve the dielectric permittivity of the polymers by incorporating high dielectric permittivity inorganic materials such as lead zirconium titanate (PZT), barium titanate ($BaTiO_3$) etc. However, very high loadings up to 50% by volume were generally required to achieve desired enhancement in permittivity. Till date, nanofillers such as $BaTiO_3$ and multiwalled carbon nanotubes (MWCNT) are reported to result in improved dielectric permittivity without compromising the flexibility of the polymer. Fig. 1 shows the variation of the dielectric permittivity of PVDF/MWCNT nanocomposites at 1 % and 3 % loading as compared to PVDF.

Functionalization of Nylon11 electrospun mats

Nanofiber mats were successfully prepared by electrospinning of Nylon11 solution in formic acid. The nanofibers mats were characterized using transmission electron microscopy, scanning electron microscopy, water contact angle measurement and EDAX. As these non-woven mats exhibit hydrophobic nature, for use in tissue engineering we need

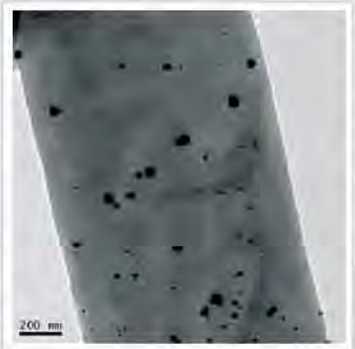

Fig. 2: TEM of electrospun fiber showing gold nanoparticles

to functionalize these mats and make them hydrophilic so as the cells can adhere and grow.

A simple treatment with Choloroaric acid was found to change the water contact angle of the mat from 135° to 93° as a result of deposition of gold nano particles on the surface of electrospun fibers. Fig. 2 illustrates the TEM of Nylon 11 nanofiber decorated with gold nanoparticles.

PHBV /ZnO nanocomposites

PHBV is a Biodegradable Polymer which has many applications in Biomedical Field. This polymer posses good mechanical properties, so it can be used in tissue engineering applications. ZnO is an inorganic biocompatible oxide with properties like photoluminescence, piezoelectricity, electroluminescence etc.

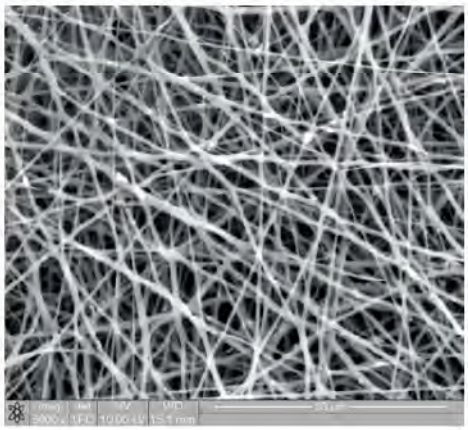

Fig. 3: SEM of PHBV/ZnO electrospun mat

Electrospinning of PHBV -ZnO system using Dichloromethane as a solvent was carried out. The nanofibers obtained were smooth and of nearly uniform size as shown in Fig. 3. These obtained mats of composite can be used in Tissue engineering applications as future materials.

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Magnetic Materials

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Publications
- *Solid State Commun.*, **2009**, 149, 2199
- *Solid State Sciences*, **2009**, 11, 714
- *Science Adv Mater*, **2009**, 1, 262
- *Nanosci. Nanotech. Letters*, **2009**, 1, 171

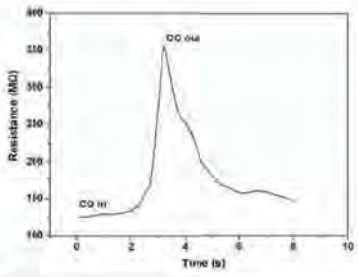
Nanomaterials

Background / objectives
- Development of magnetostrictive smart materials based on sintered ceramic oxide magnetic materials
- Nanostructured materials for various applications
- Superparamagnetic iron oxide nanoparticles capped with various biocompatible molecules for biomedical and environmental applications.
- Solid state NMR studies on bulk and nanomaterials

Work done and discussion

Nanostructured metal oxides with reduced dimensionality have ultrahigh reactivity and sensitivity to different gases due to their small grain size and large surface-to-volume ratio. Cobalt oxide (Co_3O_4), an important magnetic p-type semiconductor, has received considerable attention in the past few years due to its application potential in many technological areas. Our studies have shown that porous Co_3O_4 nanorods are very attractive as CO gas sensing materials, electrode material in Li ion batteries, as a supercapacitor material and also as oxidation catalysts.

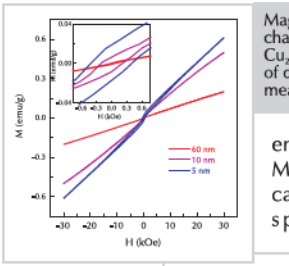
Response of Co_3O_4 nanorods to 50 ppm CO gas at 250 °C



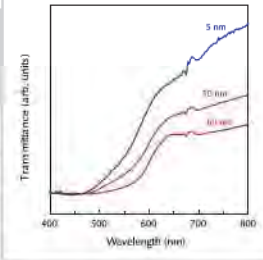
Cuprous oxide, Cu_2O, is a p-type semiconductor with a band gap of 2.17 eV and is considered as a potential candidate for use in solar energy conversion. Inducing magnetism in the transparent semiconductor Cu_2O is suitable for many potential applications.

Cuprous oxide nanoparticles capped with glucose molecules of different sizes show superparamagnetic behavior with increased magnetization as well as coercivity with decreasing particle size.

Magnetic nanoparticles can be used for biomedical applications such as contrast enhancement of MRI, magnetic carrier for site specific drug delivery, achieving local hyperthermia, catalysis, etc. Most of these applications require monodisperse biocompatible magnetic particles of size less than 10 nm or in the form of a colloidal dispersion known as magnetic fluids.



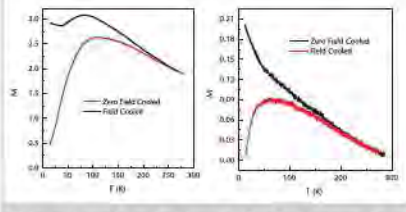
Magnetic characteristics of Cu_2O nanoparticles of different sizes, measured at 10 K.



UV-visible spectra of Cu_2O nanoparticles of different sizes

Magnetite (Fe_3O_4) is the most suitable magnetic material for the biomedical applications and magnetite nanoparticles can be functionalized by capping the magnetic nanoparticles with various biocompatible molecules.

For all the proposed applications of the magnetic nanoparticles, detailed information on their magnetic behavior, such as information on the magnetic exchange and dipolar interactions between the particles, magnitude of magnetization, superpar-amagnetism and superparamagnetic blocking temperature, etc. are very essential.



Magnetic characteristics of Fe_3O_4 nanoparticles uncoated and coated with a biocompatible molecule

Advanced MATERIALS

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Publications
- *CrystEnggComm*, **2010**, 12, 1600
- *Cryst. Growth & Design*, **2010**, 10, 1351, 2475

Porous materials for hydrogen storage and carbon sequestration

Background / objectives

The objective of our group is the focused improvement of materials for reversible gas storage (hydrogen) and sequestration (carbon dioxide, carbon monoxide) applications especially for on-board applications and clean environment. 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.

Work done and discussion

Coal-fired power plants emit flue gas comprising 15% CO_2, 7% H_2O, and 70% N_2. Selective removal of CO_2 from power plant emissions would help stabilize atmospheric CO_2 levels and help render coal a source of cleaner energy. New materials that can selectively capture CO_2 from power plant flue gas emissions in an economical and energy-efficient fashion must be developed.

Porous materials relying on physical adsorption of CO_2 are potential candidates for accomplishing this goal because they require less energy for regeneration than materials and solvents relying on chemisorption. Currently, designing and fabricating porous materials that selectively capture CO_2 is an important challenge. Metal–organic frameworks (MOFs) are being intensively investigated to address this challenge because their metrics and chemical functionality can be carefully adjusted for specific applications (Fig.1).

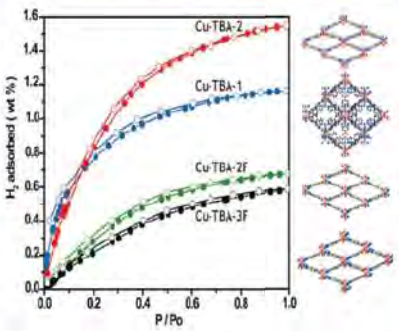


Fig. 1: Hydrogen storage in fluorinated metal organic frameworks (F-MOF)

We propose herein design and synthesis of amino functionalized (NH_2-MOFs) for selective adsorption of CO_2. Recently, researchers have begun investigating the preparation, assembly, and physical properties of amino functionalized (NH_2-MOFs) porous materials. These materials have been synthesized from a amino (-NH_2) functionalized organic building block.

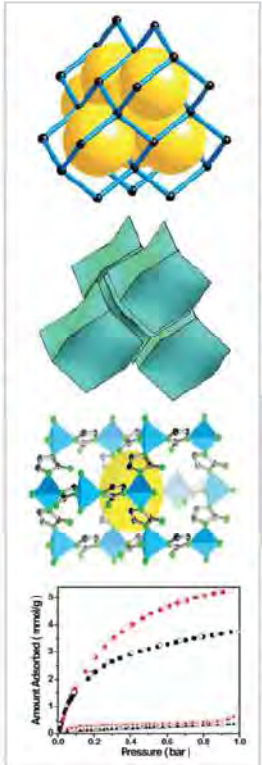


Fig. 2: Carbon dioxide capture and sequestration in amino functionalized metal organic frameworks (NH_2-MOF)

This organic links because (1) of their many potential coordination modes, allowing for the construction of a topologically diverse family of materials; (2) it is rigid, which helps enable the preparation of permanently porous materials; and (3) it is an ideal building block for constructing materials for CO_2 capture. Indeed, a recent computational study revealed that the interaction energy between CO_2 and amine (-NH_2) is higher than that between CO_2 and other MOFs. These amine groups can interact with CO_2, potentially resulting in materials

with high CO_2 adsorption energies. Therefore, amino functionalized (NH_2-MOFs) MOFs would be ideal for selective CO_2 adsorption.

Our current work represents a significant study of synthesis of amino functionalized (NH_2-MOFs) MOFs which selectively adsorbed CO_2 and exhibited rapid CO_2 uptake at low pressures (fig. 3). We attributed the selectivity to the presence of narrow pore apertures that exclude gases with larger kinetic diameters and the rapid uptake at low pressures to favorable interactions between CO_2 and the pore walls.

In this structure, the zinc 2-amino imidazole the the amino groups are exposed inside the pores and may therefore increase the material's affinity for CO_2. We reasoned that exposing these sites within the pores of a MOF should lead to materials with enhanced CO_2 adsorption properties, including high uptake and high selectivity.

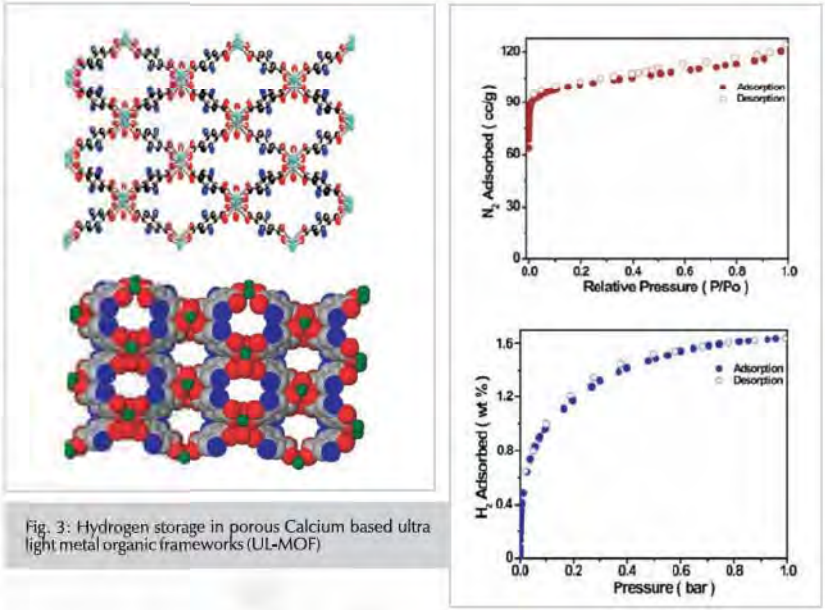
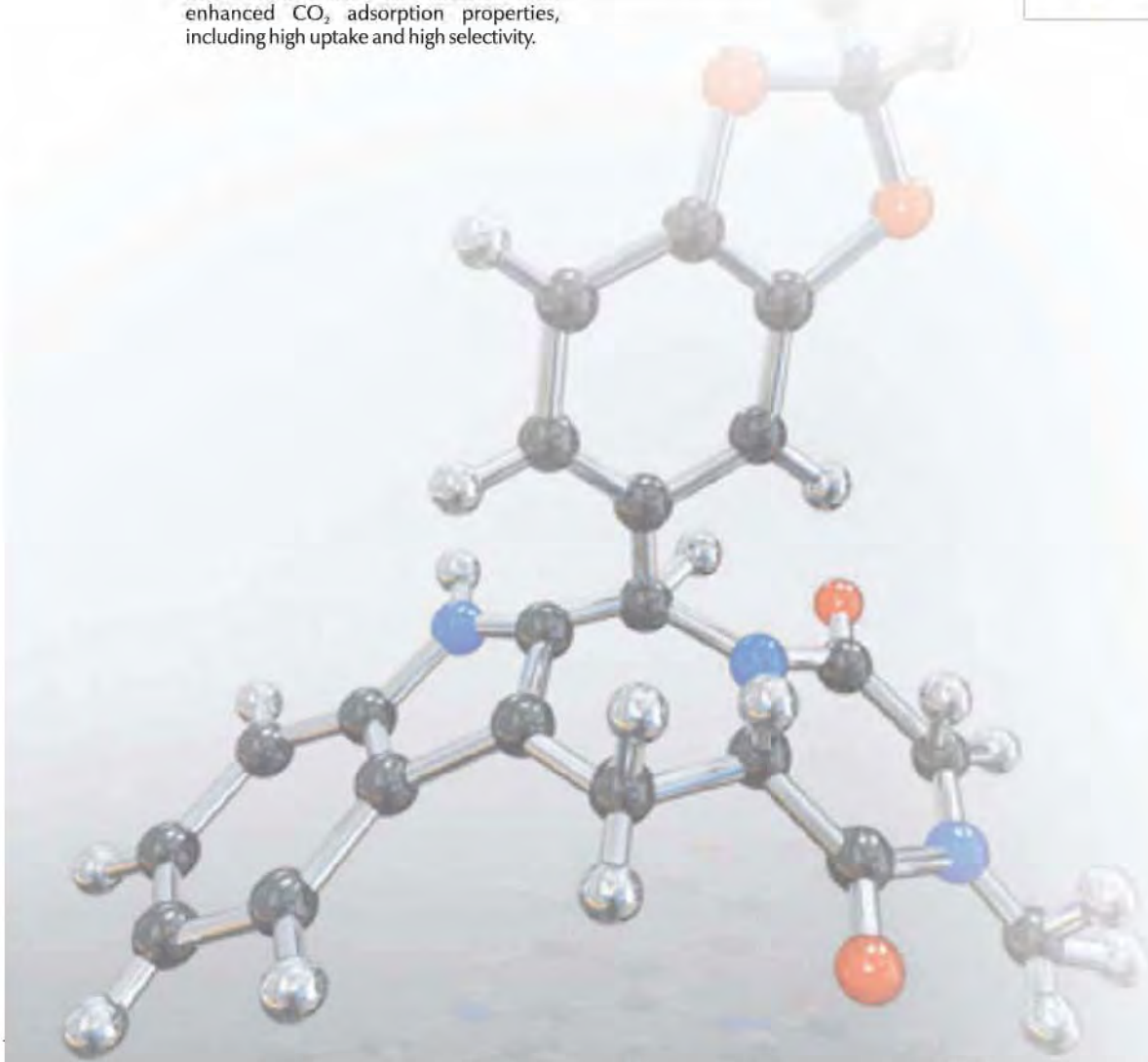


Fig. 3: Hydrogen storage in porous Calcium based ultra light metal organic frameworks (UL-MOF)



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- *J. Phys. Chem. C*, **2009**, 113, 17572
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Energy generation and storage through the development of various functional nanomaterials

Background / objectives

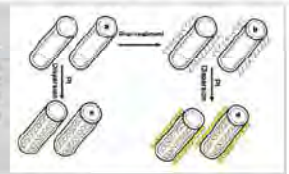
Main focus objective of our research is to advance in the area of energy generation and storage by developing various functional nanomaterials. Since Polymer Electrolyte Membrane Fuel cell (PEMFC) is an important candidate in the energy market, the main goal of our group is to design and develop advanced electrode materials which simultaneously meet all the necessary requirements to improve the commercialization aspects of the PEMFC systems. These include modifications in all the key parts including active catalyst, catalyst support, proton conducting membrane and even the ionomer-catalyst-gas pore triple-phase boundary (TPB). Some of the current approaches are listed below:

- Since the surface area of the catalyst support is an important parameter which determines the total performance of the catalyst, one of our approaches is to increase the available surface area by utilizing the inner walls of suitably structured carbon nano morphologies.
- Second is to develop potential non precious electrocatalyst systems based on iron nitride and carbon nanofiber by utilizing the slit-pores of the material.
- Third approach is to enhance the total activity of electrocatalysts by designing various multifunctional materials.
- Another approach is to increase the Pt utilization by using some foreign materials to "polish" the carbon surface.
- Synthesis of core-shell nanoparticles to reduce the Pt content and thereby the total cost reduction of the fuel cell is another activity.

Work done and discussion

An efficient electrocatalyst for PEM fuel cells based on carbon nanofiber

To overcome the surface area related issues of one dimensional carbon support materials, a novel methodology has been devolved by utilizing the inner wall of a carbon nanofiber material with open tips. Thus a new electrocatalyst with excellent Pt dispersion on the inner and outer wall of a carbon nanofiber (CNF) has been prepared by a modified polyol process in which both the surface tension and polarity characteristics of the medium were properly adjusted to favor solution entry into the tubular region by capillary filling and homogenous wetting of the inner wall surface by the solvents. The pristine CNF, which possesses inherently active inner wall surface and inactive outer wall surface, lead to selective Pt deposition along the inner wall, whereas activation of the outer wall with chemical functionalization resulted into excellent dispersion of Pt along both the inner and outer walls.



Scheme 1: Outline of the steps for the preparation of Pt decorated carbon nanofiber.

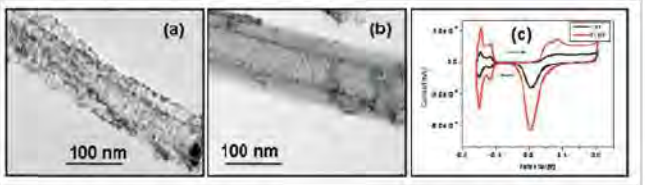


Fig. 1: (a) and (b) HR-TEM images of carbon nanofiber with Pt on both the walls and Pt only on the inner wall respectively and (c) the resulting catalytic performance

The enhanced electrocatalytic activity displayed by these materials opens up great scope in fuel cell electrode fabrication because appropriate Pt loadings can be achieved at significantly low carbon content in the system.

Facile construction of non precious iron nitride doped carbon nanofiber for PEMFCs

Despite the vast variety of Pt based catalyst for oxygen reduction reaction in PEMFCs, a novel non-Pt electrocatalyst, i.e. iron nitride doped carbon nanofiber (FeN_4CNF) electrocatalyst, has been developed by a simple method. Here, we utilized the highly active graphitic edges in the inner walls of carbon nanofibers to fill its inner pore with 1,10 phenanthroline and iron acetate and a subsequent heat treatment to obtain the unique catalyst.

Nitrogen doped CNF (N-CNF), which is a recently advancing candidate in the realm of electrocatalyst, has also been successfully prepared using the same carbon material using the same experimental procedure excluding the iron precursor. Activity evaluation using electrochemical techniques demonstrates the potential of this non-Pt material as an important candidate.

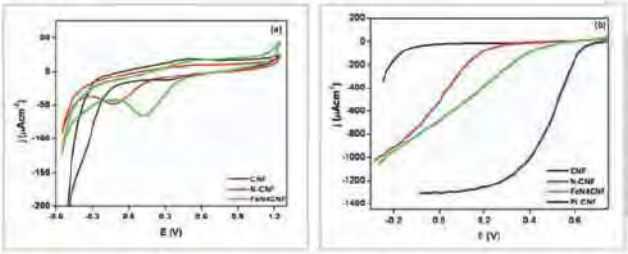


Fig. 2: Electrochemical characterizations revealing the superior activity of Iron nitride doped carbon nanofiber (FeN_4CNF) catalyst

High aspect ratio nanoscale multifunctional materials derived from hollow carbon nanofiber by polymer insertion and metal decoration

A novel high aspect ratio inorganic-organic material which can simultaneously perform multiple functions such as proton and electron conductivity and electrocatalytic activity has been developed by incorporating both platinum nanoparticles and phosphoric acid doped polybenzimidazole (PBI) along the inner and outer surfaces of a hollow carbon nanofiber.

It is accomplished by virtue of optimizing the synthesis parameters of PBI to obtain low viscosity and by manipulating the solution concentration of the PBI to facilitate its entry into the inner cavity of the CNF through the open tips.

Whereas HRTEM could directly depict the presence of PBI on the outer wall, a tracer study using Rh nanoparticles has been carried out to confirm the presence of PBI encapsulated inside the cavity based genuine fact that there is a prominent contrast difference between metal and carbon.

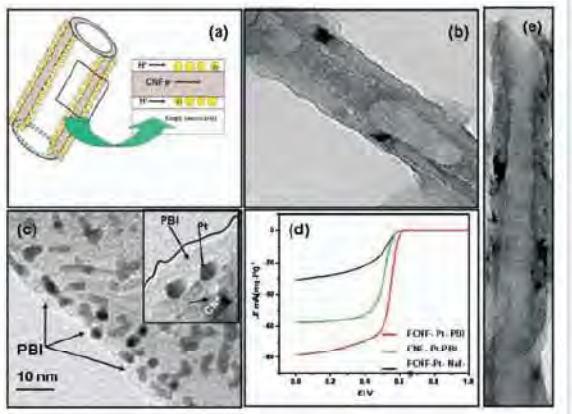
The remarkable improvement in the performance dispalyed by this material can be attributed to the synergistic effects of PBI in modulating the electronic properties of the support coupled with the improved proton conductivity and mass transport and thus this system offers intriguing possibilities of the present concept in effectively utilizing materials and creating new avenues in system developments.

Low-Pt electrocatalyst based on a core-shell approach and high Pt utilization electrodes using "polished" carbon supports

In view of reducing the total Pt content in the system, core (Cu, Fe)-shell (Pt) type catalysts with varying percentages of Pt have been synthesized by successive reduction method using ascorbic acid as the reducing agent. By a proper process modification to strictly form a thin layer of Pt on the core material, the amount of Pt could be effectively reduced to a considerable extent with notable increase in the electrochemical activity. The synthesized catalyst finds immense scope in PEMFCs as the structure of the material offers better mass activity due to a thin layer of Pt, which can be effectively prepared on the non-noble metal core.

In another approach, Pt utilization on active carbon has been significantly improved by initially utilizing polypyrrole as a moiety to "polish" the carbon surface and subsequently by dispersing Pt particles formed by a pre-precipitation process to minimize their migration into the geometrically restricted areas of the carbon surface. This process strategy has helped to significantly extend the triple-phase boundary as a greater number of Pt particles come in direct contact with Nafion, leading to a substantial improvement in the overall catalyst utilization.

Fig. 3: (a) Schematic of the novel catalyst design based on the multifunctional approach, (b) CNF with PBI incorporated inside the cavity, (c) A portion of Pt decorated CNF with PBI showing a skin layer on the surface of Pt nanoparticles, inset of (c) is the image showing the TPB formed on a single Pt nanoparticle, (d) the electrochemical activity of the so prepared catalyat and (e) CNF with Rh tracer in PBI matrix showing the one dimensional confinement of PBI phase inside the CNFs.



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Publications
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- *Appl. Phys. Lett.*, **2009**, 95, 203502
- *J. Phys. Chem. C*, **2009**, 113, 13403
- *J. Nanosci. Nanotechnol.*, **2010**, 10, 5894

Advanced nanostructures for energy, optoelectronic and biomedical applications

Background / objectives

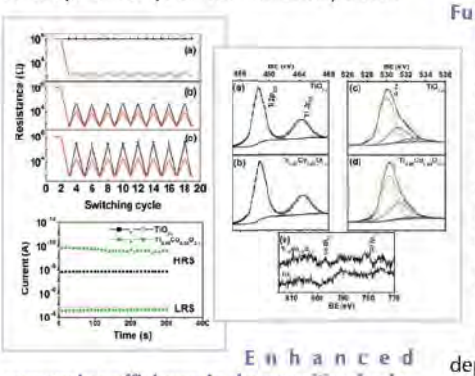
The objective of our group is to synthesize functional nanomaterial composites and their application in various field viz. energy (Dye Sensitized Solar Cells), optoelectronic devices (Sensors, Non-volatile Memory Devices, Spintronics), catalysis (Photocatalysis) and biomedical applications.

Section I: Advanced nanostructure composites for energy and optoelectronic applications.

Enhanced nonvolatile resistive switching in dilutely cobalt doped TiO_2

Incorporation of dilute concentration of dopant having a valence state different than that of the host cation enables controlled incorporation proximity vacancy defects for local charge balance. Since nonvolatile resistive switching is a phenomenon tied to such defects, it can be expected to be influenced by dilute doping.

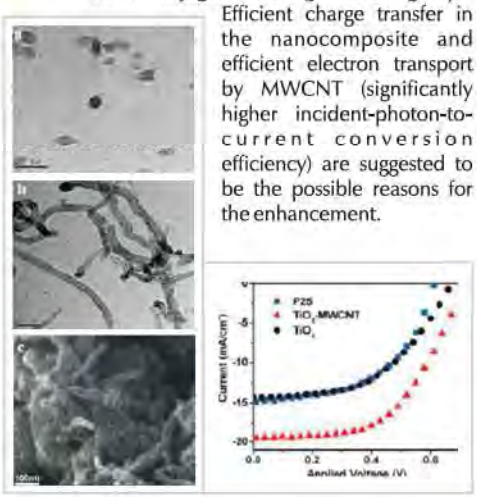
In this work, we demonstrate that enhanced nonvolatile resistive switching is realized in dilutely cobalt doped TiO_2 films grown at room temperature. We provide essential characterizations and analyses. We suggest that the oxygen vacancies in the proximity of immobile dopants provide well distributed anchors for the development of systematic filamentary tracks.



Enhanced conversion efficiency in dye-sensitized solar cells based on hydrothermally synthesized TiO_2-MWCNT nanocomposites

A 50% enhancement in the conversion efficiency (4.9-7.37%) is realized in dye-sensitized solar cells using hydrothermally synthesized TiO_2-multiwalled carbon nanotube (MWCNT) nanocomposites as compared to hydrothermally synthesized TiO_2 without MWCNT and Degussa P25.

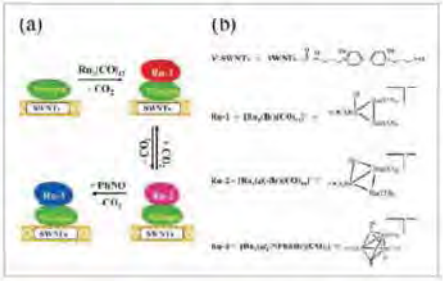
Several characterizations have been employed to reveal the nature of the modification imparted to the MWCNTs under hydrothermal processing conditions and the resulting TiO_2-MWCNT conjugation through -COOH groups. Efficient charge transfer in the nanocomposite and efficient electron transport by MWCNT (significantly higher incident-photon-to-current conversion efficiency) are suggested to be the possible reasons for the enhancement.

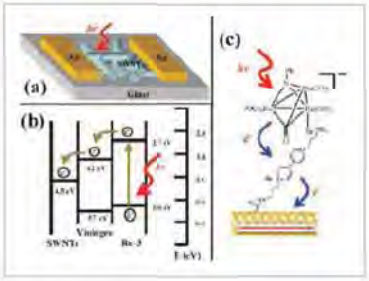


Optoelectronic Photoinduced Charge Transfer System with μ_3PhN-Ru_3 Cluster Functionalized Single-Walled Carbon Nanotubes

Optoelectronic photoinduced charges have been attracting great attention lately in view of their applicability to diverse optoelectronic device systems. Here, we report the design and implementation of a charge transfer system based on triruthenium (Ru) cluster compounds on viologen modified single-walled carbon nanotubes (V-SWNTs) by an in situ preparation method.

We examine the photoinduced (intensity dependent and temporal) changes in the transport properties of the Ru-cluster functionalized V-SWNT coating and identify the possible charge transfer mechanism. Furthermore, we demonstrate the applicability of such Ru-cluster functionalized V-SWNT films to photoelectrochemical cells.



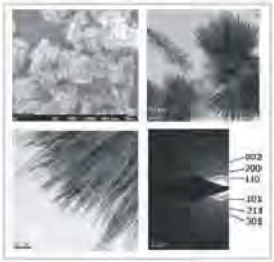


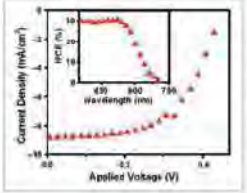
Room temperature synthesis of rutile TiO_2 hierarchical nanoneedle flower morphology for dye sensitized solar cell

Rutile TiO_2 nanoneedle flowers (representing concurrent nano-micro hierarchical morphology) with high shape anisotropy ratio are synthesized at room temperature by using a simple and efficient one step electrochemical process of anodic dissolution. This process employs highly acidic bath of perchloric acid (pH < 2) and a large current density on the surface of Titanium foil to form nanostructures. The diameter and length of rutile TiO_2 nanoneedle is ~8 nm and 100 nm respectively (aspect ratio >10). Dye sensitized solar cell (DSSC) configured using such rutile TiO_2 flowers is shown to exhibit IPCE of 30% and power conversion efficiency of ~3.6%.

Section II: Nanomaterials for biomedical application

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

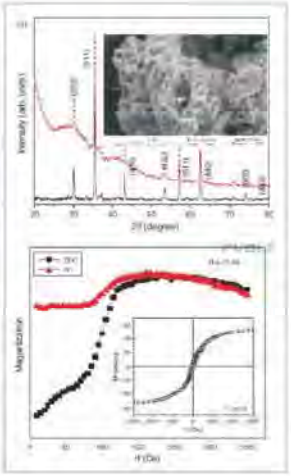




Anisotropic growth of magnetite (Fe_3O_4) nanoparticles is achieved in a hydrothermal growth process using hexamine to play a dual role of oxide forming and directing agent.

The samples are characterized by X-ray diffraction, scanning electron microscopy, high resolution transmission electron microscopy, squid magnetometry, ferromagnetic resonance technique, diffuse reflectance spectroscopy and Mossbauer spectroscopy, which collectively establish the formation of Fe_3O_4 phase. Anisotropic structures such as nanorods and nanotubules are revealed and these are shown to exhibit good humidity sensing properties.

Elucidation of the role of hexamine and other precursors in the formation of magnetite nanorods and their stoichiometry



In this work we have elucidated the mechanism of the magnetite nanorod formation by hydrothermal method. It is found that changes in the choice of iron precursors and combinations of hydrolyzing/capping agents change the constitution, shape, size and properties of phase(s) formed. Only when ferric chloride, ferrous ammonium sulfate (FAS) and hexamine are used, well defined nanorods are formed, though a small degree of non-stoichiometry, related to oxidation phenomena, is also noted.

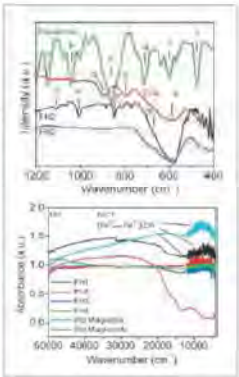
Interestingly, the decomposition products of hexamine added as precursors do not lead to nanorod formation. We conclude therefore that slow decomposition of hexamine at elevated temperature and the consequent slow rise in pH are the key factors responsible for the anisotropic growth of the iron oxide system.

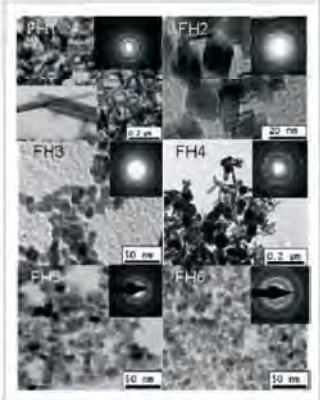
On the change in bacterial size and magnetosome features for magnetospirillum magnetotacticum (MS-1) under high concentrations of zinc and nickel

The characteristic size, shape and specific alignment of magnetite crystals synthesized by magnetotactic bacteria is a highly coordinated process with precise control over magnetosome vesicle formation, uptake and transport of Fe, and magnetite biomineralization. Magnetosome membranes along with some specific membrane proteins regulate crystal nucleation and morphology of magnetite.

Several previous works have indicated that the morphology of mature magnetite crystals is largely unaffected by environmental conditions, though some recent studies have shown the possibility of manipulation of the biomineralization process.

In this study we have examined the effects of high concentrations of Zinc and Nickel on the growth of Magnetospirillum magnetotacticum (MS-1) and the corresponding magnetosome formation. Using various characterizations it is shown that the growth of the bacterial cells, as well as the size, shape and magnetosome chain alignment is significantly influenced in the presence of high concentrations of Zn or Ni.





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Publications
- *J. Phys. Chem. C.*, **2009**, 113, 21493
- *PLoS ONE*, **2009**, 4:e7718
- *J. Phys. Chem. B*, **2009**, 113, 7927
- *J. Phys. Chem. C*, **2009**, 113, 3478

Metal ion stress induced physiological changes in bacterial cells and their real time mapping during the microbial synthesis of Co_3O_4 nanoparticles

Background / objectives

The study of elastic properties of microbial and mammalian cells using atomic force microscopy, with forcesensitivity as high as pico-Newtons and spatial resolution of a few nanometers, is proving to be a great tool for the real-time observation of the effects of drugs, biomolecules, metal ions, and nanoparticles on cell physiology in their natural environment.

It has been shown that the Young's modulus of the cell surfaces is extremely sensitive to the surrounding environment. Recently, a broad array of microbes have been used successfully to synthesize nanocrystals of several metal and metal oxides in a controlled manner at room temperature after exposing them to various metal ion precursors. However, so far there is no report on the fate of their elastic properties and cell topography etc.

during and after their exposure to the metal ions during the microbial synthesis of nanomaterials. Additionally, this information is also found to be extremely relevant to areas such as bioremediation, bioleaching, and biomineralization, where it is important to study the direct influence on the cell physiology in the presence of metal ions. Here, we reported, for the first time, the use of AFM force-distance curves on live cells, to directly monitor (in real time) the changes in the surface-topography, surface-adhesion, indentation-depth, and Young's modulus of a metal-tolerant marine bacterium, Brevibacterium casei, isolated from the coast of the Arabian Sea, after its exposure to the Co^{2+} ions during the process of biosynthesis of nanoparticles.

We earlier reported that this bacterium is capable of using the cobalt acetate as a precursor to synthesize protein-functionalized Co_3O_4 nanoparticles with very high crystallinity.

Our study indicates a significant change in the morphology as well as elastic and adhesive properties of the BreVibacterium casei, where we found an increase in the adhesive properties and the indentation depth of the bacterial surfaces and a decrease in the cell stiffness after several hours of exposure to the cobalt acetate.

Work done and discussion

For the real time observation of the Co^{2+} ion toxicity effects on the cells, the cells were incubated with an aqueous solution of cobalt acetate. In this case, the concentration of the cobalt acetate was kept similar to the concentration which was used in our earlier study for the synthesis of Co_3O_4 nanoparticles using the BreVibacterium casie culture.

The cells were dropcasted on the mica surfaces after 24, 48, and 72 h of incubation to study a time dependent effect on the cell physiology, and these results were compared with those of the untreated cells (control i.e. 0 h). Therefore, our study truly represents the changes in the morphology and mechanical properties during as well as after the biosynthesis of the Co_3O_4 nanoparticles.

Here, the 0 h measurement corresponds to the time prior to reaction, the sample taken after 24 h of incubation corresponds to the measurements "during" the synthesis process and the corresponding surface changes on bacterial cells, and the 48 h sample represent the time-scale after completion of the synthesis process and reflects the corresponding surface changes. Lastly, the 72 h sample corresponds to the time interval well beyond the formation of nanoparticles.

The atomic force microscopy measurements were performed using a Multimode scanning probe microscope equipped with a Nanoscope IV controller. All the AFM measurements were done under ambient conditions using the soft tapping mode AFM probes model-Multi75Al with proper precautions to avoid drying of the cells.

The adhesive force calculated by the force plot comes out to be 10, 40, 15, and 25 nN after 0 h (control), 24 h, 48 h, and 72 h of exposure of the cells to metal ions during the microbial synthesis, respectively. We calculated the adhesion energy for various samples by calculating the area under the force-distance curve below the zero force line of the adhesion loop, and these values were 0 h= -177.073×10^{-18} J, 24 h = -1211.45×10^{-18} J, 48 h= -197.01×10^{-18} J, and 72 h = -1067.49×10^{-18} J. It is clear that the adhesive force and adhesive energy show an enhancement during the

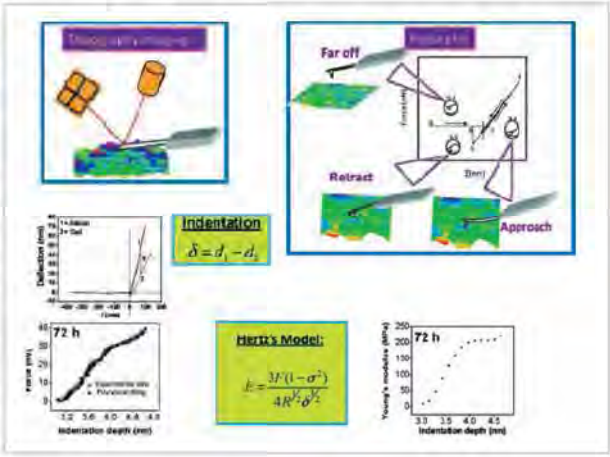
biosynthesis after the exposure of the bacterial cells to the metal ions, which is probably due to the presence of an increasing amount of exopolysaccharide and other biomolecules at the surface as the microbial reaction proceeds. For the control sample (0 h) the Young's modulus shows a gradual increase as a function of indentation depth as compared to the rest of the curves (for 24, 48, and 72 h after the reaction starts).

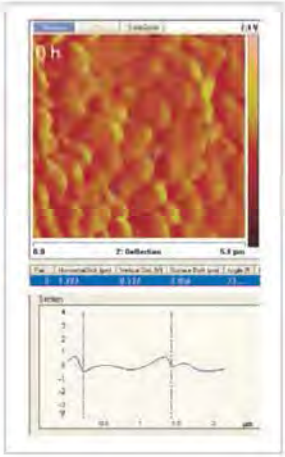
It is also evident that, at larger indentation depth values, we see an approach toward a plateau in the Young's modulus values almost for all the four cases, which is usually the situation when the applied load is proportional to the deformation produced in the sample, indicating that the region is in the elastic limit.

In this region, the calculated values for Young's modulus for 0, 24, 48, and 72 h of reaction are 769.28 ± 73.07 MPa, 170.921 ± 38.93 MPa, 82.860 ± 20.42 MPa, and 209.526 ± 6.14 MPa, respectively, which shows mostly a decreasing trend in elasticity of the cells as the reaction progresses. Young's modulus of a cell surface may originate from various sources such as (a) the cell wall itself and/or (b) underlying structures (cytoskeleton etc.) and/or (c) a pressure difference between the cell interior and the exterior (turgor pressure).

The biochemical process inside the cells and at the cell surface might be greatly affected by the presence of Co^{2+} ions, leading to the loss of turgor pressure and change in the elastic properties of the cell wall itself as well. As seen in the topographical images of the cells, we can conclude that these factors collectively lead to an overall drop in the elasticity of the cells in our case, although the approach to the plateau of Young's modulus as a function of indentation depth is faster in the 0 and 24 h samples.

This saturation point is different for each sample depending upon their exposure to the Co^{2+} ions, probably due to the clumping of cells during the microbial synthesis. Unexpected high values of Young's modulus for the 0 h sample (before reaction) indicate that the Turgor pressure is maintained. As the reaction progresses, we notice a decrease in the Young's modulus values and softness of the sample, which is probably due to turgid loss during the synthesis process.





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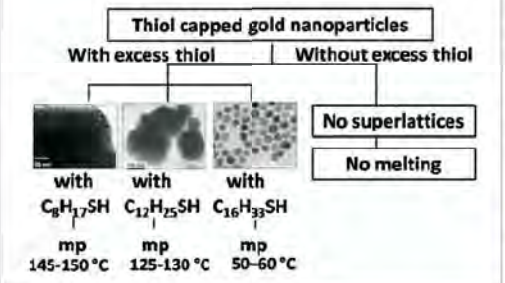
Publications
- *Chem. Mater.*, **2010**, 22, 1680
- *New J. Chem.*, **2010**, 34, 294
- *Langmuir*, **2009**, 25, 11741
- *J. Mater. Chem.*, **2009**, 19, 544

Nanoparticle dispersions in different media and diverse applications

Monolayer protected nanoparticles (aqueous and organic dispersions) and their assemblies

Gold nanoparticle superlattices obtained from nanoparticles capped by alkanethiols of different chain lengths (octane, dodecane and hexadecane) have been investigated. It is observed that as the chain length of the thiol increases; the propensity to form superlattices decreases and the melting of the superlattice is observed at lower temperature. However, the formation of the 3D superlattice is critically dependent on the presence of "excess" thiol as determined from thermogravimetric and transmission electron microscope analysis. In the absence of "excess" thiol, only 2D hexagonally closed packed arrangements were seen.

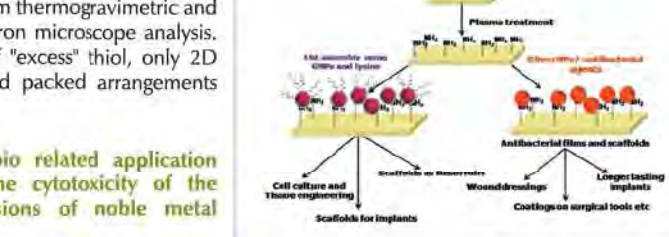


Melting characteristics of the superlattices of gold nanoparticles capped by thiols of varying chain lengths both in the presence of absence of excess thiols

Evaluating the bio related application potential and the cytotoxicity of the aqueous dispersions of noble metal nanoparticles

Recently we have made significant progress in making glycolipid conjugated metal nanoparticle where the chosen glycolipid - sophorlipid - acts as both reducing and capping agent for the synthesis of nanoparticles. These have been shown to be good as drug delivery and antibacterial agents. A systematic cytotoxic and genotoxic evaluation of glycolipid conjugated silver and gold nanoparticles is carried out on HepG2 cells.

These glycolipid conjugated nanoparticles are found cytocompatable up to their 100 μM metal concentrations. Amongst the two metallic systems investigated gold nanoparticles are found more cytocompatable than the same concentrations of silver nanoparticles. Similarly it is also demonstrated that at 100 μM silver nanoparticles cause more DNA damage as compared to gold nanoparticles of similar concentrations.



Cytotoxic and genotoxic evaluation of sophorolipid capped gold and silver nanoparticles

Polymer-metal nanoparticle conjugates for cell culture and tissue engineering applications

Ammonia plasma treatment of polymers films leads to generation of amine groups on the surface and these

Polymer membrane modification for cell-culture and tissue engineering applications

are found to be good for cell proliferation and cell attachment applications. However, longer plasma treatment is detrimental to polymer strength and leads to decomposition of the same. We developed a layer-by-layer assembly

Intracellular Ag nanoparticles have been used to prepare nanoparticle embedded in carbonaceous supports that show good antimicrobial properties.

method where the polymers are treated with the ammonia plasma for minimum amount of time and subsequently more amine groups are generated by attaching nanoparticles to surface amine groups on the polymer and grafting amino acids like lysine on the nanoparticle surfaces.

This process leads to the formation of highly hydrophilic polymers. These polymer-nanoparticle-amino acid composites are found to be extremely good for cell attachment and cell proliferation experiments.

Preparation of carbon supported metal nanoparticles through a biogenic route

Intracellular silver nanoparticles produced by exposing silver ions to the fungus Aspergillus ochraceus were heat treated in nitrogen environment to yield silver nanoparticles embedded in carbonaceous supports. This carbonaceous matrix embedded silver nanoparticles showed anti microbial properties against both bacteria (Gram-positive and Gram-negative) and virus (M 13 phage virus). The bactericidal effects were noticed even after washing and repeated exposure of these carbon supported silver nanoparticles to fresh bacterial cultures revealing their sustained activity.

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Miniaturization of capillary electrophoresis on chip for chemical analysis

Background / objectives

Interests in the miniaturization of analytical devices have grown rapidly in the past decade and the technologies based on the lab-on-chip or μTAS concept have been developing dramatically. Microfabrication technology offers much more elegant, precise and inexpensive route for the manufacturing of such Microsystems. Prime objectives of the project are:

- Development of microfluidic cells based on soft lithography.
- New cell designs.
- Surface treatments for microfluidic chips.
- Surface modification of microchannels by deposition of SAMs using μCP.
- Development of integrated detection system on chip.

Soft lithography refers to a family of techniques for fabricating or replnicating structures using, elastomeric stamps ad molds, which includes replica molding via physical contact, self-assembly of organic molecules, and templated deposition and size reduction etc.

Polydimethyl Siloxane (PDMS) is the most widely used elastomer for soft lithography applications. PDMS stamps with submicron fidelity can be generated by casting precursor solution against a suitable mold, usually a silicon master that is fabricated by photolithography.

Work done and discussion

We developed a simple new approach for the creation of unique highly ordered self assembly of micro-reservoirs through template modulated solvent vapor back-pressure.

In this scheme a viscous polymer solution is poured onto a PDMS mold bearing simple geometric patterns replicated from a silicon master. Evolution of solvent vapors through the viscous polymer solutions concurrently with cross-linking results in the generation of the patterns not present in the parent PDMS mold.

We further show that the combined patterns thus generated in the polymer can be subsequently transferred to another PDMS mold and used to generate multiple copies of the said patterns. While in principle the choice of the polymer is not limited, we demonstrated the technique using a biodegradable polymer (poly (β-amino ester) having pendant unsaturated C=C bonds, (Scheme 1).The specific polymer used was Poly [Trimethylolpropane triacrylate-co-4, 4'-trimethylenedipiperidine, poly (TMPTA-CO-TMDP)].

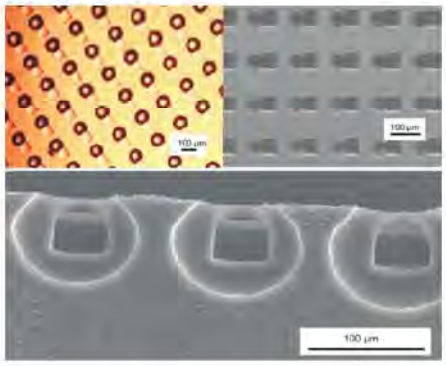

Fig. 1(a) Optical (b) SEM images of self assembled micro-cavities in micropatterned Poly (TMPTA-CO-TMDP). Fig (c) gives cross section image.

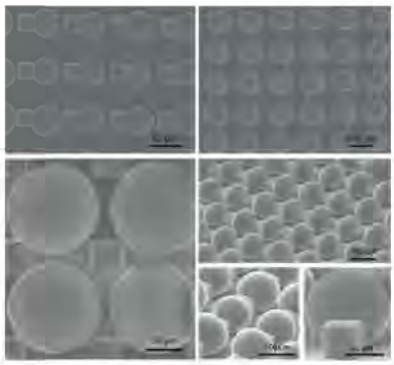

Fig. 2: SEM images of complimentary micro-mushroom PDMS patterns

Polymer MATERIALS

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Complex Fluids and Polymer Engineering

Soft condensed matter, small angle x-ray and neutron scattering and colloidal particles in surfactant mesophase

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Background / objectives
- To study the effect of inclusion of colloidal silica particles in surfactant mesophase
- To investigate the size and concentration dependence of silica particles on the surfactant phase diagram
- To investigate the structural behavior as a function of temperature

Work done and discussion

We investigate the size dependent behaviour of colloidal silica particles in the lamellar phase of a non-ionic surfactant as a function of temperature using small angle x-ray and neutron scattering (SAXS and SANS). The non-ionic surfactant Brij (Polyoxyethylene 4 Lauryl Ether, C12E4) forms lamellar phase at a ratio of 75 wt% in water below 53°C. Above 53°C, the phase is a surfactant liquid. It is known that colloids when dispersed in an ordered matrix get aggregated to form self assembled structures depending on the matrix. When colloids of different sizes are doped into the system, it modifies the interaction which stabilizes the system. We use 3 different sizes of Ludox particles namely 8 nm (S8), 11nm (S11) and 15nm (S15).

The samples were prepared at temperatures high enough so that the system is in isotropic phase. The sample is allowed to cool so as to reach the lamellar phase. The sample is prepared by vortex mixing the surfactant and the 5wt% silica dispersion keeping the surfactant-water ratio constant (75:25) so as to ensure formation of lamellar phases. Fig. 1 shows the SAXS pattern of the neat surfactant phase as well as with particle inclusions (S8, S11, S15). It can be seen that the particle inclusion does not swell or deswell the lamellar sheets.

Fig. 2-4 shows the temperature dependence of the SAXS pattern for particles S15, S11 and S8 respectively. At room temperature, the colloids are aggregated for the case of 15 nm particles (Fig.2). The structure factor peak appearing at $q=0.035$ Å^{-1} does not change till the temperature is about 53°C. At 53°C, the peak starts vanishing indicating that the particles are getting dispersed in the phase. However the behavior of smaller particles (S11 and S8) is very different (Fig. 3 and Fig. 4). Here the structure factor peak does not disappear even at a temperature of 70°C.

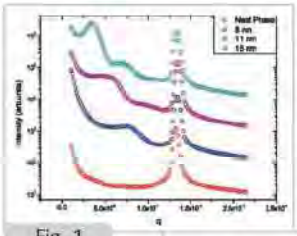

Fig. 1

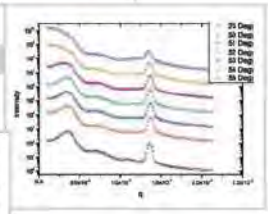
Fig. 2

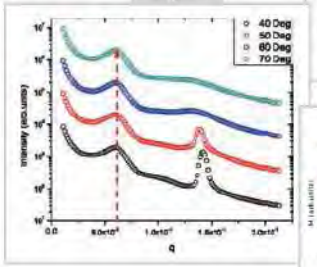

Fig. 3

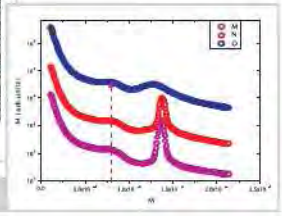
Fig. 4

We investigated the size and temperature dependence of colloidal particle inclusions in a non-ionic surfactant lamellar phase. It is seen that all the particles used does not swell or de-swell the lamellar sheets. The structure peak obtained for S15 inclusion disappears when the temperature is increased to 53°C. However for S11 and S8 particles, the structure does not disappear even at a temperature of 70°C.

It seems that for smaller particle sizes, the particles get trapped between some of the bilayers and are forming some sheet like structures so as to give a peak in SAXS pattern which is coming from the local correlation of sheet like structure of the particles. Once the particles go into the bilayers, it makes some water channels so that there is a tendency for other particles to follow the same path and form sheet like structures.

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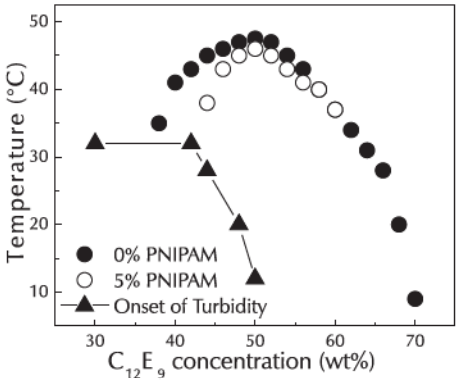
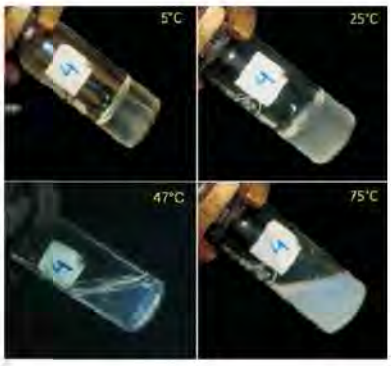
Publication
- *Macromolecules*, **2010**, 43, 4782

Assembly in surfactant mesophases

We demonstrated, for the first time, that for a thermoresponsive polymer, poly(N-isopropylacrylamide), PNIPAM in a weakly interacting surfactant matrix, it is the phase behavior of the matrix rather than the matrix chemistry that governs the coil–globule transition. This investigation combined turbidimetry with optical microscopy, NMR, and SAXS to follow the volume transition of the PNIPAM and the H_1-isotropic transition of the surfactant/water system.



Nonionic surfactants such as $C_{12}E_9$ are known to interact weakly with PNIPAM - thus, there is only a small change in the volume transition temperature for the PNIPAM in isotropic micellar solutions of $C_{12}E_9$, even for relatively high concentrations of $C_{12}E_9$.



Interestingly, once the surfactant forms an H1 phase, there is a dramatic decrease in the coil?globule transition onset temperature. We believe that this behavior results from a competition between $C_{12}E_9$ in the H_1 phase, and PNIPAM to associate with water.

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Publication
- *J. Non-Newtonian Fluid Mech.*, **2009**, 21

Numerical simulations of polymer extrusion processes

Background / objectives

The processing performance of polymers is governed to a large extent by the rheological properties of the polymer melt, which in turn are decided by the molecular architectural attributes such as a molecular weight distribution and long chain branching. The objective of this work is to use rheological constitutive equations that are derived from coarse-grained molecular models to predict polymer extrusion processes, which often involve free surfaces. For this purpose a special ALE algorithm developed by TRDDC for metal processing has been adapted to perform CFD simulations of viscoelastic materials.

Work done and discussion

We have demonstrated successful application of the ALE algorithm to the simulation of axisymmetric and quasi-planar die swell of extrudates of polyethylenes of two different molecular architectures: linear low density PE (containing only short chain branching) and long chain branched PE (containing long chain branching in addition to short chain branching).

Fig.1 shows experimental rheological measurements of LLDPE and LDPE in shear and extensional flows. Lines through the data show fits of the pom-pom constitutive equation to the data. Fig. 2 shows experimental flow birefringence measurements of the LLDPE and LDPE through a slit die and ALE simulations of the flow. Fig. 3 shows experimental measurements of the extrudate swell of LLDPE. The lines through the data points are results of ALE simulations. For LDPE quantitative comparisons were obtained for equilibrium swell data only.

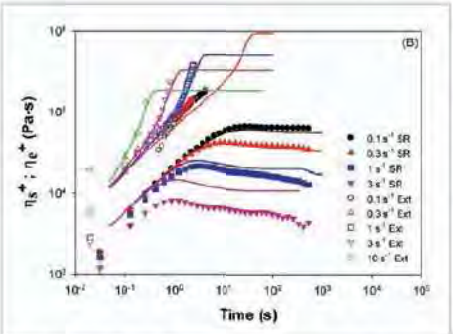

Fig. 1: Non linear rheology of LDPE (left) in shear and extensional flows. Lines show fits of pom-pom constitutive equation to the data. Flow birefringence data for flow of LDPE through a slit die. Lines show ale simulations using pom-pom constitutive equation.

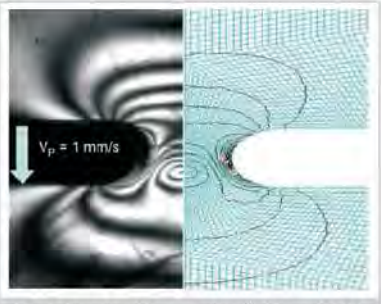

Fig. 2. Flow birefringence data for flow of LDPE through a slit die. Lines show ale simulations using pom-pom constitutive equation data.

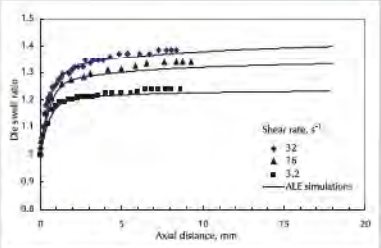

Fig. 3: Experimental measurement of extrudate swell and comparison with ale simulations

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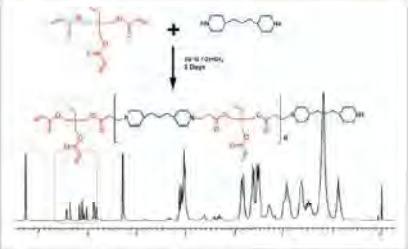
Template assisted highly ordered novel self assembly of micro-reservoirs and its replication

Micro-patterned polymers are being increasingly used in micro-nano-devices, biomimetics, tissue engineering scaffolds and biosensors. Photolithography has been extensively used for the fabrication of such uniform, ordered two-dimensional microstructures. For micro patterning of polymer surfaces, UV micro-embossing and hot embossing are commonly used. Pattern geometries that can be processed by replication are limited to those that can be obtained by optical lithography.

More complex topologies such as spheres or ellipsoids are difficult to fabricate and creative modifications of existing techniques are needed to develop cost competitive solutions. A new approach has been developed for the creation of highly ordered mixed micro-cavity pattern comprising replica of the parent mold and an additional correlated self generated one (not present in the parent mold) through template modulated solvent vapor back-pressure.

Synthesis of poly (trimethylol-propane triacrylate -co-4,4'-trimethylene-dipiperidine)



Scheme 1: Synthesis of Poly (TMPTA-CO-TMDP)

Fabrication of PDMS mold and micropatterned polymer films

PDMS molds with desired micro-patterns were fabricated using widely used PDMS prepolymer Sylgard 184. These PDMS molds were then used for UV embossing of poly (Trimethylol propane triacrylate-co-4,4'-trimethylene dipiperidine).1-hydro-xycyclohexyl phenyl ketone dissolved in dichloro methane (DCM) was added as a photoinitiator The polymer was then exposed to UV light for 15 min and was peeled off after curing from the PDMS mold. Viscosities of the polymer solution were adjusted by varying solvent content.

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Functional Polymers

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Development of materials/chemicals for PJ-10 system

A project entitled "Development of Materials/Chemicals for PJ-10 System" was sponsored by DRDO, India in Feb. 2009. The aim of this project was "the indigenization of polymeric and chemical materials for air frame of BrahMos missile".

BrahMos is a supersonic cruise missile that can be launched from submarines, ships, aircraft or land. It is a joint venture between India's Defense Research and Development Organization (DRDO) and Russia. BrahMos missile travels at speeds of Mach 2.5 to 2.8 and is the world's fastest cruise missile. More than 200 polymeric and other materials are used in the fabrication of BrahMos. Out of those, 15 critical materials are being developed at NCL.

Polyimide is most important polymeric material used in BrahMos missile for air frame. NCL has completed the lab scale technology for the synthesis of polyimide binder resin and has transferred it to DRDL/ASL (Defense Research and Development Laboratory/Advanced Systems Laboratory) Hyderabad. A vendor has been identified by DRDL/ASL for its manufacture. In close association with NCL and ASL scientists, the vendor has progressively scaled up polyimide technology in 4 steps to a 20 kg batch size. Simultaneously, the polyimide is being evaluated for the preparation of composites. In this exercise, NCL, ASL, BrahMos as well as scientists associated with 3 vendors are working closely with L&T.

NCL has also completed the preparation of special solid resole resin as well as urethane systems. These will soon be transferred to DRDO for further action steps towards eventual commercialisation.NCL has filed six patent disclosure letters (PDL) as below:

PDL No	Title of the PDL
1	Amino functionalised polyimide telechelics
2	Amino functionalised polyimides with enhanced stability
3	Amino functionalised polyimides with crank-shaft amines for enhanced processibility and stability
4	Ethyl oligo-silicates with strong acid heterogeneous polymer catalysis
5	Amino-phenol-formaldehyde resins by strong base macroreticular polymer supported catalysis
6	Amino-phenol-formaldehyde resins by in-situ generation of catalyst

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Polymers from Renewable Resources

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Publications
- *Carbo Polym,* **2009**, 76, 23, 63
- *Bioresources*, **2009**, 4, 1669
- *Biores Technol,* **2009**, 100, 6679
- *Trends Carbo Research*, **2009,** 1(2), 10

Studies in biomass polymers, natural polymers and environment friendly polymers: lignocelluloses, cellulose, chitosan, and biodegradable polymers

Background / objectives

Lignocellulosic biomass constitutes the largest group of natural materials for sustainable development of chemicals, fuels, polymers, and composite materials available to mankind. 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. Investigation of the reactions, derivatives of such polymers is therefore a prime area of current R & D worldwide.

Technologies for obtaining these individual polymers in a pure state, as well as derivatising it to value-addded 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.

Similarly, another aspect of this field of work concerns the development of the science and technology of biodegradable polymers synthesized from synthetic polymers as well as from natural polymers 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, we mainly concentrated on certain aspects of cellulose chemistry, especially new derivatives that are difficult to characterize, such as Schiff's bases based on 2,3-dialdehyde cellulose and 2,3-dicarboxy cellulose The polymers so derived were characterized for their structure, morphology, molecular weights, antimicrobial and biodegradable properties based on fungal strains.

In the area of chitin/chitosan chemistry also we are exploring antimicrobial derivatives for applications in packaging applications.

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. Several novel polymers with multi-group moieties have been anchored onto styrene-butadiene-styrene and thoroughly characterized by a variety of tools. The work has thrown new light on the antimicrobial properties of such polymers

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Value added chemical from cashew nut shell liquid

Background / Objective

The aim of this project is to design and synthesize difunctional monomers, such as, diphenols, diacids and diamines starting from cashew nut shell liquid (CNSL), an inexpensive and abundantly available renewable resource material, and to utilize them for the synthesis of processable high performance polymers.

Work done and discussion

As a continuation of our program on the utilization of CNSL, a range of difunctional monomers, such as, diphenols, diacids and diamines were synthesized starting from CNSL making use of simple organic transformation reactions (Fig. 1).

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

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

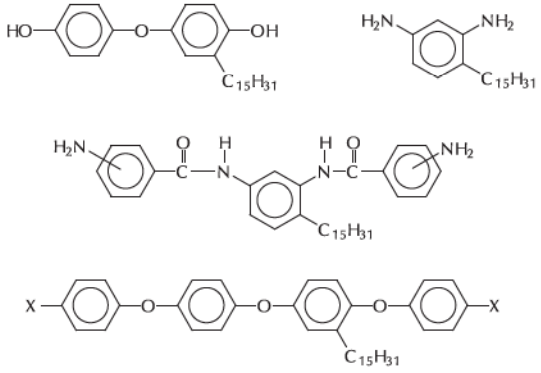

Fig. 1

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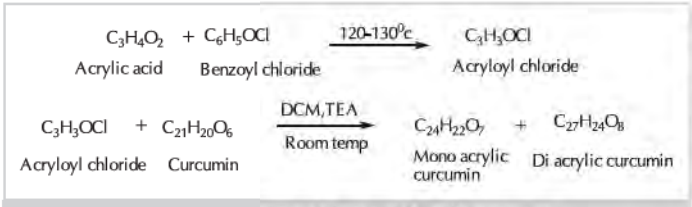
Publication
- *Patent application INV-2009-33*, **2009**

Development of drug conjugated and metal chelated polymers and their nanofibers

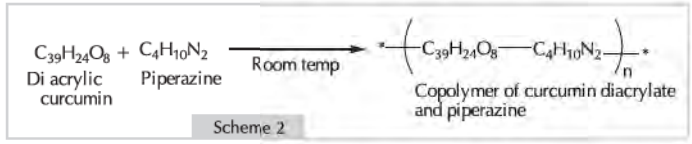
Background / objectives

Nanotechnology is well advancing in many areas including biomedical and biotechnological applications because the products created with nanotechnology are smaller (1-1000 nm), cheaper and more efficient with unique properties. We are focusing our research in developing the nanomaterials to meet the requirements such as efficient wound healing and metal extracting materials. Curcumin is antibacterial, antioxidant and anti tumor agent. Hence is being used for various biomedical applications.

Synthesis of polymer immobilized curcumin by conjugating or derivatizing curcumin with acrylic monomers



Scheme 1: Curcumin derivative with acrylic monomers



Scheme 2

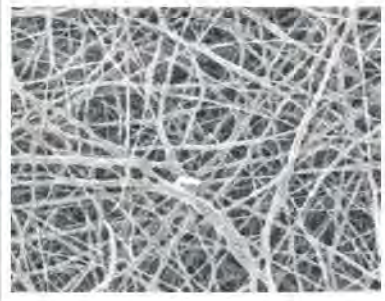
We were successful in developing curcumin derivatives with monomers of acrylic and methacrylic acid. The obtained diacrylic curcumin monomer was reacted with piparizene to achieve co-polymer of piparizene and polyacrylic curcumin. The molecular weight of the polymer is yet to be determined. For example, the reaction methods are reported in scheme-1 and scheme-2 to obtain co-polymer of curcumin diacrylate and piperazine.

Biomedical applications [scaffolds, wound dressings, bone implants]

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 were on average 100 nm in diameter.

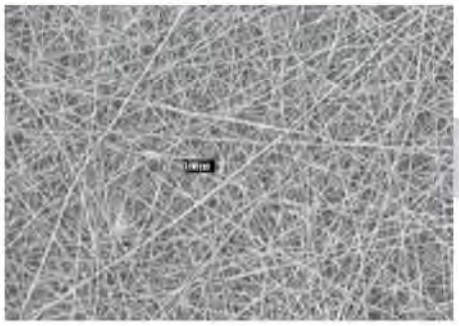
The nanofibers were loaded with 15 % diltiazem hydrochloride, crosslinked and controlled drug release studies were done in pH 7.4 at 37°C. The drug release experiment recorded only 70 % of release over 24 h and 30 % of it still remained in network which would further release over an extended period.



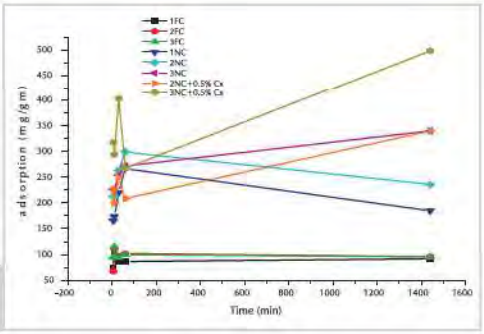
Drug loaded nano-fibers of sodium alginate and PVA blends

Metal extraction materials

Sodium alginate and PVA nanofiber mats were also evaluated to determine the efficiency to metal adsorption. The results indicated that the metal adsorption by the nanofibers was three times more than the films of the same composition of sodium alginate and PVA. The



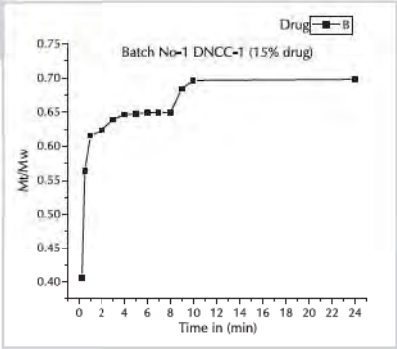
Egg albumen and polyvinyl alcohol nanofibers



Metal adsorption studies of films and nanofibers

reason for more adsorption is due to increased surface area of nanofibers. The nanofibers immobilized with metal chelating agent, cyanex 272 has record highest adsorption of copper metal. Also the metal adsorption increased with increase in sodium alginate.

Controlled drug release studies of nanofibers



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Carbohydrate Chemistry

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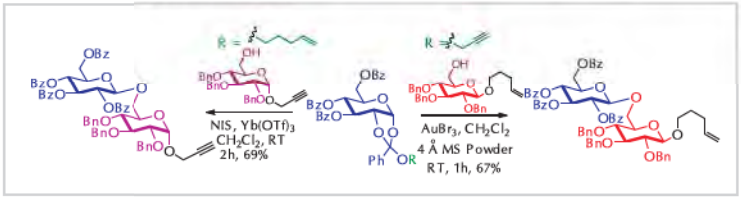
Publications
- *J. Org. Chem.*, **2009**, 74, 9233
- *Chem Commn*, **2009**, 2505
- *Langmuir*, **2009**, 25, 2339

Carbohydrate chemistry/ chemical glycosylation

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 number of oxygen atoms and chiral centers as well as they 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, easily prepared 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.

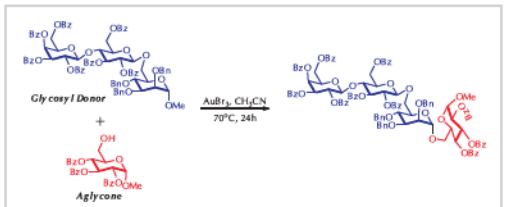
Gold mediated glycosylations

In continuation of our studies on the propargyl glycosides as glycosyl donors, the orthogonal activation of propargyl glycosides/1,2-orthoesters in the presence of pentenyl glycosides/ orthoesters using a catalytic amount of $AuBr_3$ was investigated. It is interesting to note that the propargyl 1,2-orthoesters can be activated using Au(III) salts in the presence of n-pentenyl glycosides and pentenyl 1,2-orthoesters can be activated in the presence of propargyl glycosides. Resulting propargyl/pentenyl saccharides can be utilized to synthesize pseudo-oligosaccharides, neoglycoconjugates and higher saccharides.

Methyl glycosides as glycosyl donors

Methyl glycosides were identified as novel and stable glycosyl donors. A diverse range of aglycones are shown to react with methyl glycosides, resulting in the formation of corresponding glycosides and disaccharides in good yields.

The anomeric configuration of either the glycosyl donor or the glycosyl acceptor did not influence either progress of the reaction or the anomeric diastereoselectivity of the resulting disaccharide. Interesting to note that tri- and tetra- saccharides were synthesized from respective di- and tri- saccharides exploiting salient features of this novel glycosylation protocol.

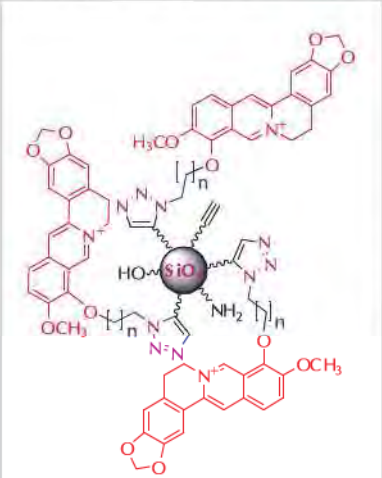


Natural product-silica conjugates as biological probes

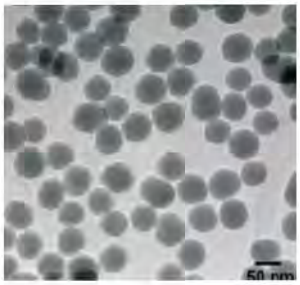
The synthesis and biological characterization of novel prototype, namely, silica nanoconjugates bearing a covalently linked berberine, a plant alkaloid known to have antiproliferative activity was studied. The effect of synthesized

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.

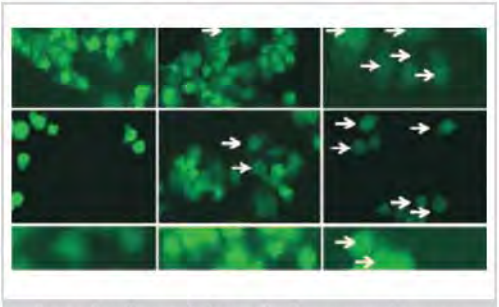
Our results show that all the nanoconjugates display higher antiproliferative activity than free berberine. The ability of these nanoconjugates to inhibit cellular proliferation is mediated by the cell cycle arrest at the G1 phase. Moreover, silica nanoconugates caused selective apoptotic arrest with a higher efficiency than free berberine followed by apoptotic cell death.



Silica–berberine nanoconjugates



Morphology of nanoparticles after capping



Apoptotic cells morphology under florescence microscopy

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Publication
- *J. Str. Chem.*, **2010**, 51, C.693

Reactions in crystals

Background / objectives

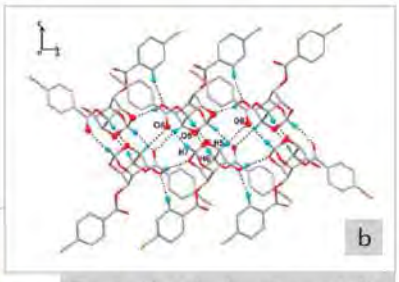
To study quantitative structure - reactivity correlation and mechanism of acyl transfer reactions in the solid state and create supramolecular structures that exhibit acyl transfer reactivity.

Work done and discussion

The crystal structure of racemic 2,6-di-O-benzoyl-*myo*-inositol 1,3,5-orthoformate (1) which underwent a facile intermolecular benzoyl transfer reaction in the solid state, revealed a helical assembly of molecules along the two-fold screw axis *via* O-H···O hydrogen bond bringing the electrophile (C=O) and the nucleophile (-OH) in close proximity along the helical axis. But, structurally related racemic 2,6-di-O-(p-halobenzoyl)-*myo*-inositol 1,3,5-orthoformates (bromo-2 and chloro-3) produced triclinic dimorphs (both P-1) when crystallized from methanol and ethyl acetate.

Molecules in either form did not assemble spirally (like 1) instead, exhibited a one-dimensional isostructurality, bridging O-H···O linked identical molecular strings via C-H···O interactions across the inversion center (Fig. 1). However, the molecules of 2 and 3 assembled in a helical manner similar to 1 with inclusion of solvent molecules in the crystal lattice when crystallized from other common organic solvents (Fig. 2). Remarkably, in all the solvates the host molecules formed strikingly similar helices around the crystallographic 2$_1$-screw axis through O-H···O bond involving -OH group and carbonyl oxygen of the equatorial C2-O-benzoyl group.

Comparison of the crystal structure of dimorphs and the solvatomorphs revealed that the solvent molecules, which interact with the orthoformate-bridge, trigger the helix formation of the host. The helical organization achieved through solvent mediation and inclusion is of significance in creating molecular packing for intermolecular acyl transfer reactions in crystals.



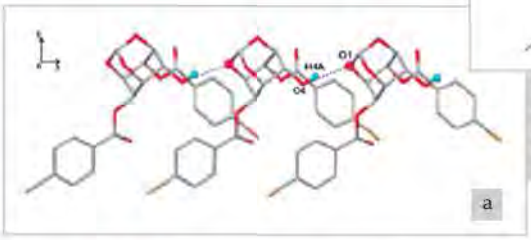


Fig. 1: (a) Molecular strings and (b) subsequent bilayers formed by O-H...O and CH...O interactions in Forms I and II crystals of 2.

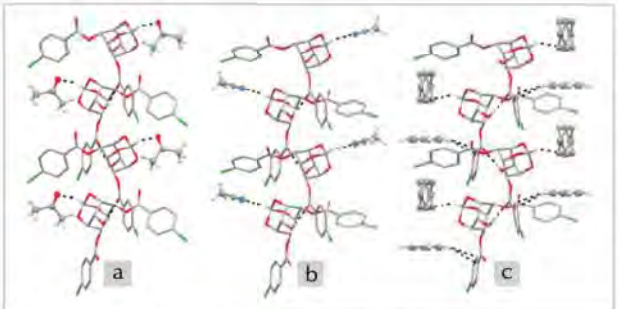


Fig. 2: The solvent molecules in crystals keep the orthoformate bridge engaged in solute-solvent interactions, coaxing the molecules of 2 and 3 to assemble in helical pattern.

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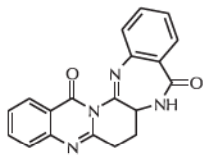
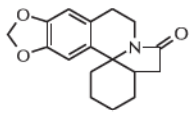
Publications

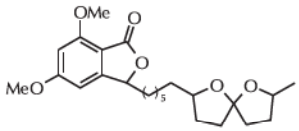
- *J. Org. Chem.*, **2010**, 75, 2702, 3121
- *Tetrahedron*, **2009**, 65, 5244
- *Tetrahedron: Asymmetry*, **2009**, 20, 220

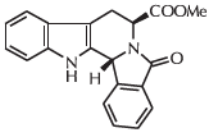
Total synthesis of recently isolated bioactive natural products

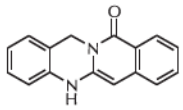
Total synthesis of bioactive natural products occupies keystone position in organic chemistry. The real challenge lies in designing these molecules using highly efficient and practical routes. Past several years, we have been busy in total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors, employing variety of new synthetic strategies. The list of nitrogen/oxygen containing natural products synthesized during the past year includes Auranthine, Erythrina Alkaloid, CJ-compound, Isoindolo-β-carboline and Nuevamine.

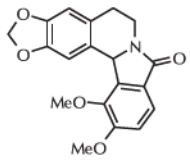

Auranthine


Erythrina alkaloid
(Basic Skeleton)


CJ-Compound


(+)-Isoindolo-beta-carboline


Isoquinolinoquinazolinone
(Unnatural)


(+)-Nuevamine

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Methodologies, Asymmetric Synthesis and Organometallics

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Publications
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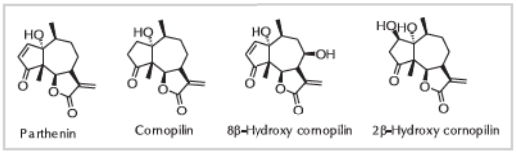
- *Bioorg. Med. Chem. Lett.*, **2009**, 19, 5590
- *Tetrahedron Lett.*, **2008**, 49, 2598

Natural products chemistry

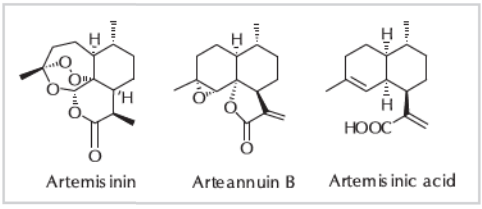
Chemical examination of *Parthenium hysterophorus* for bioactive secondary metabolites

Our efforts in the chemical examination of the plant, Parthenium hysterophorus for bioactive secondary metabolites has led to the isolation of following compounds. Besides these, two more compounds have been isolated and their structure elucidation is in progress. At present, the identified molecules are being evaluated for their antimalarial efficacy.

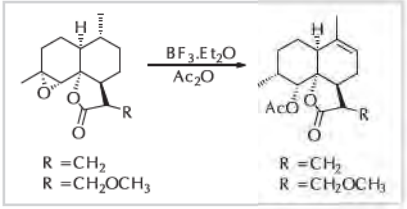


Chemical transformations of abundant natural products into bioactive molecules

The three major secondary metabolites isolated from the plant, *Artemisia annua* are artemisinin, arteannuin B and artemisinic acid.



In an attempt to chemically convert arteannuin B to artemisinic acid, we treated arteannuin B with $BF_3.Et_2O$ and Ac_2O at 0-5 °C, an interesting rearranged product was obtained which might have formed due to 1,3- or 1,5-hydride shift. Also, the Michael addition product of arteannuin B furnished the similar rearranged product under similar reaction conditions. This type of rearrangement in sesquiterpene lactones is hitherto unknown and at present we are trying to generalize this reaction with different sesquiterpene lactones.

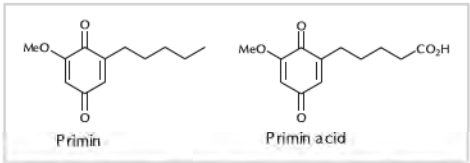


Synthesis of the antibacterial benzoquinone primin and its water-soluble analogue, primin acid

Primin, 2-methoxy-6-pentylbenzoquinone, has been isolated from a variety of plants, including *Primula obconica* (primrose) and *Miconia sp*. In addition to its antimicrobial and insect feeding activities, this benzoquinone is also known for its allergenic properties. Primin is indeed a strong sensitizer and has long been recognized to induce contact dermatitis.

Synthetic primin has been included for some time in the European standard patch testing series, which is used to identify plant sources in people subject to contact dermatitis. The immune response is believed to be mediated by the formation of antigenic adducts resulting from the Michael addition of the nucleophilic protein residues to the quinone.

The limited solubility of primin (LogP 2.99) in aqueous media prompted us to carry out synthesis of a more water-soluble analog, primin acid (LogP 0.96, i.e. about 100 times more hydrophilic) was selected.



We have achieved synthesis of antibacterial benzoquinone, primin and its water-soluble analog primin acid using Grignard reaction and Johnson-Claisen rearrangement as the key steps. The overall yield of primin and primin acid is 34 % and 25 %, respectively.

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Methodologies, Asymmetric Synthesis and Organometallics

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Publications
- *Tetrahedron Lett.*, **2009**, 50, 6562
- *Bioorg. Med. Chem. Lett.*, **2010**, 20, 722

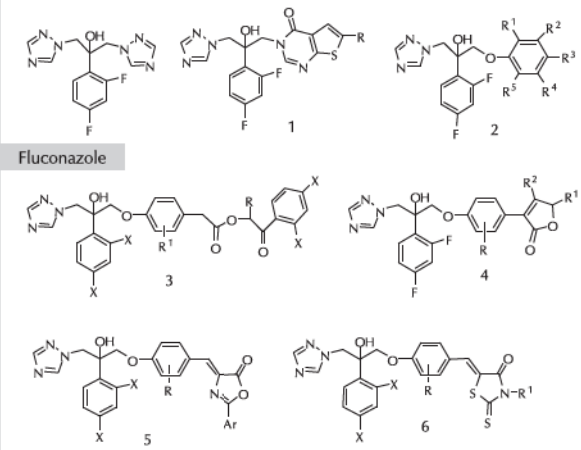
Synthesis of novel antifungal compounds

Background / objectives

Azole antifungals are widely used in the treatment of various fungal infections and fluconazole is an important member of this class of drugs. Its extensive use has resulted in emergence of fluconazole-resistant fungal strains and it is necessary to have new antifungal agents to take care of the infections caused by the resistant fungal strains. We have undertaken synthesis of fluconazole analogues and our research has resulted in synthesis of novel antifungal compounds which are being studied further.

Work done and discussion

A number of fluconazole analogues were synthesized as a part of our current efforts in the direction of developing novel antifungal agents. A series of compounds with general formula 1 were prepared in order to improve the pharmacological properties of the lead compound of this group. It was observed that compound 1 with R=C_5H_{11} exhibited highest activity and it is being studied further at FDC Ltd Mumbai.



Fluconazole analogues with general formula 2 were also synthesized at NCL and screened for antifungal activity at FDC Ltd and it was observed that most of these molecules exhibited good activity against *Candida* strains. Efforts are on to modify these molecules to get compounds with maximum antifungal activity and broad spectrum of activity.

These compounds were further converted into the new chemical entities 3 and hybrid molecules 4 in an attempt to get more active molecules. The compounds with general structure 4 were found to have significant antifungal activity. Some of the compounds with general structure 2 were converted into hybrid molecules 5 and 6 to check their potential as antifungal agents and it was observed that they did not exhibit significant activity.

This made us to synthesize new compounds of a different class and most of the compounds of the new group have exhibited very good antifungal activity and further work is in progress. A patent will be filed for this group after making a few more molecules of this group.

Resolution of some of the active molecules was done to check the activity of individual enantiomers. The active enantiomers are being scaled up for further study.

Organic CHEMISTRY

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Methodologies, Asymmetric Synthesis and Organometallics

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Publication
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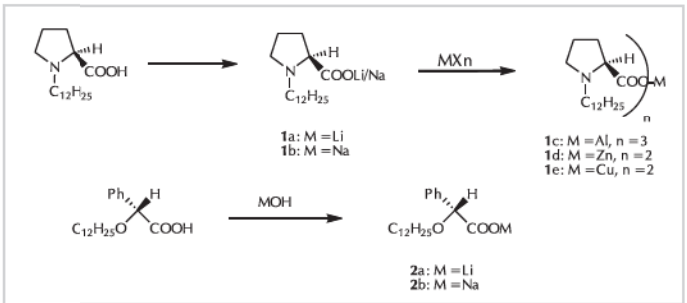
Asymmetric synthesis

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

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.
Last year we reported that we have succeeded in the preparation of a variety of RZnX (X = halogen) through direct insertion reaction with specially activated zinc.

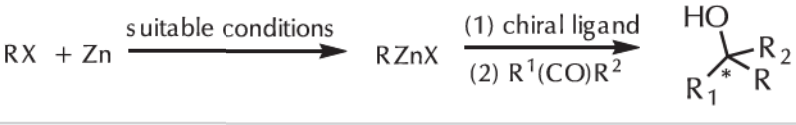


Unfortunately these reagents were found to unreactive towards aldehydes, ketones and imines. Although we could not isolate RZnX reagents for spectroscopic characterization, experimental evidence was collected to establish their oligomeric structure.

One of the ways to make these react, would be to use stoichiometric amount of bidentate ligands e.g. morpholine derivatives. Alternative strategy would be to provide intramolecular chelation, for example in RZn(OAc). We have now proved that indeed both protocols are feasible. We are thus closing on to our long pursued target of a general, reliable and enantioselective procedure for the alkylation of carbonyl group.

Micellar catalysis

Very recently, we have undertaken work on enantioselective reactions in aqueous media. This is more of a concept-driven exploration. We envisaged that suitably designed organometallic complexes could prove to be useful amphiphilc catalysts. A series of simple lipophilic ligands and their water-stable complexes were therefore prepared. Amongst these, molecules like **1**a,b & **2**a,b are Bronsted bases whereas **1**c,d,e are Lewis acids. Target reactions for these catalysts are Mukaiyama aldol reaction, Michael reaction, Henry reaction and cleavage of *meso*-epoxides. The findings are still under preliminary stage and work is in progress.



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Publications

- *Org. Lett.*, **2009**, 11, 2611
- *Tetrahedron Lett.*, **2009**, 50, 3425
- *Tetrahedron*, **2010**, 66, 3159
- *Synthesis*, **2010**, 1479

Developing new synthetic methodologies and enantioselective synthesis of biologically active natural products

The theme of the work is to develop new methodologies and their application to the enantioselective synthesis of biologically active natural products. Our research in this area is mainly focused on asymmetric synthesis of naturally occurring lactones and amino alcohols.

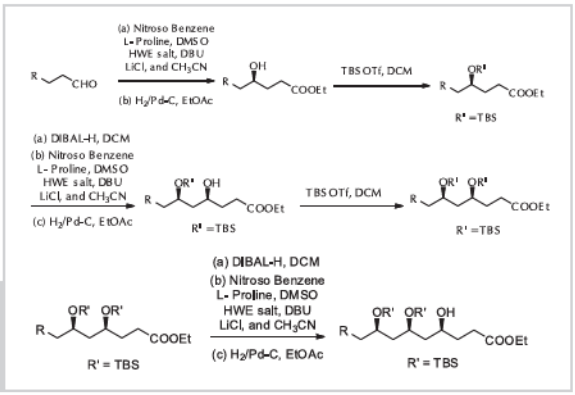
Asymmetric synthesis of naturally occurring amino alcohols and lactones

We ahve worked on the total asymmetric synthesis of a wide variety of biologically useful compounds mainly employing the AD/AE/AA/ Jacobsen hydrolytic kinetic resolution or organocatalysis as the source of chirality and ring closing metathesis as one of the key steps. These target molecules include phytosphingosine, aspinolide, decarestrictine J, aculeatins, galantinic acids and hydroxylated piperidine and pyrrolidine alkaloids. We have developed proline catalyzed iterative approach for the construction of enantiopure syn- and anti-1,3-polyols and 1,3-amino alcohols via organocatalysed aminoxylation of aldehydes which were successfully employed for the synthesis of some important biologically useful compounds. The Highlights of this methodology are following.

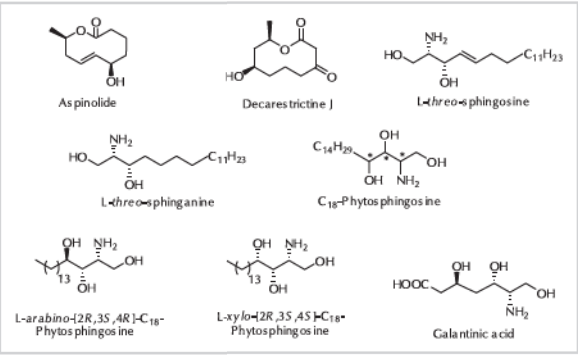
One-pot method was developed for the synthesis of γ-hydroxy ester starting from phenyl propanal by sequential aminoxylation with proline followed by HWE olefination reaction. The ee was found to be 98%.

- First cycle of iteration using L-proline gave the 1,3-syn-diol in 10:1 ratio while D-proline afforded the anti-diol in more than 95% de. Each iteration consists of DIBAL-reduction of ester, aminoxylation, HWE olefination and H_2-Pd/C reduction.
- Second cycle of iteration using L-proline-catalyzed sequence of reaction provided syn/syn-1,3,5-triol as 10:1 inseparable mixture of diastereomers which were nicely separated after TBS protection of the hydroxyl group.

The above methodology was applied to the synthesis of pheromone component (2S, 3S)-2-hydroxyhexylcyclopentanone



Strategy for making 1, 3-polyol building blocks by repetitive sequential α-aminoxylation and HWE olefination of an aldehyde



Some of the molecules we have accomplished the total synthesis recently are following

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- *Tetrahedron Lett.*, **2009**, 50, 2643
- *Synth. Commun.*, **2010**, 40, 1391
- *US patent*, **2007**, 7, 227,039

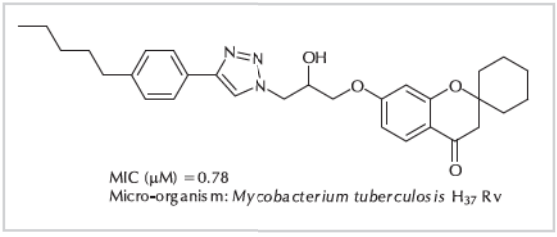
Design, synthesis and biological evaluation of natural product-like small molecules/ Asymmetric synthesis of pharmaceutically important compounds

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

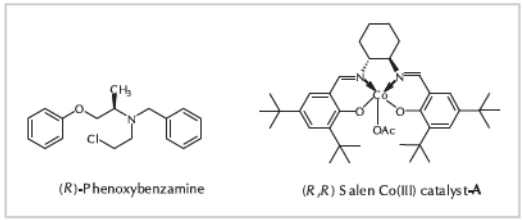
In recent years, there has been re-stimulated interest in nature's repertoire of structures and many strategies are being adapted to exploit advantageously the features of natural products in the design of novel small molecules for various biological applications, especially in the area of drug discovery and chemical biology.

In this context, as part of our ongoing program dealt with design, synthesis and biological evaluation of novel small molecules, we prepared many natural-product like small molecules based upon privileged chromone motif as a parent scaffold.



The new compounds synthesized are systematically being applied for their biological properties. During preliminary evaluation, we identified a novel triazole fused spirochromone conjugate, showing significant in vitro anti-TB activity against *Mycobacterium tuberculosis* and its potency is better than first line antibacterial drug ethambutol.

Further, in continuation of our work in the area of asymmetric synthesis of pharmaceutically important compounds, we recently developed a practical and highly enantioselective synthetic route to an α-adrenergic receptor blocking agent (R)-Phenoxybenzamine (DibenzylineR) using Jacobsen's hydrolytic kinetic resolution method as a key step.



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Publications

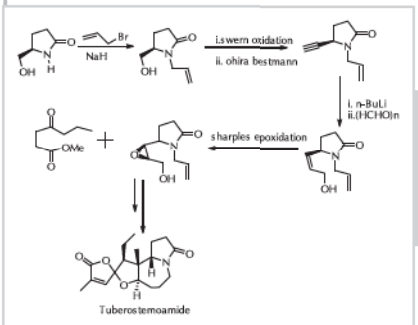
- *Org. Lett.*, **2009**, 11, 2547
- *Org. Biomol. Chem.*, **2009**, 7, 3300
- *Tet. Lett.*, **2009**, 50, 3296

Total synthesis of complex bioactive natural products and azasugars

The total synthesis of Tuberostemoamide

As there are large numbers of natural products containing pyrrolidine rings with substituents at the 1-, 2-, 3- and 5- positions, we were attracted to the idea of developing a chiral building-block based on a pyrrolidine ring, such that this might serve as a versatile entry into many of these natural product systems. Some representative natural products are manzamine A, stemonine, nirurine and berkleyamide A. The stemona group of alkaloids has received considerable attention from synthetic chemists in the past decade. Root extracts from stemona species have been used in traditional Chinese medicine to treat respiratory disorders. Insecticidal, anti-feedant, and neuromuscular activities of some members of the stemona group have also been noted in the literature.

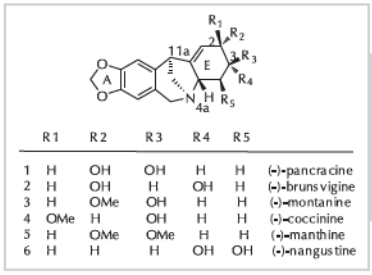
A key feature of this class of alkaloids is the 1-azabicyclo [5.3.0] decane core which is present in most members of this family. (S)-Pyroglutamic acid would serve as the starting material similar to the several reported synthesis of stemoamide. The possible key step for the synthesis of tuberostemoamide will be epoxide opening by enolate followed by cyclisation(Scheme-1)



Scheme 1

Synthetic studies towards the montanine tye of alkaloids

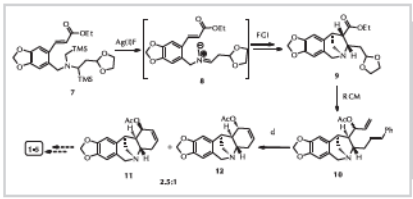
The montanine type of alkaloids belongs to Amaryllidaceae family are known to have common structural feature including challenging 5,11-methanomorphanthridine framework and biological activities such as anxiolytic, antidepressive, anticonvulsive and weak hypotensive activities. Owing to the challenging linearly fused pentacyclic skeleton and some important biological activities associated with these alkaloids, we have been attracted towards the synthesis of these molecules. These are the molecules (1-6) belongs to montanine class of alkaloids.



	R1	R2	R3	R4	R5	
1	H	OH	OH	H	H	(-)-pancracine
2	H	OH	H	OH	H	(-)-brunsvigine
3	H	OMe	OH	H	H	(-)-montanine
4	OMe	H	OH	H	H	(-)-coccinine
5	H	OMe	OMe	H	H	(-)-manthine
6	H	H	H	OH	OH	(-)-nangustine

Fig. 1: Representatives of *Amaryllidaceae* with 5,11-methanomorphenthridine skeleton

Our synthetic scheme employ the 1,3-dipolar cycloaddition of non stabilized AMY for the stereospecific construction of CD-ring and RCM metathesis of the building of E-ring. The cyclized products (11 and 12) were realized to be advance intermediates for the synthesis of these alkaloids by functional group interconversion exploiting the allylic acetoxy functionality for directing the hydroxylation of double bond (Scheme-2).



Scheme 2

A novel organocatalytic asymmetric approach towards prismatomerin type Iridoid class of terpenes

Iridoids are large family of structurally diverse natural cyclopentanopyran monoterpenes that show wide range of biological activities. They are biosynthesized from isoprene and they are often intermediates in the biosynthesis of alkaloids. We are especially attracted to this family since-

- Members of this family exhibit cytotoxic, antileukemic, antimicrobial and antifungal activity,
- Their densely functionalized skeleton possesing the synthetic challenge,
- Interesting cyclic hemi-acetal ring portion, which also makes up part of a cyclic acetal,

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one 'ether' residue of which constitutes the β-oxygen of a spiro-fused α-ethylidene-β-oxy-γ-butyrolactone ring system,

- No asymmetric total synthesis of prismatomerin type Iridoid is known till date.

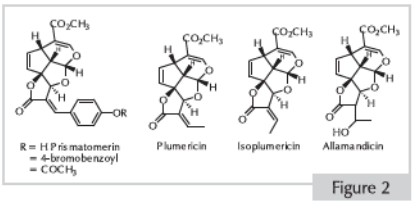


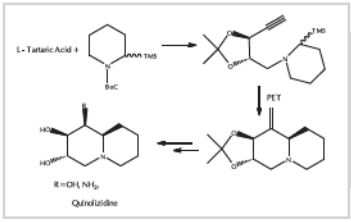
Figure 2

Thus, the objective of the present work is to develop a short, organo-catalytic route towards the asymmetric synthesis of prismatomerin and its analogs of this class of iridoids.

Synthetic studies towards the synthesis of azasugars as potent glycosidase inhibitors

Polyhydroxyazasugars are potent drugs for HIV, cancer, influenza and other diseases because of their glycosidase inhibitory activity. Several new inhibitors have been designed and synthesized by employing a novel and innovative method by the generation of amine radical cation, followed cyclization to electron rich multiple bonds. The olefin functionality generated is utilized to create synthetic diversity.

The Conformationally restricted aza-sugars which resembles to both charge and shape of the presumed half chair transition state (oxocarbenium ion), have also been synthesized as shown below and have shown encouraging carbohydrate specific inhibition.



Scheme 3

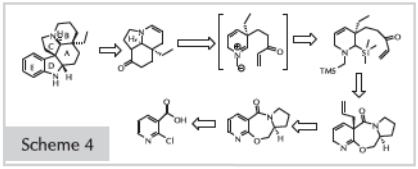
Progress towards total synthesis of (-) - Aspidospermidine employing intramolecular [3+2] cycloaddition of non-stabilized Azomethine ylide

Biological activities and interesting structural features of these alkaloids have generated considerable attention from the many research groups.

The basic skeletal features of these compounds, particularly the complex pentacyclic frame work, that is conformationally rigid due to the cis- relationship of the contiguous stereocentres at C(7), C(21), & C(20).

The construction of the quaternary carbon centre & A/C ring junction is a particular challenge toward the synthesis of this family of natural products.

Impressed by the [3+2] cycloaddition strategy if non-stabilized AMY towards the total synthesis of bioactive molecules, we planned to explore this methodology towards the synthesis of Aspidosperma alkoloids. This method involves the formation of key precursor tricyclic keto amine structure stereo selectively in a single step. So our design of synthesis of aspedospermidine would involve intramolecular [3+2]- cycloaddition of Non-stabilized AMY as a key step.



Scheme 4

Total synthesis of (-)- Lycorine through [3+2] cycloaddition approach of non-stabilized azomethine ylide

Lycorine is an amaryllidaceae class of alkaloids first isolated in 1877. It is found in several plant species such as *clivia miniata*, *Lycoris*, *narcissus* etc. It is an emetic alkaloid. It has other potent biological activities such as antivirul, apoptosis induction etc.

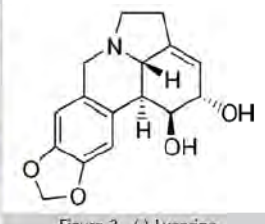
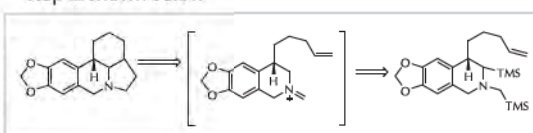
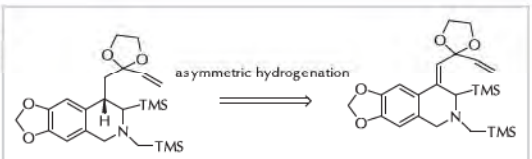


Figure-3 (-)-Lycorine

We have designed to make its core structure through [3+2] cycloaddition of non-stabilized azomethine ylide as a key step as shown below



Scheme 6

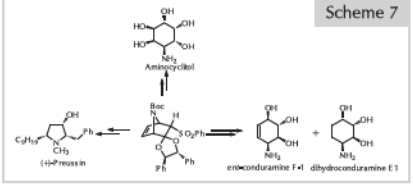


The cycloaddition precursor will come from asymmetric hydrogenation

Studies toward the syntheses of highly functionalised cyclohexanes via asymmetric desymmetrization approach

Aminocyclitols, due to their structural similarity, are a family of carbohydrate mimics, which have attracted a great deal of attention amongst organic and medicinal chemists due to their profound biological activities towards glycosidases. These polyhydroxy glycosidase inhibitors are a widely diverse class compounds often isolated from plants and microorganisms and they have significant therapeuticuse.

Scheme 7

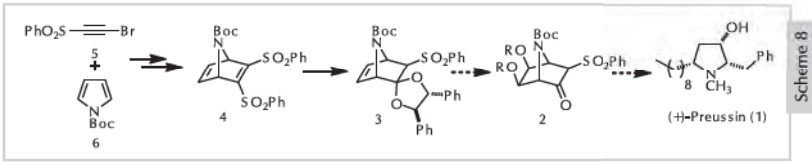


Asymmetric desymmetrization of *meso*-(1R, 4S)-tert-butyl 2,3-bis (phenylsulfonyl) -7-azabicyclo[2.2.1]hepta-2,5-diene-7-carboxylate - Application to the total synthesis of (+)-Preussin

(+)-Preussin (1), a potent antifungal agent possessing a pyrrolidine skeleton, was isolated from fermentation broths of both *Aspergillus ochraceus* and Preussia sp. in the late 1980s. Recently, preussin has been shown to be a potent inhibitor of cell growth in yeast mutants with defective cdc 2 regulatory genes and a potent inhibitor of cyclin E kinase in human tumor cell lines.

(+)-Preussin (1) could be obtained from optically pure 7-azabicyclo [2.2.1] hept-2-one 2, which could easily be obtained via asymmetric desymmetrization of meso-4 (Scheme-8).

The key precursor meso compound 4 was prepared by (4+2) cyclo addition of N-Boc pyrrole 6 and 1-bromo-2-(phenyl sulfonyl) acetylene 5, followed by introduction of second phenyl sulfonyl group on the cycloadduct via conjugate addition of sodium salt of thiophenol followed by subsequent oxidation utilizing the procedure reported in the literature.



Scheme 8

Then desymmetrization of meso compound 4 with disodium salt of (1R, 2R)-1,2-diphenylethane-1,2-diol at -100°c gave optically pure compound 3.
Double bond oxidation of compound 3 followed by removal of chiral auxiliary and subsequent ring opening of bicyclic skeleton under progress.

Desymmetrization of meso olefinic C=C via chiral ketalization: Application in the total synthesis of validamine, valiolamine and 2-epi-valiolamine

Biochemically, carbasugars and cylitols themselves are recognized as the pseudosugars in a living system, and they show interesting biological activities based on the structural similarity to sugars.

The C7N aminocyclitol units which mainly consist of validamine 7, valienamine 8 and valiolamine 9, also called as aminocarbasugars (Figure 4), has been tested as inhibitors of glycosidases enzymes besides being used as biosynthetic building blocks in many antibiotics.

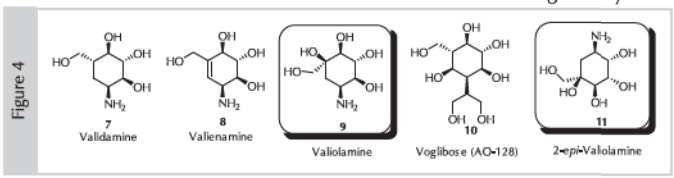


Figure 4

We have designed the Retrosynthesis of 2-*epi*-Valiolamine and Validamine such that both of these molecules can be prepared from the single meso precursor.

This meso precursor on asymmetric Desymmetrization with (R,R)-Hydrobenzoin and ketal deprotection is expected to give Keto 19a from which 2-*epi*-Valiolamine will prepared. While meso precursor on asymmetric Desymmetrization with (S,S)-Hydrobenzoin and on ketal group deprotection is expected to give keto 19b from which Validamine will be prepared.

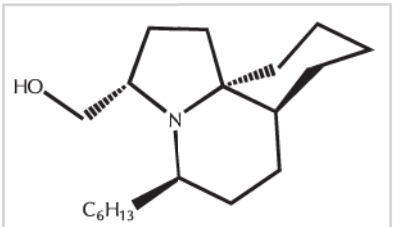
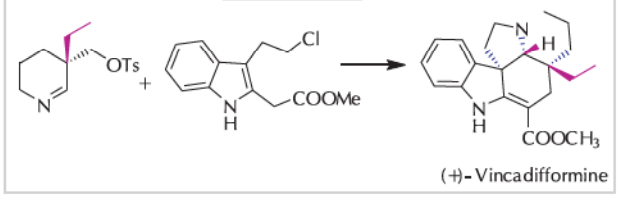


Figure-6: (-)-Lepadiformine

Synthetic studies towards total synthesis of (-)-Lepadiformine

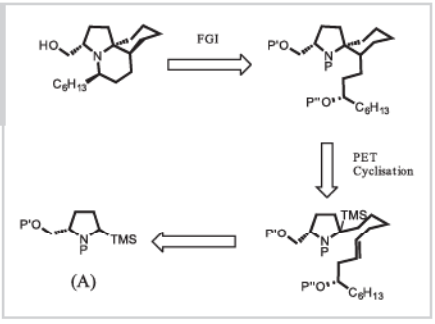
(-)-Lepadiformine is an important marine alkaloid, isolated from marine tunicates Clavelina lepadiformis and Clavelina moluccensis. It shows moderate cytotoxic activity towards various tumor cell lines, also it shows strong activity in the cardiovascular system. (-)-Lepadiformine possesses pyrroloquinoline tricyclic framework with trans-azadecaline ring system. Because of its unique structural feature and important biological activity we have planned a very short and conceptually new route towards enantioselective total synthesis of (-)-Lepadiformine, using our PET cyclization methodology.



Scheme 10

Total synthesis of anticancer agent (+)-Vincadi-fformine

Iminium ion triggered cascade reaction is developed for the total synthesis of anticancer agent (+)-Vincadifformine by the coupling of 3, 3-substituted tetrahydropyridine and indole derivative. The strategy allows simultaneous construction of two new rings, three new sigma bonds and two new stereogenic centers in one pot with complete stereochemical control.



Scheme 9

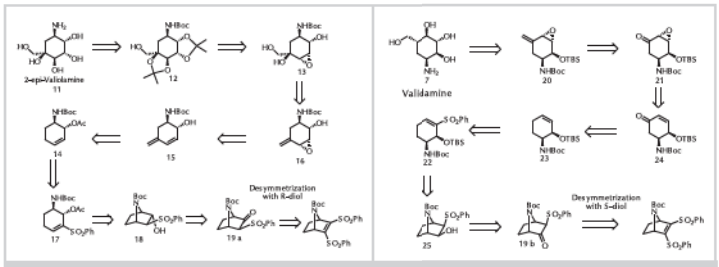


Figure-5
Synthesis of these molecule and other analogues of aminocarbasugar are currently in progress.

Organic CHEMISTRY

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Methodologies, Asymmetric Synthesis and Organometallics

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Publications
- *Tetrahedron.*, **2009**, 65, 9819, **2010**, 66, 390
- *J. Org. Chem.*, **2009**, 74, 2842
- *Tetrahedron Lett.*, **2009**, 50, 271

Total synthesis, metal catalysis and synthetic carbohydrate chemistry

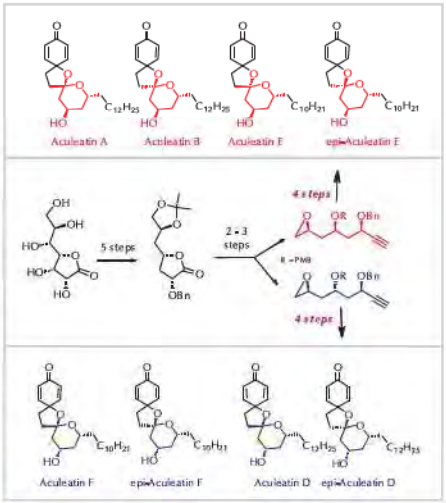
Total synthesis of Natural Products forms the central theme of our research group. Since, their co-existence and their optimization along with the evolution of life, natural products were regarded as pre-validated lead structures for chemical biology and medicinal chemistry research. Secondly, because they have been accommodated in some living organism, either during their own bio-synthesis or through their involvement in the modulation of respective biological processes, natural products and to a major extent natural product like small molecules can move fast across the critical pharmacokinetic and bioavailability barriers when compared with a randomly synthesized small molecule.

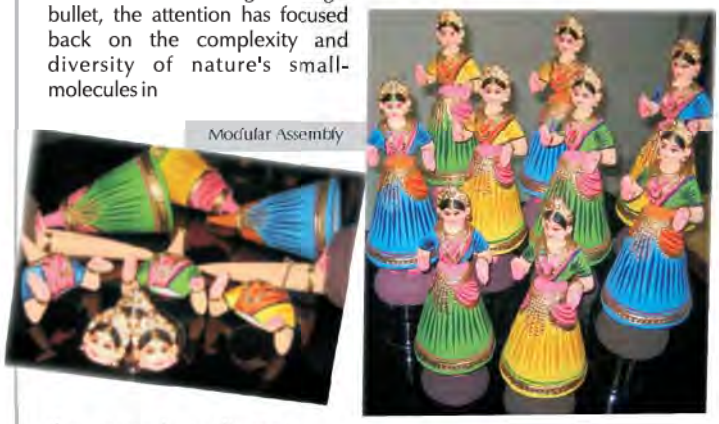
As a part of our total synthesis program, we aim to develop new strategies and methods that make the process of synthesizing natural products as efficient and flexible as possible. We will explore this to generate small libraries of the congeners of the identified natural products with proven biological activity and their further biological evaluation.

Target cum flexibility concepts for the natural product like small molecule library synthesis

In the wake of the failure of the combinatorial libraries in delivering a magic bullet, the attention has focused back on the complexity and diversity of nature's small-molecules in the new drug discovery programs. Concepts funded upon the designing around, and of the synthesis of natural products and natural product like small molecules have provided a direct entry of "total synthesis programs" 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 product 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 programs. In this presentation, we describe a simple yet powerful technology to addresses the synthesis of natural product like small molecules with a flexibility window to modulate the chemical properties.



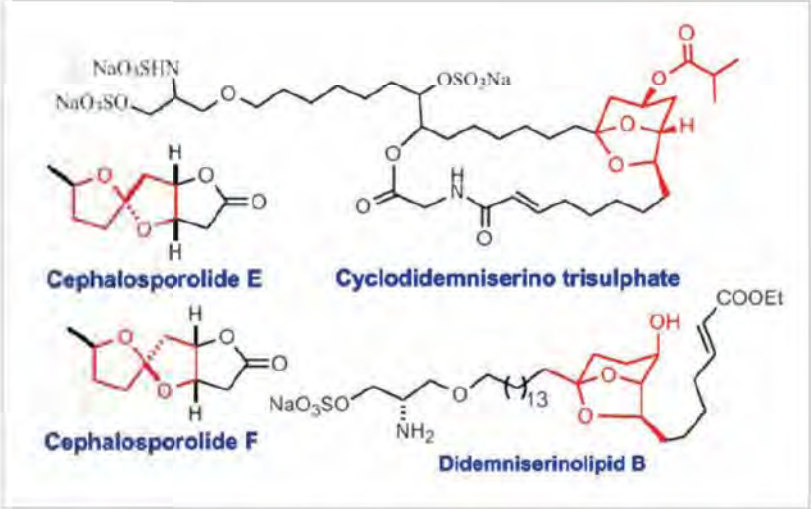

Modular Assembly

The underlying motive of our approach will be the identification of complexity generating transform(s) that should address the critical skeletal construction at an advanced stage and be flexible for employing the simple, inexpensive, easily available materials so as to create natural product-like small-molecule libraries rapidly. In essence, this approach could be identified as "Target cum Flexibility Oriented Synthesis".

Metal catalysis

In this program we aim to bring together excellence in catalysis and organic synthesis for discovering efficient and economic tools for small molecule synthesis. One of the active areas in our group is developing catalytic methods that address the molecular complexity present natural products. Inspired with the wide spread presence of bridged and spirobicyclic systems in a wide range of natural products with diverse biological activities.

We have initiated a program that exploit the dual role of the alkyne unit as functional unit for the C-C bond formations and also as the neutral surrogate of the carbonyl groups. We have studied the details of the Pd-mediated cycloisomerization by employing a range of substrates that addressing the key issue of these cyclizations i.e. *exo-dig* vs. *endo*-dig competitions. This information has been used to design the key substrate and complete the total synthesis of cephalosporolides E & F, didemniserinolipid B and also the synthesis of the central core of cyclodidemniserinol.



Organic CHEMISTRY

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Publications
- *Tetrahedron: Asymmetry*, **2009**, 20, 2173, 2287
- *Tetrahedron:Asymmetry*, **2010**, 21, 558.
- *Chem. Commun.*, **2010**, 46, 5012.

Asymmetric synthesis of bioactive molecules and development of new synthetic transformations

Asymmetric Synthesis of bioactive molecules

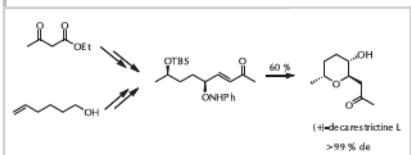
Basic chemistry leading to the asymmetric synthesis of optically active alcohols, amines, amino acids etc., particularly synthesis of drugs such as antibiotics, antiinflammatories, antihypertensives, antiulcer, antidepressants, antimalarials, antibacterials, antiTBs, etc was carried out.

Several asymmetric reactions like asymmetric reductions, epoxidations, dihydroxylations, oxidative kinetic resolutions, C-H insertions and proline based organocatalysis were employed in order to achieve the target molecules.

A concise enantioselective synthesis of (+)-decarestrictine L via proline catalyzed sequential α-aminooxylation and Horner-Wadsworth-Emmons olefination

The Decarestrictine L were isolated from a culture broth of Penicillium simplicissium and its absolute configuration (+)-(2R,3S,6R) was subsequently confirmed by total synthesis by Kibayashi et al. Decarestrictine have been shown to inhibit the biosynthesis of cholesterol in both a HEP-G2 liver cells assay and in vivo.

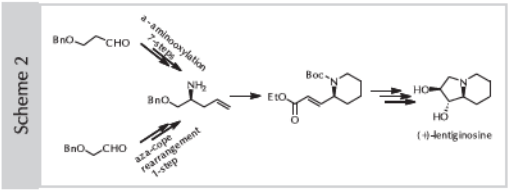
Several other syntheses of decarestrictine L have been reported but many suffer from one or more disadvantages, which include the use of chiral building blocks, long reaction sequences, and low yields. Herein, we report an efficient synthesis of (+)-decarestrictine L in 99% de from the readily available raw materials via a D-proline-catalyzed sequential aminooxylation-olefination reaction followed by intramolecular conjugate 1,4-addition as the key reactions



Scheme 1

A concise enantioselective synthesis of (+)-lentiginosine

A high yielding enantioselective synthesis of indolizidine alkaloid, (+)-lentiginosine has been described based on asymmetric aza-Cope rearrangement and l- proline catalyzed α-aminooxylation of aldehydes. The strategy also makes use of ring closing metathesis for the construction of piperidine core.



Scheme 2

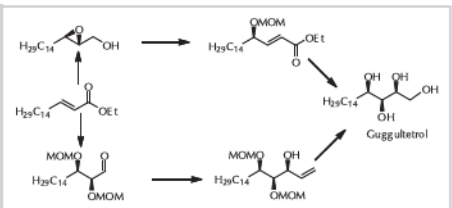
Polyhydroxylated alkaloids such as (+)-lentiginosine, (—)-swainsonine and (+)-catanospermine constitute a class of azasugars exhibiting potent and selective glycosidase inhibitory activities and are found to be useful as anti-cancer, anti-diabetic and anti-viral agents and immune stimulants.

For instance, (+)-lentiginosine, a dihydroxylated indolizidine alkaloid isolated from the leaves of *Astragalus lentiginosis* was shown to be a selective inhibitor of amyloglucosidase, an enzyme that hydrolyses 1,4- and 1,6-α-glycosidic linkages.

Due to the enormous biological importance as well as structural complexities of this class of compounds, numerous reports describing the synthesis of these natural products and their analogues have been published. Although the majority of the reported enantiospecific synthesis of (+)-lentiginosine relies mostly upon the chiral pool, the low-cost L-tartaric acid is the most widely employed since it allows the direct construction of the (1S,2S)-configuration of (+)-lentiginosine

A short enantioselective synthesis of guggultetrol, a naturally occurring lipid

An enantioselective synthesis of guggultetrol, is



Scheme 3

described from commercially available l-pentadecanol. The key steps includes a Sharpless asymmetric epoxidation of allylic alcohol and a dihydroxylation of an α β-unsaturated ester.

Asymmetric catalysis provides a practical, cost-effective, and efficient procedure for the synthesis of bioactive natural products containing multiple stereogenic centers. Tetrols, in particular, with contiguous stereogenic centers are useful intermediates in the synthesis of a number of biologically active compounds such as phytosphingosines.

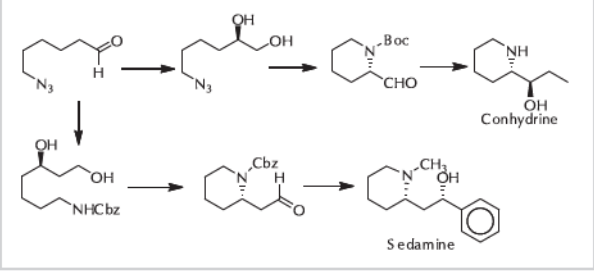
For instance, guggultetrol is used in the treatment of arthritis, inflammation, obesity, and disorders of lipid metabolism. There are only a few literature reports available for the synthesis of guggultetrol; all of them have made use of a chiral pool approach for its asymmetric synthesis. We have reported a short and efficient enantioselective synthesis of guggultetrol, by employing Sharpless asymmetric epoxidation of allylic alcohol as the chiral-inducing step.

Enantioselective synthesis of (+)-α-conhydrine and (-)-sedamine by L-proline-catalysed α-aminooxylation

An efficient organocatalytic enantioselective synthesis of (+)-α-conhydrine and (-)-sedamine via L-proline-catalyzed approach to the enantioslective synthesis of two important piperidine alkaloids, namely (+)-α-conhydrine (98% ee) and (-)-sedamine (95% ee), by L-proline-catalysed α-aminooxylation of aldehydes has been developed.

The strategy involves an intramolecular cyclization to construct the piperidine core. Alkaloids with piperidine structural units often display interesting biological activities and include (+)-conhydrine, (-)-sedamine, (-)-lobeline and their stereoisomers. In particular, these alkaloids have been shown to display memory-enhancing properties and are effective in the treatment of cognitive disorders. Their stereoselective synthesis is important for organic and medicinal chemists, and they have been the subject of intense study due to their structural diversity and varied biological activities.

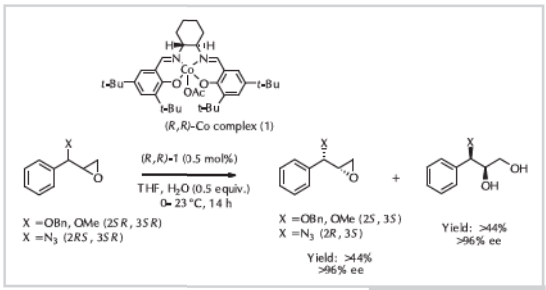
Scheme 4



However, many of the reported methods either make use of chiral building blocks or involve longer reaction sequences, often accompanied by low product selectivity. As part of our research we developed a stereocontrolled synthesis of bioactive molecules, we herein report an organocatalytic approach to a high-yielding synthesis of (+)- -conhydrine and (-)-sedamine, namely by L-proline-catalysed - aminooxylation of azido aldehyde as the chiral inducing step.

Co(III)(salen)-catalyzed HKR of two stereocentered alkoxy- and azido epoxides: A concise enantioselective synthesis of (S,S)-reboxetine and (+)- epi-cytoxazone.

A novel method for two stereocentered hydrolytic kinetic resolution (HKR) of syn, anti-alkoxy/azido epoxides to corresponding enantiomerically pure syn, anti-alkoxy/azido epoxides and diols was developed. The application of this protocol to the enantioselective syntheses of biologically important molecules (S,S)-reboxetine, (+)-epi-cytoxazone and (+)-2-oxazolidone is also described.



Scheme 5

This synthesis describes the generation of two stereocentres of high purities in a single step using hydrolytic kinetic Resolution (HKR) of recemic alkoxy and azido epoxides with Co(salen) complex. The (salen) Co(III)-catalyzed HKR of recemic alkoxy- and azido epoxides provides a highly practicle route to enantiopure syn- or anti- and azido epoxides and the corresponding diols in a single step.

Earlier methods for the preparation of enantiopure alkoxy or azido epoxides and their corresponding diols show that the reaction routes are very tedious with more number of reaction steps. Whereas our procedure for the same preparation is very simple and the reaction is convenient to carry out under mild conditions displaying a wide range of substrate scope

We believe that this HKR strategy will find applications in the field of asymmetric synthesis of bioactive molecules owing to the flexible nature of synthesis of recemic alkoxy and azido epoxides and the ready availability of catalyst in both enantiomeric forms.

Aminobromination of olefins

The metal catalyzed aminohalogenation of alkenes leading to vicinal haloamines has attracted considerable attention due to their importance as building blocks and they are also useful structural moieties in organic and medicinal chemistry. The objectives of this study are:

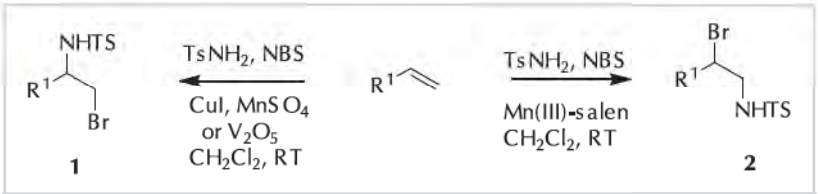
- Explorative studies towards 1,2-haloamination of alkenes using metal catalysis as well as organo catalysis.
- Synthetic methodologies for obtaining chiral vicinal aminohalogens directly from alkenes employing chiral catalysts
- Enantioselective synthesis of optically active drugs, particularly highly active anti-cancer and anti- HIV drugs by employing these methods extensively.

Transition metal-catalyzed regio- and stereoselective aminobromination of olefins

We have developed a new catalytic method for the preparation of 1, 2-aminobrominated products (1 & 2) in preparative yield from a variety of olefins including α, β- unsaturated carbonyl compounds at ambient conditions (Scheme 6).

The method employs CuI, $MnSO_4$, or V_2O_5 as catalysts and NBS/$TsNH_2$ combination as the bromine and nitrogen sources, respectively.

Organic CHEMISTRY



Scheme 6: Metal catalyzed aminobromination of olefins

Surprisingly, both catalysts and olefinic substrates have shown unprecedented regio- and stereoselectivity toward the aminobromination process.

Variety of α, β-unsaturated carbonyl compounds reacted smoothly to afford the corresponding bromoaminated products in good regio- and diastereoselectivity. MnSO4 proved to be better catalyst than those of either CuI or Mn (III)-salen.

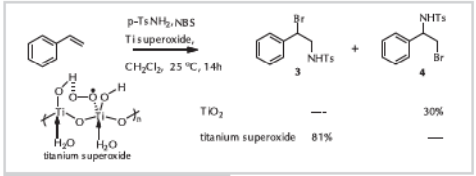
Titanium superoxide: a heterogeneous catalyst for anti-Markovnikov aminobromination of olefins

We have also developed a titanium superoxide-catalyzed regiospecific aminobromination of styrenic and other conjugated olefins to give exclusively anti-Markovnikov products in high yields using p-$TsNH_2$ and NBS as amine and bromine sources respectively under ambient conditions (Scheme 7).

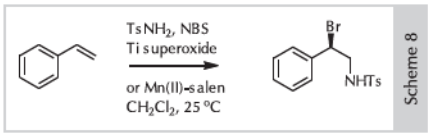
The protocol makes use of stable and readily accessible titanium superoxide as a new solid catalyst for the aminobromination process. The regiochemistry of 1, 2- addition was ascertained on the basis of ^{13}C and DEPT NMR spectra. The isomeric ratio was determined from the ^{1}H NMR spectrum

Asymmetric version: Screening of commercially available chiral ligands

We then turned our attention to develop an asymmetric version of aminobromination process using chiral metal catalysts. Thus, we have screened a variety of chiral ligands in similar reaction conditions. Unfortunately, asymmetric aminobromination proceeds with low ee. A maximum 20% ee was achieved with (R)-BINOL as a ligand. Further studies for improving the ee are in progress.



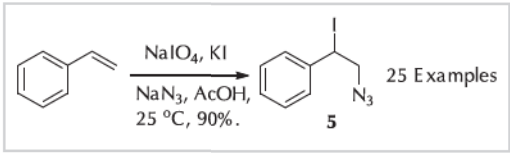
Scheme 7: Aminobromination of styrene



Scheme 8

NaIO4-mediated regioselective azidoiodination of alkenes, using sodium azide and potassium iodide as a halide sources under mild acidic conditions

We have developed a mild, inexpensive and highly regioselective azidoiodination of alkenes using NaIO4, as an oxidizing agent, sodium azide and potassium iodide as a halide source under milder acidic conditions (Scheme 9). This method is mild and high yielding when compared to other reported literature methods.



Scheme 9: $NaIO_4$-mediated regioselective azidoiodination of styrene

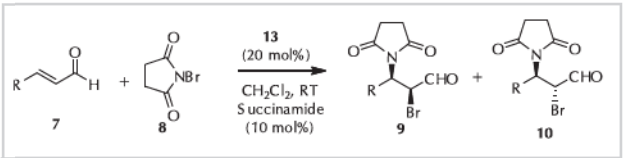
Asymmetric version

Asymmetric version of azidoiodination was carried out using β-CD complexes of styrene under the reaction conditions ($NaIO_4$, sodium azide and potassium iodide as a halide source). Chiral azidoiodides were indeed obtained in good yields with poor enantioselectivities

Asymmetric aminobromination of olefins using organocatalyst

We began the asymmetric aminobromination reaction between cinnamic aldehyde 7 and N-bromosuccinimide 8, as a successful merging of the two catalytic cycles in the domino process has the potential to push the equilibrium towards product formation. A small amount of succinimide (10 mol %) was also added in order to initiate the reaction.

The highest enantioselectivity was achieved in dichloromethane solution when chiral amine was the catalyst. The two diastereoisomers 9 and 10 were readily separated and isolated by silica-gel column chromatography with 99% and >96% ee, respectively. We have presented an easy and organocatalytic approach to form α-aminated aldehydes with high enantioselectivity and yields by using a



Scheme 10: Catalytic asymmetric amino bromination of enals

cheap and commercially available nucleophile i.e. succinimide.

We have also shown that a one-pot syn diamination of α, β-unsaturated aldehydes by using succinimide as a nucleophile and diethyl azodicarboxylate as the electrophile is possible, giving good yields and excellent diastereo- and enantioselectivity of the syn-aminated products.

Structural CHEMISTRY

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Publications
- *Macromolecules*, **2010**, 43, 4782
- *Chem. Mater.*, **2010**, 22, 1633
- *Chem. Commun.*, **2009**, 3446

NMR for structural characterization

a) Studies on structural architecture of aromatic oligoamides containg sterically controlled building blocks

A wide variety of organic backbone architectures exhibiting novel features and functions have attracted attention of chemists in recent past. These structural scaffolds, known as foldamers, show very interesting features and functions that mimic biological molecules. Abiotic backbones, especially that containing aromatic rings, have been proved to be attractive targets in foldamer research due to the predictable and stable conformation.

Tough majority of them display helical conformations sheet and rod conformations can also be attained. Hydrogen bonding has been of considerable utility in structural pre-organization owing to its directionality and specificity. Aromatic oligoamides can attain a stable conformation if the rotations about the Ar-CO and Ar-NH bonds are restricted. This can be achieved by S(6) or S(5) hydrogen bonding between side chains and backbone, within the backbone, or between side chains.

Continuing with this program, a novel class of abiotic hybrid oligoamides with cofacial structural architecture based on 1,8-diarylnaphthyl unit has been synthesized and characterized extensively by NMR, X-ray and molecular modeling. 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. The molecules synthesized using 2,6-diamino pyridine as a co-building block demonstrated the existence of symmetrical co-facial structural architecture (Fig 1).

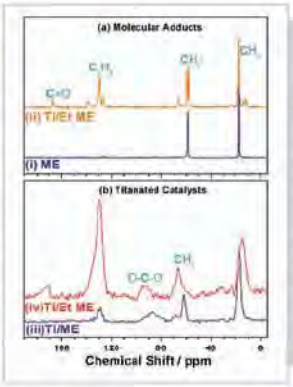


Fig.2 . 13C CP-MAS NMR spectra of (a) molecular adducts, (i) $MgCl_2$-6EtOHE (ME) (ii) $MgCl_2$-EtCOOC6H5 (Et ME), and (b) titanated catalysts, (iii) Ti/ME and (iv) Ti/Et ME.

b) Characterization of $MgCl_2$ support for Ziegler Natta catalysts

The development of $MgCl_2$ supported Ziegler Natta catalysts have revolutionalized the polymer industry by improving the quality of the polymers. The quality of the polymer in turn depends on the nature of the support materials and the other additives used to activate the catalyst. Lewis base such as esters or ethers, which are generally referred to as the electron donors (ED), is commonly used to activate the Ziegler Natta catalyst. The electron donors interact strongly with $MgCl_2$ -alcohol adducts, the support system commonly used. It is believed that the ED blocks particular sites on the $MgCl_2$ surface which otherwise, upon coordination with $TiCl_4$, would generate precursors of non-stereospecific active sites. The aim of this investigation is to understand the molecular level properties and activities of $MgCl_2$.ethanol adduct in presence of ED such as benzoyl chloride and ethyl benzoate using solid state NMR methods.

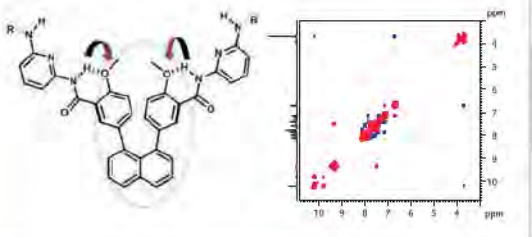


Fig .1 Structure of the co-facial oligo amide and the 500 MHz NOESY spectrum of it in $CDCl_3$ showing the cross peak between the NH and the OMe group.

The formation of esterified adduct from $MgCl_2$-6EtOH and benzoyl chloride was very much evident from the ^{13}C CP-MAS NMR spectrum which showed partial replacement of the alcohol. In addition, the presence of

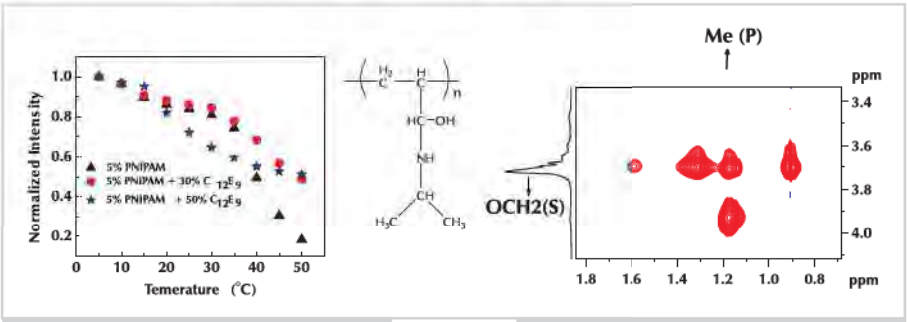
Structural CHEMISTRY

the ester (ID) in the final titanated catalyst (Ti/Et ME) was also confirmed from the ^{13}C CPMAS spectra shown in Fig-2 which clearly show that the catalyst preparation doesn't remove the ester group from the support.

c) Investigations of the Volume Transition of PNIPAM in a Nonionic Surfactant Hexagonal Mesophase

On heating an aqueous solution of poly(N-isopropylacrylamide) (PNIPAM) to above its lower critical solution temperature (LCST) of around 32°C, the polymer chains collapse and aggregate, and the solution goes from clear to cloudy. The LCST of PNIPAM can be tailored and is influenced by the presence of surfactants, especially the anionic surfactants. . Nonionic surfactants such as C12E9 are known to interact weakly with PNIPAM. In this investigation, volume phase transition of PNIPAM chains in a hexagonal mesophase of nonionic surfactant C12E9.

^{1}H and ^{13}C NMR methods have been used to study the volume transition of poly(N-isopropylacrylamide),PNIPAM, in presence of an aqueous solution of nonionic surfactant, C12E9. The study shows that there is only a small change in the volume transition temperature (~32°C) for the PNIPAM in isotropic micellar solutions of C12E9. But, in the H1 phase of surfactant, a decrease to ~15°C in the coil-globule transition temperature was observed. The NMR studies provide more insight to this phenomenon and show that the LCST of PNIPAM is strongly influenced by the matrix phase. In addition the 2D ROESY data showed finer details about the surfactant-polymer interactions prevailing in the system investigated.



Temperature dependence of the area of methyl carbon signals of the polymer in 5% PNIPAM in D2O.. The area of the signal at a particular temperature is normalized with the area of the same signal at 5°C for each system

400 MHz ROESY spectrum of PNIPAM in the micellar phase (30% C12E9). Only cross-peaks in the region of interest are shown. Polymer signal is marked as Me(P) and the surfactant signal as OCH2(S)

GIAO/DFT calculation of NMR Parameters

^{1}H, ^{13}C and ^{15}N NMR shielding constants of different organic molecules varying form hetero cycles, bioorganic molecules and natural products were calculated by employing the gauge-including - atomic-orbital (GIAO) method at B3LYP density functional theory (DFT). The geometry of each compound has been optimized using a 6-311^{++}G (d,p) level basis set. The calculated values were compared with the observed NMR chemical shifts of various nuclei to get information about nature of tautomers in 1,2,4-triazoles and stereochemistry in natural products and bioorganic molecules.

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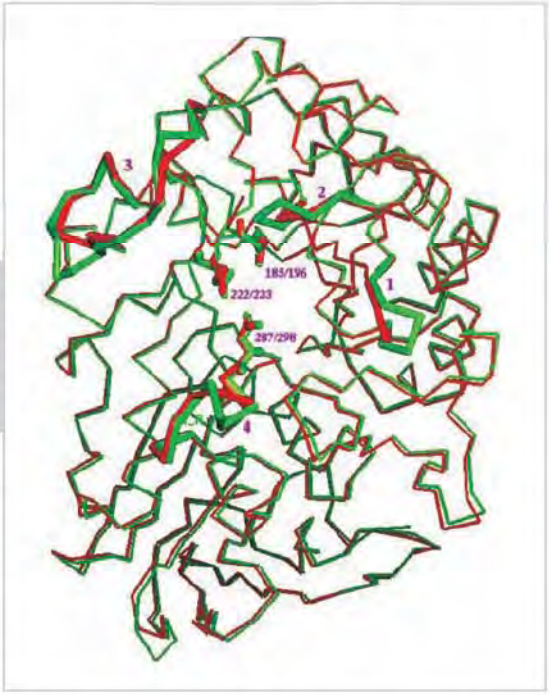
- *J. Fluoresc.*, **2009**, 19, 239
- *Acta Crystallogr.*, **2009**, D65, 1
- *Biochem. Biophys. Res. Commun.*, **2009**, 390, 273
- *Int. J. Ins. Sci.*, **2009**, 1, 29

Structure-function study of selected plant and microbial proteins

Synchrotron data were collected on crystals of lectin with complex sugar specificity purified from *Cicer arietinum* seeds. Further calculation for structure determination is in progress. The characterization and structural studies of a similar protein from *Moringa oleifera* seeds is continuing. Biophysical characterization of a lectin from *Ariesaema curvatum* has been carried out.

Refinement of the structures of recombinant penicillin G. acylase from *Alcaligence faecalis* in two crystal forms is completed. Bioinformatics analysis for understanding the substrate specificity and identifying the substrate dependent sub-groups in Ntn hydrolase family members is in progress. Modeling of the structures of some enzymes involved in the biosynthetic pathway of lignins is initiated.



Superposition of the modeled structure of *Scirpophaga incertulas* Walker amylase (green on the reported structure of *Tenebrio molitor* L. α-amylase (red, pdb: 1jae. The active site residues and the loops where the structures differ are numbered.

Modeling study of the structure of an amylase from the rice pest *Scirpophaga incertulas* walker and its interaction with a wheat inhibitor has been published. The biophysical study of the human eukaryotic initiation factor 2α is published. Similarly, biophysical study is carried out on the heme-regulated eukaryotic initiation factor 2α kinase.

Study of human mitochondrial genetic disorders at molecular level

Some selected Mitochondrial proteins of the mitochondrial complex-1 have been cloned for overexpression. Structural studies on these mitochondrial proteins have been initiated to understand at molecular level the effects of mitochondrial related pathogenic DNA mutations.

Chemical BIOLOGY

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Publication
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Biotech process development

Cellulose based porous membrane for bio-separation and bio-conversion

This process comprises a novel membrane casting solution for the preparation of cellulose based highly porous, chemically stable, chromatographic or adsorption membranes.

The process was developed to utilize fully the advantages of membranes in bio-separation and bioconversion. e.g., high mass transfer efficiency and to overcome fouling arising due to pore blockage that reduces productivity and increases maintenance and operating costs. The market size for such type of membrane is $2 billion per year and this is growing at a rate of 13%.

The membranes are biocompatible, because the base polymer of developed membrane is ethyl cellulose which is being used conventionally as a food additive, pharmaceutical tablet binder, etc.

it is cost effective and environment friendly, because its preparation process is simple and does not involve heating, cooling and use of highly hazardous chemicals. It minimizes post use disposal problems due to inherent biodegradability property of cellulose.

The membrane is suitable for bio-separation, bioconversion operations, because it is highly porous and chemically stable [Flux - ~2500 LMH (L m^{-2} h^{-1}) at 0.5 bar; Average pore size - ~ 6.37μm]. This allows its chemical modification without compromising on its operational flux. This is highly essential to overcome the conventional chromatography technology problems related to scale-up, mass transfer and throughputs. It is unique, because it can be used without any chemical modification for single step purification of blood albumin (Fig. 1).

Albumin is being used as a therapeutic agent and dietary supplement worldwide. The annual production of albumin from human blood using conventional ethanol precipitation process is estimated to be around 300 tons.

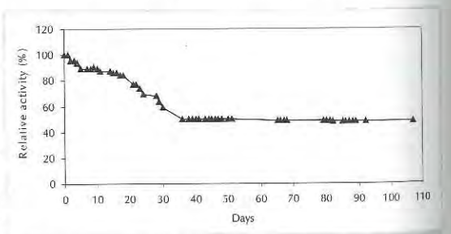

Fig. 2: Operational stability of an enzyme penicillin G acylase immobilized on the developed membrane and shows suitability of developed membrane in bioconversion operations].

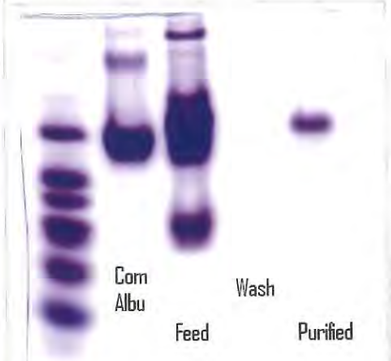

Fig.1: [MW M – Molecular weight markers (Sigma); Com Albu – Commercial human serum albumin (Sigma); Feed - Diluted horse serum, adsorption pH 4.0; Wash - Last Wash; Purified - Eluent pH 7.0].

The chemical stability of the membrane allows different chemical modifications that are required for immobilizing enzymes for carrying out different bioconversion operations in biotech industries. For example, the enzyme penicillin G acylase which is being used commercially for the production of β-lactam antibiotics was immobilized on the chemically modified developed membrane and used for 107 days that indicates significant operational stability and suitability for such operations (Fig. 2).
Single step purification of blood albumin using the developed membrane without any chemical modification shows suitability of developed membrane in bio-separation operations.

Use of black liquor for the production of *E. coli* whole cell containing penicillin G acylase

The growing demand from legal and social sources for the safe disposal of environmentally hazardous industrial waste material has put an economical burden on concerned industries. The conversion of these materials to high value product may help to ease this burden significantly. Black liquor is a most polluted waste material of pulp and paper industry because of its toxicity and poor biodegradability.

Approximately, annual world production of black liquor is around 500 million tonnes. Considerable effort is going on to make black liquor suitable for safe disposal. However, not much has been done to produce commercially viable products using black liquor. In the present study, we have used black liquor for the production of high value product such as an enzyme penicillin G acylase.

Penicillin G acylase (EC 3.5.1.11) is being used in industrial syntheses of various semi-synthetic penicillins. It hydrolyzes penicillin G and other phenyl-acetic derivatives, is also involved in synthesis of the anti-platelet agents and in the enzymatic activation of pro-drugs in cancer therapy.

Six different *Escherichia coli* were obtained from the NCIM and the whole cell production was carried out using growth medium containing black liquor (6%) and conventional growth medium using standard procedure. The whole cell penicillin G acylase activity of all the strains were checked. All the strains showed 39 ± 7.6% average increase in whole cell penicillin G acylase activity (Fig. 3).

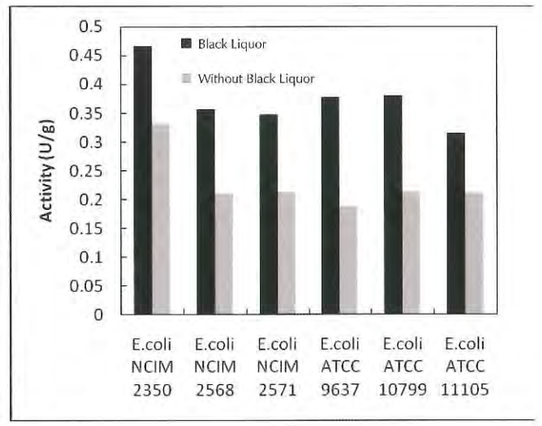

Fig. 3: Effect of black liquor on different whole cell PGA activity. [U/g - moles of 6-aminopenicillanic acid formed per minute per g wet weight of cell at pH 7.0 and 40 ºC].

This clearly indicates that the black liquor has significant role in the overall enhancement of whole cell penicillin G acylase activity. As the industrial production of 6-aminopenicillanic acid (precursor of the semisynthetic penicillins) using penicillin acylase is around 9000 tonnes per year. This is likely to further increase in the coming years.

For such large scales, the use of industrial waste as a nutrient may help in the reduction of overall production costs as well as in the management of environmental pollution. Further studies are needed to verify this using microbial strain for use at industrial levels.

Chemical BIOLOGY

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Bioprocess engineering

Mammalian cells such as Chinese Hamster Ovary (CHO) cells are extensively used for production of complex recombinant proteins used as therapeutic. The use of chemically defined (CD) media for culturing CHO cells is well documented. Most CD media compositions are optimized for growth potential.

Rapid cell growth is an important parameter in large scale protein production. However, maximizing the viable cell density and duration of culture are also important for increasing the volumetric productivity of a cell culture process. Maximizing viable cell density and increasing culture longevity can however be accompanied with an undesirable accumulation of waste metabolites like lactate and ammonia at inhibitory levels.

Another 'inhibitory' parameter especially in longer duration fed batch cultures could be high levels of osmolarity which increases during the course of the culture. Several approaches have been proposed to reduce waste metabolite production such as metabolic shift, use of alternate nutrients with slower uptake rates or genetic engineering of the cell to decrease the expression of enzymes catalyzing the formation of the waste metabolites e.g. lactate dehydrogenase.

It should be noted here that though lactate and ammonia are the most widely studied inhibitory waste metabolites for cell culture, there might be other hitherto unrecognized inhibitors as demonstrated in a recent report describing D-lactate and methylglyoxal accumulation in cell culture. In this study, we were interested in testing whether dilution of a long duration culture in shake flasks could lead to improved performance.

CHO clone expressing IgG was cultured in CD CHO media in shake flasks and fed with glucose and protein hydrolysate at two instances during the culture. After the last feed addition, the culture was diluted and an increase in protein yield per ml of media was observed. An unstructured mathematical model was used to simulate the behavior of cells in batch and fed batch mode of operation to assess if the experimentally observed increase in protein yield per ml of media could be predicted using previously used kinetic models for cell growth and protein production. The model assumes that growth is affected by limiting nutrient concentration and accumulating inhibitor concentration.

Since growth rate was seen to decrease even when glucose concentration was significantly above previously reported Km values, we assume the presence of another unmeasured pool of nutrients (denoted by N) which limits growth. I is assumed to represent waste metabolites which can affect growth and productivity.

Inhibitors could include a combination of waste metabolites and physical factors like increase in osmolarity. The specific antibody production rate is assumed to comprise of a growth associated and growth independent term as previously reported.

The model predictions for cell density and glucose consumption are similar to the experimental data. The model also predicts the observed increased yields of IVCD and protein per ml of media.

In order to test the hypothesis that dilution of inhibitors was at least partly contributing to the observed increased yield of recombinant protein, the model was simulated with the specific production rate of inhibitor (I) set to zero i.e. assuming there is no production of inhibitor. In the absence of I, the model predicts no change in protein yields, supporting this hypothesis.

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Publication
- *Chem. Commun.*, **2009**, 6646

Organic biomolecular chemistry

Background / objectives

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.

Work done and discussion

After confirming that the α-amino acid alternating with nucleoside α-amino acid form

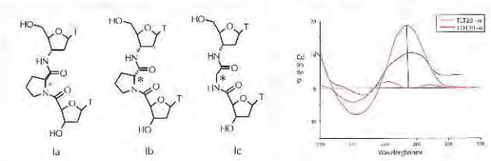

Fig. 1. Dimer blocks containing L-pro Ia, D-pro Ib and glycine Ic as linker amino acids and their CD spectra

stable duplexes with complementary DNA and RNA, we further studied the effect of backbone chirality while using the both L/D- α-amino acids and a prochiral amino acid, glycine. The Thyminyl-Thymine dimer blocks (1a, 1b and 1c) were synthesized by using thyminyl-5'-acid component coupled with L/D proline or glycine followed by coupling with 3'-amino-3'-deoxythymidine. The dimer blocks containing D-proline, L-proline and prochiral glycine exhibited very interesting CD-curves. A strong CD maximum for D-pro/ a weak minimum for L-pro and an intermediate positive band for prochiral glycine was observed. The CD profile exhibited by the D-pro containing dimer is similar to the LNA dimers that induce increased stability to DNA:RNA duplexes. The CD data obtained shows differential base stacking features that may have implications in recognition of DNA/RNA sequences. We then incorporated the amide linked thymidine dimer blocks in DNA sequences. The RNA/DNA binding ability of the modified DNA strand was found to be dictated by the chirality of the amino acid.

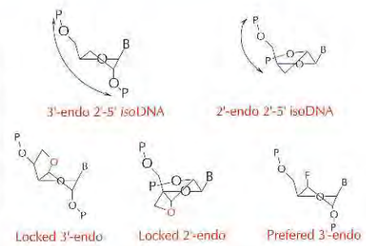

Fig. 2: Preferences of sugar geometry in isoDNA:RNA duplexes. The locked monomers showing the extended and compact backbone

The oligonucleotides joined by 'non-genetic' 2', 5'-linkages (isoDNA) (Fig. 2) 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. Synthesis of locked 3'-endo, locked 2'-endo and 3'-xylofluoro -uracil and thymine nucleoside monomers was accomplished and these units were incorporated in isoDNA.

As expected, it was found that when the 2'-endo locked monomers that would give rise to compact geometry were incorporated into isoDNA, duplexes formed with RNA were stabilized (+1-2.5°C). Conversely, the 2'-endo locked/preferred monomers that form extended geometry destabilized isoDNA:RNA complexes (-5 to-7.5°C). Also the incorporation of 3'-xylo configured 3'-fluoro thymine nucleoside, known to be in 3'-endo preferred geometry, destabilized isoDNA:RNA duplexes.

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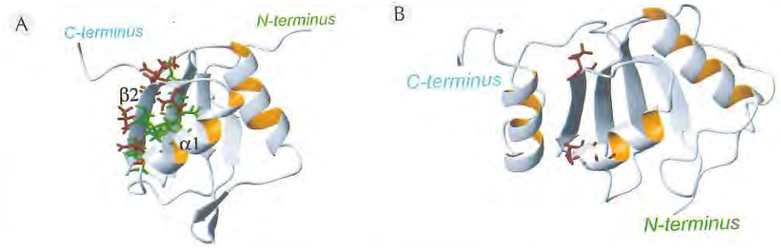

Fig. 2: Preliminary structures of PTB-RBD1 (a) in the free state and (b) when bound to a stem-loop RNA.

measured relaxation rates and the correlation plots between pairs of spectral density functions are being analyzed to obtain insights into the dynamics of PTB-RBD1. The correlation plots show a clear separation between regions with different types of molecular motions (Figure 3). For example, there is a clear separation between residues from the globular domain and the N- and C-terminal segments, with a greater contribution from high frequency spectral density functions at the highly flexible terminal regions.

Some of the residues which show indications of slow motion are located in the the α1 helix and β2 strand. Preliminary structural studies have suggested contacts between these regions and the C-terminal segment in the RNA bound state. It is possible that these contacts are also present in the free form but are of a transient nature.

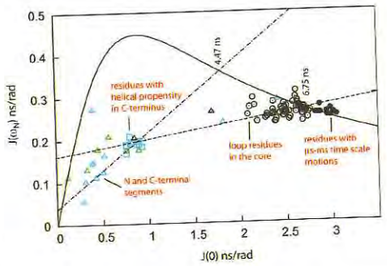

Fig. 3: Plots of $J(\omega_N)$ versus J(0) in free PTB-RBD1 showing residues from the core (circles) and residues from N and C-terminal segments (in color). The part of the C-terminus which seems to be partly structured is indicated by squares. Filled circles correspond to residues undergoing slow conformational exchange

The dynamics of residues 105 to 115 in the C-terminal segment is distinctly different from the other terminal residues and indicates that even though there may not be a clear helix formation, there must be some partial ordering in this region. Further studies are in progress to examine the folding event which takes place on RNA binding resulting in the formation of a helix in the C-terminal segment.

The spectral density correlations are being analyzed to examine the possibility of modeling the dynamical processes in PTB-RBD1 in terms of motions of two domains. Linear fits to data points from N-terminus and core residues intersects the parametric curve for isotropic motion at a point corresponding to a correlation time of 6.75 ns for global motion whereas a linear fit involving the C-terminal segment gives a correlation time of 4.47 ns. Since full length PTB consists of RNA binding domains separated by flexible linkers, the dynamics is being modeled in terms of two ordered domains linked by flexible residues. How RNA binding affects motions of the two domains is currently being investigated.

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Publications
- *Chem Commun.*, **2009**, 3446
- *Org. Biomol. Chem.*, **2009**, 7, 2458

Development of conformationally restricted synthetic oligomers

Background / objectives

The major thrust of my search focus over the years has been to generate conformationally ordered synthetic scaffolds capable of displaying diverse secondary structural features. Conformationally ordered synthetic oligomers, called "foldamers", have attracted considerable attention in recent years primarily due to their enormous ability to display discrete folding propensities similar to biopolymers.

The initial efforts ushered by Seebach and Gellman showed that oligomers made from beta-amino acids form stable secondary structures, akin to the conformations displayed by native peptides and proteins. Subsequent studies revealed that oligomers of the higher homologous amino acids are also able to form definite secondary structures.

To extend the repertoire of foldamer design, oligomers containing different residues of independent conformational preferences have been suggested. For instance, several groups demonstrated that hybrid peptides composed of alternating amino acids of different backbone substitution adopt special helix types. Interestingly, such oligomers are resistant against proteases and some of them display promising biological activities. The search for building blocks to construct synthetic oligomers with predefined conformational preference has also led to the discovery of a myriad of molecules with aromatic frameworks showing intriguing structures and properties

Work done and discussion

Inspired by our recent success in the development of de novo designed "hybrid foldamers" containing conformationally constrained aliphatic and aromatic amino acids of varying substitution pattern, in repeating sequences (Sanjayan et al. J. Am. Chem. Soc. 2008, 130, 17743), we recently ventured into the development of novel synthetic oligopmers displaying unusual structural architecture. In this context, we achieved the development 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 to an excellent template for building cofacial structures. It was anticipated that positioning of hydrogen-bond directing conformationally restricted aryl units on the 1,8-peri- positions of naphthalene building blocks would pave the way for the creation of conformationally ordered structural units with cofacial arrangements of the aryl rings. For this purpose, we selected 2,6-diamino pyridine as a co-building block, anticipating that the resulting oligomer would have suitable intramolecular hydrogen bonding arrangements which would help the molecule to adopt symmetrical cofacial structural architecture.

In addition to this, use of pyridine rings on the backbone can aid the molecule to participate in processes like molecular recognition and self-assembly, which are known for these classes of systems. Given below are representative examples of recently developed conformationally ordered synthetic oligomers from this lab.

Novel Foldamer Structural Architecture from Cofacial Aromatic Building Blocks. Panchami, P.; Gonnade, R.; H.- Hofmann, and Sanjayan, G. J. Chem Commun, 2009, 3446

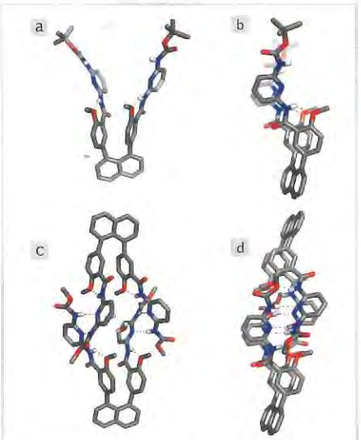

Fig. 1: Solid-state structure of an oligomer. Various views of the crystal structure (a,b); and various views of the H-bonded duplex (c,d).

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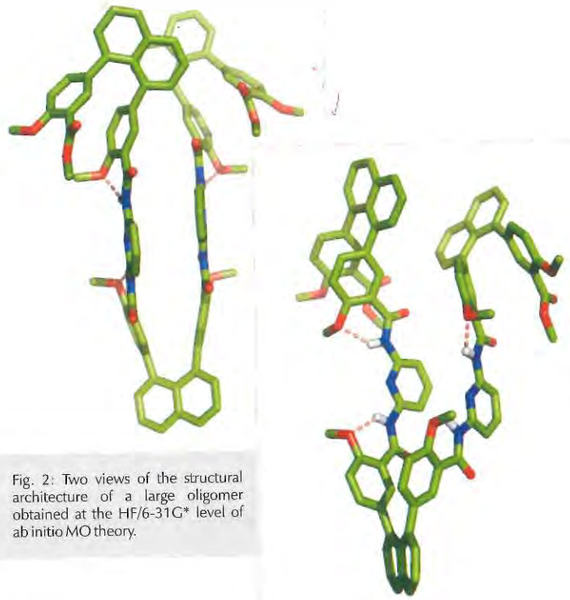

Fig. 2: Two views of the structural architecture of a large oligomer obtained at the HF/6-31G* level of ab initio MO theory.

Sterically controlled Foldamers

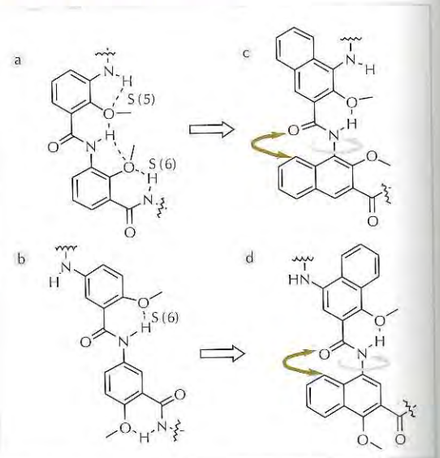

Fig. 3: Iillustration of the design strategy of sterically controlled foldamers

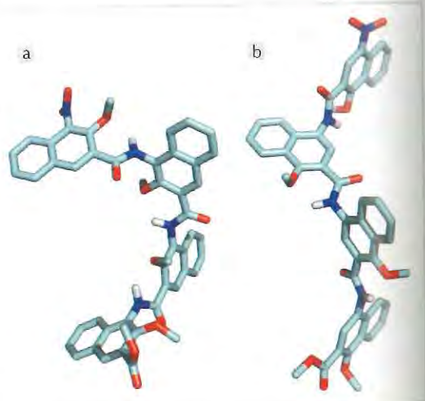

Fig. 4: Structural architecture of oligomers at the HF/6-31G* level of ab initio MO theory

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Biocatalysis and biosynthesis

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

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 the isoprenoid biosynthetic pathways with special emphasis on establishing the mechanisms of the enzyme-catalyzed transformations and how the enzymes promote the reactions.

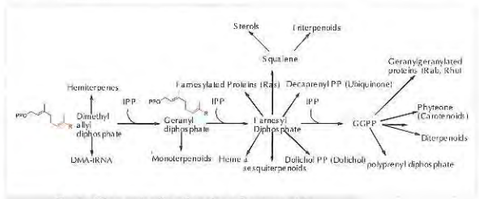


Fig.1: Biosynthesis of various isoprenoids

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.

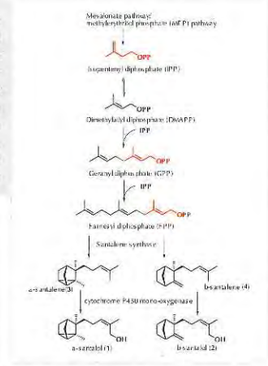
Work done and discussion

Biosynthesis and biotransformation of sesquiterpenoids from sandalwood oil

The endangered, Sandalwood or Chandan (*Santalum album* L.) is highly valued for its oil. The sandal wood oil mainly consists of santalene derivatives. The sesquiterpene alcohol, α-santalol, which is the major component (~90%) of essential oil from well matured tree (≥80 years old), is responsible for most of the activity of the oil. α-Santalol has particularly attracted increasing attention for its neuroleptic property and chemopreventive effect in *in* vitro and *in* vivo bioassay systems.

α and β -Santalols have been purified from the sandalwood oil using silver nitrate coated silica gel column chromatography. Biotransformation of both the santalols was carried out using the soil isolated versatile fungal culture (SFT11). The fungal strain carries out the hydroxylation at the allylic methylene and methyl groups of the both α-andβ-Santalols.

Fig. 2: Proposed Biosynthetic pathway for Santalene Derivatives in Indian Sandalwood, *Santalum album*



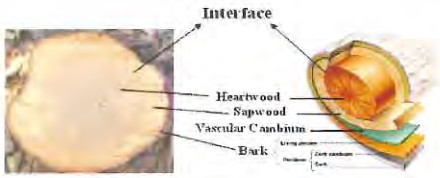
The genes responsible for santalene synthases are expressed at the transition zone of sapwood and heartwood of S. album and the first committed step in santalol biosynthesis is cyclization of farnesyl diphosphate (FPP) by santalene synthase to yield santalene (2 or 3; fig. 2) which will be converted into santalols (1 and 2; Fig. 2) by cytochrome P 450 system. Till this date no efforts were made towards the understanding of biosynthetic pathway and mechanism of production of santalene derivatives in the heartwood of *S. album* and very little is known about the mode of biotransformation of these santalene derivatives in living systems.

We have successfully isolated the RNA from the tissue from the heartwood and sapwood interface is standardized (Fig. 3) and used for cDNA library construction. Screening of cDNA library is progressing for santalene synthases.

Metabolic profiling, and biotransformation of neem (*Azadirachta indica*) limonoids

We have standardized the method for the isolation of major limonoids from neem seed kernel by simple extraction method. We have isolated and characterized (figure 4) the following major limonoids- Epoxyazadiradione (1), Azadiradione (2), Nimbin (3), 6-

Chemical BIOLOGY



Cross-section of sandalwood trunk

Legend:
Lane 1: 1Kb DNA ladder
Lane 2: RNA

28S RNA
18S RNA

$A_{260/A280}$ = 1.92
$A_{260/230}$ = 2.15

Fig. 3: Total RNA from interface of heartwood and

Deacetylnimbin (4), Salanin (5), 17β - Hydroxyazadiradione (6), 3-Deacetylsalanin (7), Azadirachtin B (8), Azadirachtin A (9), Azadirachtin-H (10), and 11-Epi-azadirachtin-D (11).

Fig. 4: metabolic profiling

We have carried out the metabolic profiling of neem seeds at the different developing stages (figure 5) to find out whether limonoids synthesized in seeds or transported to seeds as neem seeds are the major source for tetranor triterpenoids, azadirachtins.

Fig. 5: Neem seed kernels of the five different growing stages

From the profile of the developing stages, it is clear that limonoid content is in same ratio throughout the different developmental stages of seed kernel and fruit coat. The major limonoids present in the seed kernel are salanin, nimbin, their deacetyl derivatives; Azadirachtin A and B where as azadiradione and epoxyazadiradione are the major contents of the fruit coat.

Very little known regarding the mode of metabolism of these limonoids in living system. We have carried out the biotransformation studies on azadiradione and epoxyazadiradione by using soil isolated versatile fungal system SF11. The fungal system initiates the biotransformation of these compounds by hydroxylating at C11 and C17 positions.

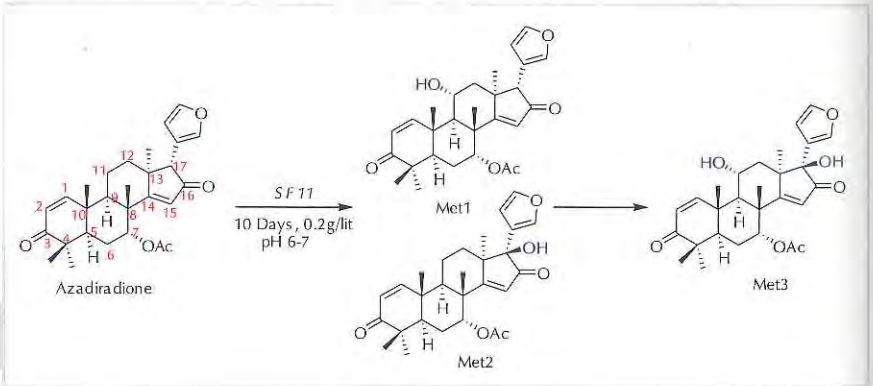
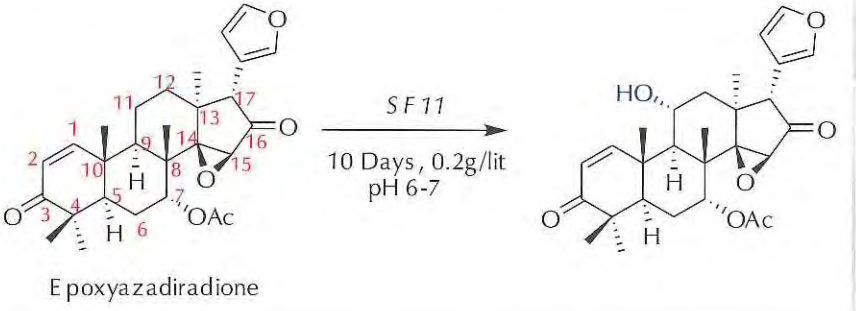


Fig. 6. Biotransformation of azadiradione and epoxyazadiradione by Sf11



Epoxyazadiradione

Fig. 7. Biotransformation of epoxyazadiradione and epoxyazadiradione by SF11

Chemical ENGINEERING SCIENCE

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Biochemical Engineering

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Microbial fermentation/ microbial production of erythritol

Erythritol is a natural polyol produced commercially by fermentation using osmophilic yeasts and fungi. It can be used as a bulk sweetener with the necessary "mouth feel" in reduced calorie foods. It can also be used to make a "syrup", an important feature of Indian traditional sweets. Erythritol is absorbed in the small intestine and eliminated by the body within 24 hours. The cold drink manufacturers are known to use erythritol in their low-calorie soft drinks. The market for erythritol is slowly increasing in the world and also in India. A project funded by Department of Biotechnology was completed in the current year on development of mutants for production of erythritol.

A mutant of *Candida magnoliae* was developed and studied for erythritol production. The mutant was studied in 10 L fermenter for production of erythritol and suitable fermentation conditions. It was observed that the production of erythritol is delicately controlled by the pH, temperature and dissolved oxygen tension in the fermenter. Using suitable conditions, the erythritol production could be increased to 70 g/l in batch fermentation. The results also showed that concentration of fermentable sugar affects production of the other metabolites like glycerol and ethanol during fermentation. A fed-batch approach is more suitable for maximal erythritol production. Further optimization and fed-batch fermentation studies are necessary to increase the erythritol production and yield based on the sugar consumed.

Fermenter set-up

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Materials and surface-based approaches in proteomics

Comprehensive analysis of complex biological samples containing proteins, peptides and various metabolites is challenging. Existing generic analytical methodologies, usually involving a separation dimension such as HPLC followed by detection mechanism, have many limitations leaving scope for simpler, quicker and more efficient tools.

Some of these tools can also be aimed at providing tailor made solutions depending on the analytical need. Thus, the first long-term goal and objective of this work is to develop novel chromatography platforms and/or methods that could enable 'high throughput' and 'minimal sample preparation' methodologies for bioanalysis including 'bottom up' proteomics and metabolomics.

Key aspects of the planar platform would include optimization of the planar stationary phases as well as the mass spectral interface to enable direct detection of separated analytes from planar surfaces.

In yet another pursuit, surface chemistry based approaches are being explored to stabilize enzymes for their catalytic activity and therapeutic release applications. Protein and enzyme stability as well as activity in non-aqueous media are attractive in several applications such as biocatalysis, green chemistry and in formulations. Microemulsions are macroscopically homogenous but microscopically heterogenous systems with different proportions of oil, water, surfactant and a co-surfactant.

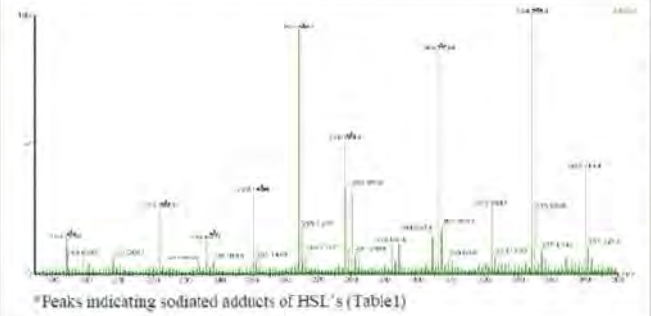
Microemulsions as media for enzymatic reactions have gained relevance due to their excellent solubilizing properties, presence of controlled ratios of water, possible control of enzymatic activity by tuning the microemulsion composition, their lower toxicity when compared to organic solvents, excellent conductivity and recyclability of the solvent. In this work, our objective was to understand the stability of proteins/enzyme, incorporated into microemulsions.

Laser desorption ionization mass spectrometry (LDI MS) from surfaces for bioanalysis

Small molecule pattern analysis, especially biological metabolite analysis, using LDI MS has unique advantages such as simplified sample preparation and high throughput analysis.

Conventional matrices used in MALDI MS have multiple mass peaks in the 1-500 m/z range thereby making metabolite analysis from complex mixtures difficult. Titania was used to perform the preliminary experiments to understand the overall process of LSI MS. Bacterial signaling molecules (N-acyl homoserine lactones) representing various bacteria with a wide ranging applications such as health to agriculture and food industry were analyzed individually and molecular ion peaks without matrix interference were obtained.

Sodiated and potassiated peaks were observed in addition to the molecular ion peaks for the individual standards in many cases (Fig. 1). Traditionally, electrospray ionization (ESI MS) or fluorescence assays are used for the analysis, and using LDI MS, the analysis can be done in a high throughput manner with minimum sample preparation.



*Peaks indicating sodiated adducts of HSL's (Table1)

Fig. 1: Resolution of a mixture of various the bacterial signalling homoserine lactones using LDI MS yields sodiated and potassiated adducts

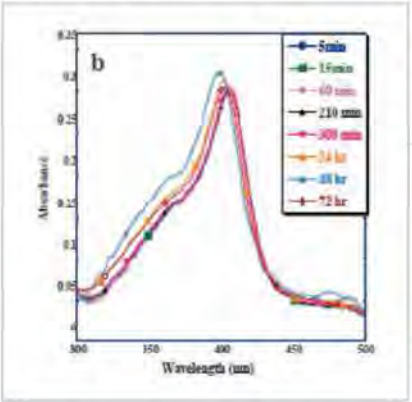
Stability of protein and enzymatic activity in microemulsions

Our results on proteins incorporated in

microemulsions indicate that myoglobin and HRP, both having heme reaction centers, are stable in the bicontinuous microemulsions as indicated by their Soret band absorbance maxima centered around 403-410nm (Fig. 2).

The feasibility of using microemulsions as hosts for enzymatic reactions with the enzyme incorporated in the microemulsion was investigated using the peroxidase activity of HRP. This activity was measured as a rate of pyrogallol oxidation to purpurogallin at various HRP concentrations.

The enzymatic reaction was monitored spectrometrically based on the production of purpurogallin that has an absorbtion maximum at 420nm. HRP showed a linear dependence of its enzymatic activity on the concentration of HRP (Fig. 3). Thus, HRP exhibits its peroxidase activity in the bicontinuous microemulsion.



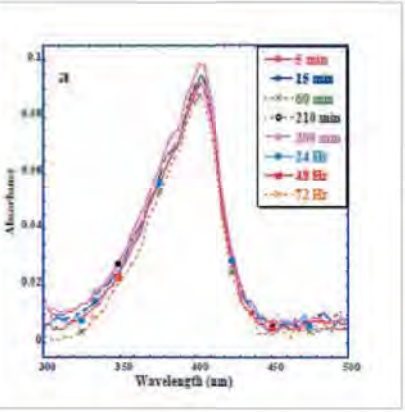


Fig. 2: Native Soret band absorption spectra of horseradish peroxidase (HRP) (a) and myoglobin (b) in bicontinuous microemulsion at 403 and 410nm respectively, indicating their stability in the media

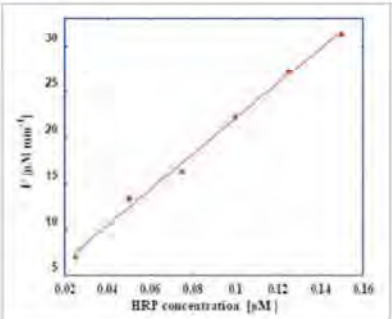


Fig. 3: Effect of the HRP concentration variation on the enzymatic activity represented as the initial rate (v) of the enzyme catalyzed pyrogallol oxidation at 25°C

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Process Development

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Publication
- Indian patent filed Application No: NF115/2009

Process development for the synthesis of vinyl ester (NAVE-10) or vinyl neodecanoate

With the expertise in the development of vinyl monomer using semi-continuous/ continuous process, we have already developed a new continuous / semi-continuous process based on transvinylation using BA/2-EHA acid and vinyl acetate monomers in the presence of transition metal complex catalyst. M/s Celanese was looking for the process development for synthesis of vinyl neodecanoate. The synthesis of vinyl neodecanoate is associated with the challenges such as:

- The purity of C-10 acid for transvinylation reaction is very important and
- Analysis of reactants and products are tricky because of C-10 acid and vinyl neodecanoate esters involve number of isomers.

Methodology
A unique semi continuous / continuous reactive distillation process has been developed for the transvinylation of C-10 acid using VAM and palladium-complex catalyst. In order to optimize the process, the effect of various operating parameters such as reaction time, catalyst loading, reaction temperature was studied.

The Acid: VAM molar ratio and reusability of catalyst on conversion of C-10 acid was studied and optimum conditions for transvinylation reaction were suggested. The rate expression for kinetics of transvinaylation of C-10 acid was also developed.

For proof of concept in the laboratory scale (preferably in a 3 or 5 L reactor set up) a semi-continuous reactive distillation assembly has been designed. The process safety procedure was developed for transvinylation of C-10 acid using Pd-complex catalyst.

Results
A unique semi-continuous/ continuous reactive distillation process has been developed for the transvinylation of C-10 acid using VAM and palladium-complex catalyst. The Process will be transferred to MEHK Chemicals Pvt. Ltd, Thane.

Development of eco-friendly route for the preparation of pure alkyl esters
The process involves preparation of pure alkyl esters from alkali metal salt of carboxylic acid using carbon dioxide and alcohols. The group of alkyl esters is one of the most important derivatives of lactic acid. For instance ethyl ester is a biodegradable substance with excellent solvent properties and can replace toxic and halogenated solvents for a wide range of industrial applications.

Alkyl esters can be used as additives in a variety of products, including paints, grease removers, packaging and cleansers. Low-cost salts esters can potentially be used to produce other chemicals such as copolymers of biodegradable plastics, acrylates, glycol and other specialty chemicals. Ethyl ester is a natural flavoring compound and therefore used as a valuable food and perfumery additive.

Methodology
A novel green and a promising process for the preparation of pure alkyl esters from corresponding salt of carboxylic acid such as calcium lactate, sodium lactate, potassium lactate etc. using carbon dioxide and alcohol like methanol, ethanol, butanol etc. has been developed.

The alkali metal salts of carboxylic acid are prepared from natural sources by a process of fermentation of carbohydrates like sugar juice, food grains (seagram, wheat, and corn), beat etc. The other alkali metal salts of carboxylic acid are like sodium benzoate, sodium acetate, sodium salicylate etc. can be used.

The reaction route for synthesis of pure alkyl esters is pollution free by avoiding formation of calcium sulfate as byproduct.

Schematic experimental setup for continuous synthesis of pure lactic esters using high pressure reactor (10 L capacity)

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Process Modeling and Simulations

Publication
- *Fluid Phase Equilibria,* **2009**, 282, 65

Evaluation of repulsive particle swarm method for phase equilibrium and phase stability problems

A persistently difficult problem in chemical engineering is the phase equilibrium and stability problems, which is of crucial importance in simulation, design and optimization of several process separation applications. Under the conditions of constant temperature and pressure, a necessary condition for a multicomponent & multiphase system to achieve equilibrium is total Gibbs' free energy must be at global minimum. This is a classic problem in thermodynamics- how to distinguish between unstable, metastable and absolutely stable phases.

In this study, *Repulsive Particle Swarm method* is applied to solve phase equilibrium and phase stability problems. RPS is a computerized search and optimization algorithm, similar to GA applied on real world variables, which is significantly fast at numerical optimization and is also more likely to find a function's true global optimum.

It is based on the social behavior of a swarm of birds or a school of fish, which searches for food in a very typical manner. Every member of the swarm searches for the best in its locality-learns from its own experience. Additionally, each member learns from the others, typically from the best performer among them.

The RPSO consists of three steps, namely, generating positions and velocities of particles, velocity update, and finally, position update. Efficacy of the RPS has been demonstrated by considering a binary n-butyl acetate-water system, and a ternary system, ethylene glycol-lauryl alcohol- nitromethane.

There are two optimization objective functions, one for phase equilibrium and the second for phase stability. A severe problem causing computational difficulties in phase equilibrium calculations is that the number and identity of phases present at equilibrium are not known a priori.

Secondly, it is to be established, whether the phases and equilibrium are stable or not. A phase whose stability is in question must be assured to be at the lowest possible Gibbs' free energy before instability can be ruled out. This can be checked by global minimization of tangent plane distance function (TPDF), which is different between the Gibbs' free energy and tangent plane drawn at equilibrium composition.

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Process Modeling and Simulations

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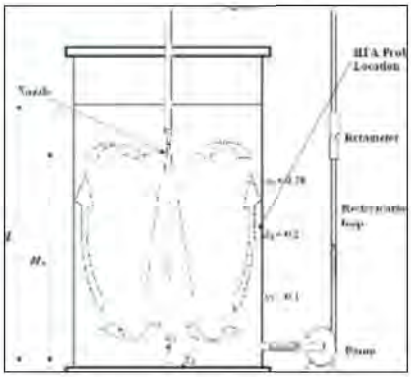
Publication
- *Ind. Engg. Chem.*, **2009**,

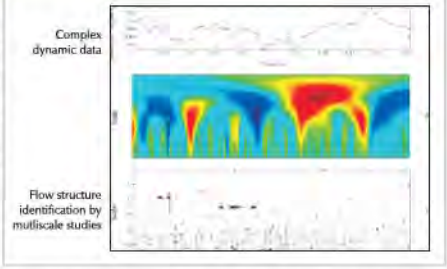
Studying flow structures and heat transfer in jet reactors by multi-scale analysis

It is important to develop multiscale methodologies for studying complex data monitored from chemical reactions and reactor systems. With sophisticated methods of data collection like LDA, PIV, HFA etc. the extent of data monitored data available is large and exhaustive. Concomitantly, the information content in the data is also much more and the need exists to develop suitable methodologies to understand the information content in it. The methods that need to be developed would require to consider not only the multiple time scale and spatial scales associated with the process but also the inherent multi-stationarity where the associated frequency content/ wave numbers is not constant, both varies in the space-time domain.



Schematic of Jet Reactor

We have been carrying out work to analyze complex data monitored from complex systems for multiscale systems using wavelet transforms and detrended fluctuation analysis of data. The results of analysis bring out applications of the Wavelet Transform Modulus Maxima Methodology (WTMM) where the passage of flow structures is viewed as an intermittent events of varying energy magnitude.



A multi-scale analysis algorithm for flow structure identification has been devised from velocity data based on (i) zero crossings and (ii) continuous wavelet transform (CWT) to study the properties of systems at iinterfaces (gas-liquid, liquird-liquid). The wavelet transform algorithm is especially found to be useful in accurately estimating both the age and size distributions of eddies near interfaces. Using these distributions, it is shown that the calculated values of properties like heat and mass transfer coefficients at interfaces show remarkable correspondence with the values obtained independently from experiments.

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Separation Science

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Publications
- *Ind. Eng. Chem. Res.*, **2009**, 48, 7893
- *Sugar J.*, **2009**, 217
- *J. Hazardous Materials*, **2009**, 167, 873
- *Mater. Res. Soc. Symp. Proc.*, **2009**, 1151

Reaction kinetics and separations

The overall objective of our work is the application of principles of chemistry and chemical engineering for (i) understanding chemical processes, (ii) the solution of diverse problems and (iii) the generation of knowledge. Some specific areas of research are: adsorption, ion-exchange, hybrid processes, and kinetics of reactions.

Work done and discussion

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, cymenes), 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.

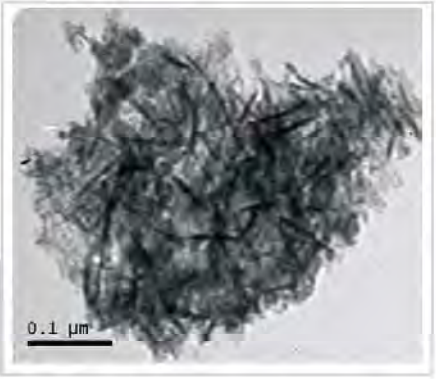


Fig. 1: Scanning Electron microscopic image of zinc aluminium hydroxide ZA-13

Fluoride/selenium decontamination from water

Anionic clays with varying amounts of bi-valent and tri-valent metal ion (M2+, M3+) 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/Cl anionic clay has been synthesized by co-precipitation method and applied for adsorption of fluoride in aqueous medium. Equilibrium adsorption data were fitted to Langmuir, Freundlich, Temkin, and Generalized isotherm equations. Thermodynamic parameters like ΔG and ΔH values showthe feasibility and exothermic nature of the adsorption process.

Influence of solution pH and presence of other anions on fluoride adsorption by the clay has also been studied. Presence of carbonate inwaterwas found to have an adverse effect on fluoride adsorption by the clay. pHpzc of the clay has been found to be 8.97.

A two-step 1st order kinetic model was used to explain the fluoride adsorption kinetics of the as-synthesized clay. It was possible to regenerate the adsorbent with an aqueous solution of 0.01M NaOH and the effect of regeneration on fluoride adsorption was reported up to five regeneration cycles.

Layered double hydroxide materials (Zn/Al, Mg/Al, Zn/Fe) with varying composition (M^{2+}:M^{3+} molar ratio, x) 3, 2, 1, and 0.33) were synthesized and evaluated for their selenium adsorption characteristics in aqueous medium.

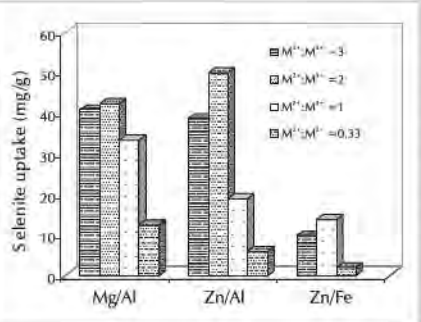


Fig. 2: Selenite uptake on Mg/Al, Zn/Al and Zn/Fe LDHs with varying M^{2+}: M^{3+} molar ratios (Initial selenite conc. 50.34 mg/l; volume: 100 cm3; adsorbent dose: 0.1 g; contact time: 240 min; temp: 25°C).

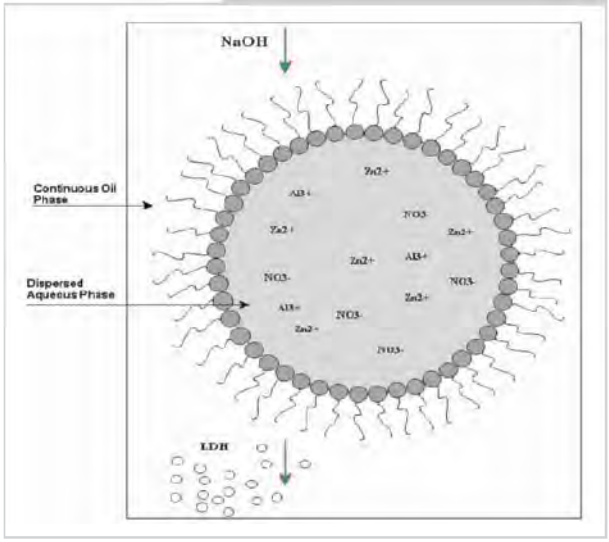
Zn/Al and Mg/Al LDHs with x) 3 and 2 exhibited very high selenite adsorption capacity. XRD patterns of the pristine LDHs, LDH after selenite adsorption, and chloride ion leaching studies revealed that adsorption of selenium on the LDHs occurred through both surface adsorption and ion-exchange mechanism.

The adsorption data was fitted to Langmuir and Freundlich isotherm models. A pseudo second-order kinetic model was used to describe the adsorption kinetics of selenite on LDH materials. Desorption of selenite ions in water from the LDH-Se matrix was studied up to 5 h.

Zn/Al layered double hydroxide was synthesized in micro-emulsion system with the oil phase comprising of cyclohexane + TX100 (surfactant) + n-hexanol (co-surfactant). Aqueous NaOH solution was used as the precipitating agent. The XRD pattern showed Zincite as the primary and hydrotalcite as the secondary phase.

The d_{003} diffraction peak corresponded to interlayer hydroxide ion. There was no interlayer NO3 - ion. The synthesized LDH showed much higher BET surface area (116.3 m^2/g) than similar LDH synthesized by conventional co-precipitation technique (4.2 m^2/g). Well defined flaky nano-crystals having an average dimension of 5-20 nm were observed by HRTEM.

Fig. 3: Schematic diagram of the synthesis of LDH in w/o micro-emulsion technique



CATALYSIS

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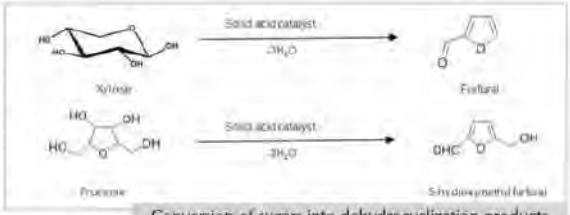
Publication
- PCT Application, PCT/IN2010/000047

Conversion of biomass and biomass derived chemicals using heterogeneous catalysts

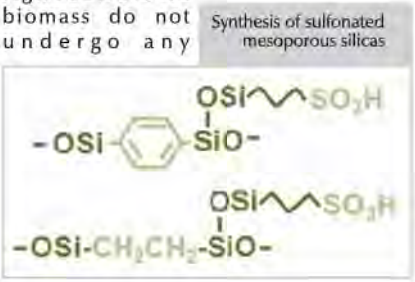
Recently, conversion of biomass especially non-edible biomass (lignocellulosic materials) into chemicals, fuels, and energy is attracting lot of attention under the biorefinery concept because of dwindling fossil feedstock resource.

The mismatch in demand and supply of conventional resources such as fossil feedstock are also responsible for the increasing interests in the conversion of biomass. Since several governmental rules and regulations across the globe regarding environmental pollutions etc. are becoming effective, it is desired to develop green routes for the known processes or for future processes. The heterogeneous catalyst based process can overcome drawbacks associated with enzyme and mineral acid based processes such as difficulty in the recovery of the catalyst, corrosion, using buffer etc. The heterogeneous catalysts could be of different types such as solid acids, solid bases, supported metal catalysts etc. which can be used for the conversion of biomass.



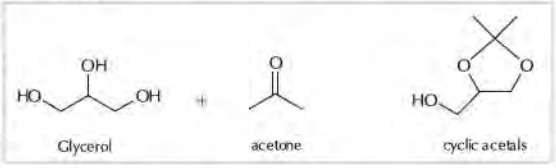
Conversion of sugars into dehydrocyclization products

We have carried out work on the selective conversion of hemicellulose from bagasse (crop waste) using solid acid catalysts. The results indicate that under certain reaction conditions it is possible to achieve ca. 50% xylose+arabinose yield from bagasse. By tuning the reaction conditions it is also possible to achieve ca. 60% furfural yield. While converting hemicellulose from bagasse, cellulose and lignin the other components of lignocellulosic biomass do not undergo any degradation reactions. The catalysts are recyclable but with loss of activity (ca. 10% after each run). The detailed characterization of the catalysts was done and it was observed that catalysts undergo morphological changes after the catalytic reactions.



Synthesis of sulfonated mesoporous silicas

The synthesis and characterization of sulfonated mesoporous silicas and sulfonated carbon materials as the solid acid catalysts was also carried out. These catalysts showed ca. 1 mmol/g of acid amount and were used in the synthesis of furfural and 5-Hydroxymethyl furfural (HMF) from xylose and fructose, respectively. Although our catalysts were active the other solid acid catalysts such as zeolites, clays and metal oxides also showed better or comparable activity.



The effect of solvent (water and organic solvent) was studied and it was found that if the reactions are done without water (only with organic solvent) or with <10% water concentration, yields of furfural and HMF increases.

The other work which was done is acetals formation from glycerol using solid acid catalysts. Since glycerol is a side product in the biodiesel synthesis it is desired to use it for the synthesis of value-added chemicals. The acetals are useful as the intermediates in various chemical industries.

Catalysis

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Publications
- *J. Mol. Catal. A.*, **2009**, 310, 150
- *Appl. Catal. A.*, **2010**, 374, 103
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- *App. Catal. B.*, **2009**, 90, 416

Development of catalyst for organic transformations and environmental applications

Development of catalyst for removal of NOx from automobile exhaust engines

Hydrocarbon selective catalytic reduction (HC-SCR) of NOx is a powerful technology for the removal of NOx, CO and unburned hydrocarbon from automotive emissions under a large excess of oxygen. Ag/Al_2O_3 is one of the most active and selective catalyst for the SCR of NO_x to N_2 however it has poor activity in low temperature range which is required for automobile applications, as well as it is highly prone to sulphur poisoning.

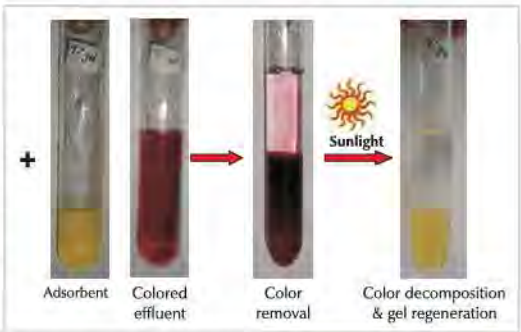
Hence there is a need for development of catalyst active at low temperature range which is sulphur tolerant. We have modified the support of Ag/Al_2O_3 by doping it with SiO_2 or TiO_2.

These modified catalysts have shown very good sulphur tolerance during the selective catalytic reduction (SCR) of NO_x using propene under lean conditions. In situ FTIR studies have shown the mechanism for improved sulphur tolerance. We have also prepared Au/Al_2O_3 catalyst to test its low temperature activity and the highest activity was found in the temperature range of 300-350 °C for reduction of NOx with 100% selectivity for N_2.

initially separated and subsequently decomposed in presence of sunlight thus regenerating the gel which can be reused many times. We are also exploring its application for various organic transformations. Some of the advantages of this process are as follows:

- Fast separation of organic dyes from aqueous solution
- Decomposition of dyes in sunlight
- Easy regeneration, needs only sunlight
- Contains 99.997 % water only 0.003% active component hence cost effective
- Two-step effluent treatment
- No secondary effluent generated

This technology was awarded the gold medal in Indian Innovation programme 2010 organized by DST, FICCI & IC2 Institute of Texas.



This technology has fetched gold medal in Indian Innovation programme 2010 organized by DST, FICCI & IC2 Institute of Texas.

Titanium based gels for separation and degradation of organic pollutants and dyes

We have developed titanium based gels for environmental applications like separation and degradation of the organic dyes and organic contaminants from aqueous solution.

The effluent coming out of dye and ink manufacturing as well as textile industries is highly colored. This color needs to be removed as well as decomposed before the effluent water is let in the main stream due to regulatory restrictions.

Using this gel adsorbent the colored contaminates from aqueous effluent can be

Synthesis for dioxo molybdenum acetylide complexes for catalytic oxidations

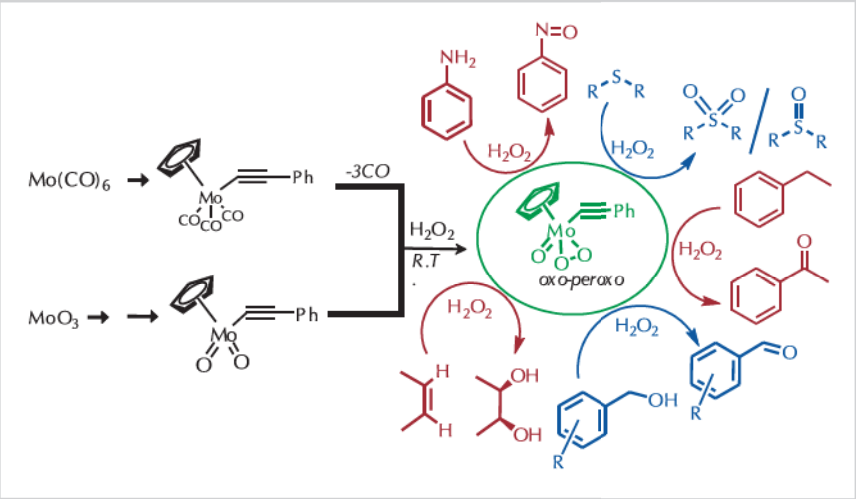
We have already reported the preparation of the molybdenum carbonyl acetylide complex $CpMo(CO)_3$(-C CPh) from $Mo(CO)_6$ and its catalytic applications for oxidation of variety of organics using hydrogen peroxide or TBHP as oxidants.

This complex though homogeneous, could be recycled very efficiently without any problems. As Mo carbonyl complex loses CO in presence of H_2O_2 and forms corresponding Mo(VI) oxo-peroxo complex $CpMo(O_2)O$(-C CPh), we have developed a novel and very simple methodology for preparation of $CpMoO_2$(-C CPh) from MoO_3 which forms corresponding

Mo-oxo peroxo complex in presence of H_2O_2.

Preparation of Mo carbonyl complex involves use of expensive molybdenum hexacarbonyl, it is multi step reaction involving tedious work up procedures due to which the yield of final complex is low and hence it becomes expensive.

The strategy which we have developed for dioxo molybdenum acetylide complex involve use of very cheap MoO_3 as precursor, the number of steps in the synthesis are reduced substantially and also the work up is very simples because of which this methodology is very simple and cost effective compared to corresponding carbonyl complex.



The dioxo molybdenum acetylide complex has also shown very high catalytic activity for oxidation of various organics and was recycled efficiently. We are in process of filing patent for the synthesis procedure. One multinational industry has shown interest in this catalyst for industrial applications.

We are also preparing various Mo-dioxo complexes using variety of azole ligands. Our aim is to study the catalytic / biological activity of different Mo complexes when different donor atoms like N and S are present in the ligand with acetylide group.

Heterogeneous catalysts for valorization of renewable

Synthesis of acrylic acid by dehydration of lactic acid

Lactic acid is prepared from sugarcane juice and hence becomes renewable material. Lactic acid is said to be sleeping giant, which can be converted to many value added chemicals.

We have developed a process for converting lactic acid to acrylic acid which is important raw material for polymer industry. This continuous down flow process gives 100% lactic acid conversion with ~60% selectivity for acrylic acid with acetaldehyde as the only by-product.

This performance is much superior to the previously reported methods (patents and publications) where number of products formed is more with less selectivity for any particular product as well as very high CO_2 formation. We are in process of filing patent for this process.

Glycerol value addition

We have developed a range of high surface area mesoporous solid acid catalysts by simple sol-gel method which has been used for value addition to glycerol by acetylation and etherification of glycerol.

During the synthesis of solid acid catalyst specially MoO_3/SiO_2 by sol-gel synthesis we have observed in situ formation of heteropoly acid on the surface of the support. Extensive characterization for these catalysts is presently in progress.

Catalysis

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Publications
- *Chem. Biochem. Eng. Q.*, **2009**, 23, 267
- *J. Rare Earths*, **2010**, 28, 1
- *Sepn Sci. Technol.*, **2009**, 44, 2626
- *Anal. Lett.*, **2009**, 42, 3018

Sequestration of carbon dioxide over regenerable adsorbents at post and pre combustion conditions

Investigations have been carried out using liquid cation or anion exchanger for the transport of metal and carbonate ions with supported liquid membrane. The objective of this research includes the screening of liquid anion exchangers for sequestration of carbon dioxide at the post-combustion conditions.

The main objective of research is to develop dry regenerable porous solid lithium or calcium silicate, zirconate and aluminates adsorbents with or without modifications for pre-combustion high temperature CO_2 removal (IGCC conditions). The present research activitiy includes development of porous solid lithium or calcium silicate, zirconate, aluminates adsorbents for carbon dioxide sequestration at pre-combustion high temperature (IGCC conditions).

Fiber supported membrane

A novel idea of transport of yttrium (III) metal ions through fibers supported liquid membrane in two stage processes namely source to membrane and membrane to receiving phase has been investigated. The fibers supported liquid membrane was impregnated with different concentrations carrier. The pre-concentration of yttrium (III) ions was investigated from the dilute solutions.

The two-channel fibers supported liquid membrane solvent extraction was investigated for the transport of yttrium (III) ions from the source to membrane and membrane to receiving phase. The scheme below illustrates the transport of yttrium ions from source to membrane and membrane to receiving phase through fibers supported liquid membrane.

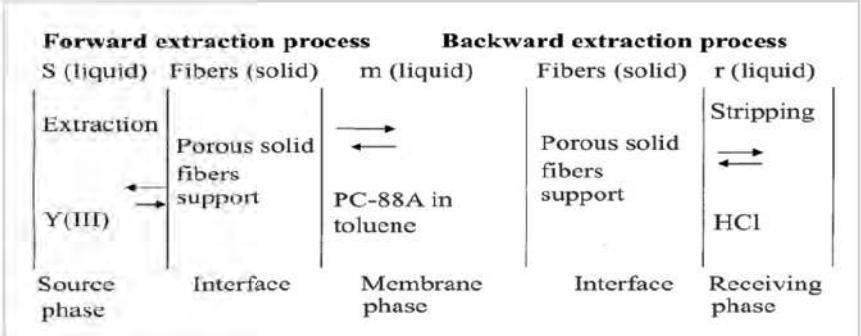
The continuous yttrium ion transport through fibers supported liquid membrane can be simultaneously carried out as extraction from source to membrane phase and stripping from membrane to source phase. There is no continuous flow of mobile phase (either source or membrane or receiving) through the fibers membrane support, but, there is a transport of metal ions through the interface of the source, membrane and receiving phase.

Therefore, the solute or metal ion transport mechanism is considered to be the supported liquid membrane. The capillary action mechanism in the fiber is very significant for the transport of yttrium ions due to the gradient concentration difference in the both sides of the interface. The fiber supported liquid membrane solvent extraction is a dispersion free technique, no need of phase separation and can continuously be operated for several hours.

Cotton fibers are eco-friendly natural material, no need to be separately manufactured and no environmentally disposal problems. Thus, cotton fibers have added advantages over the synthetic polymer fibers.

CO_2 Sequestration

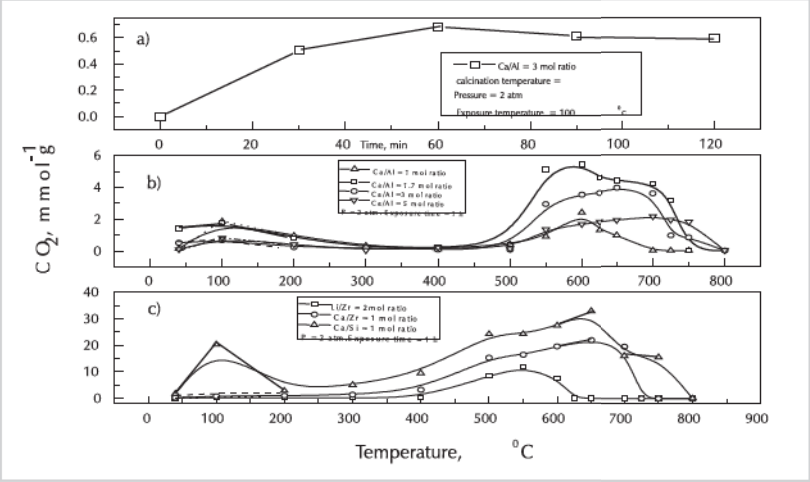
The atmosphere of an earth, global warming an important issue, is warming up with the released heat from the heat liberation sources such as refineries, industries, thermal power stations, vehicles, growing population, cooking burners, aircrafts, volcano, sun, etc,. The liberated heat and CO_2 from these different sources should be balanced by the increasing the forestry.



The concentration of carbon dioxide in the atmosphere is increased from 250 to 350 ppm during the last several years. We could reduce the global warming heat by reducing the use of natural gas, petroleum and coal fuels, and also developing the commercial process for the capturing the carbon dioxide. There are different ways to control the carbon dioxide emission either by reducing use of petroleum products and coal, and the development of non-conventional energy sources.

The bio-fuel is an alternative but it also generates carbon dioxide during its combustion. It is very difficult to meet the required demand of energy from the other sources except petroleum product. Therefore, there is a need to develop the method for the sequestration, capture and storage of carbon dioxide.

There are several ways to sequester the carbon dioxide such as by deposition underground, reacting with rocks, by dissolving in the water in the underground, by adsorption over porous solid adsorbents zeolites and carbon, by making complex with amines, ionic liquids, metal oxides etc. The figure shows that the sequestrations of carbon dioxide over calcium aluminate, calcium zirconate, calcium silicate and lithium zirconate at pre-combustion temperatures in a quartz reactor by using temperature controlled split furnace. The gases connection systems were set to sequester the carbon dioxide over the adsorbents. The sequestration of carbon dioxide over these adsorbents were studied in the temperature range 40 to 800 °C. The trend of sequestration of carbon dioxide over these adsorbents observed was in the increase in order as calcium aluminate < lithium zirconate < calcium zirconate < calcium silicate.



Catalysis

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Synthesis, characterization, catalytic benign processes and scale- up

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Publications
- *Ind. Engg. Chem. Res.*, **2009**, 48, 9408
- *Fuel*, **2009**, 88, 1773
- *Cat. Lett.*, **2009** ,133, 175
- US Patent Appln No.: US20090326252A1 (2009)

R & D activities focus on the development of catalyst or support / synthesis route / catalytic process / protocol for characterization and scale up studies. Some of the activities are described below:

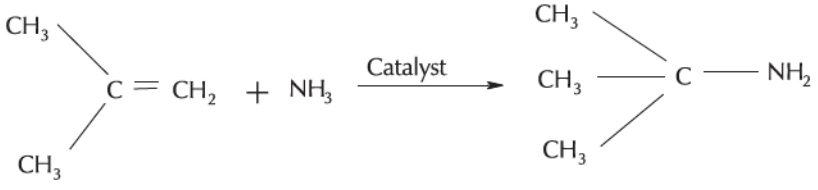
Development of catalyst for tert-butyl amine from isobutylene and ammonia

We have developed a process for production of tertiary butyl amine from isobutylene and ammonia using heterogeneous catalyst that operates at lower pressure of 30 bars to give 40 to 48% isobutylene conversion with a selectivity of 93 to 97%. None of the prior arts mention high conversion of isobutylene.

Detail studies were carried out on the optimization of the process parameters.

The conversion of triglycerides (TG), diglycerides (DG) and monoglycerides (MG) appeared to be second order mechanism for the forward and reverse reactions, where the reaction system could be described as a pseudo heterogeneous catalyzed reaction. Reaction rate constants for TG, DG and MG hydrolysis reactions were 0.12 - 0.84 h^{-1} and higher for the MG reaction than for the TG hydrolysis.

The proposed kinetic model fitted the experimental results well. The efficacy of Flyash



Isobutylene Ammonia tert-Butyl Amine

The process for the preparation of catalyst was also successfully scaled up to 10kg/batch level.

Synthesis of Si-MCM-41 by dry gel conversion route

Steam-assisted dry-gel conversion method was employed for the synthesis of Si-MCM-41 from ternary SiO_2: CTAOH: H_2O systems wherein fumed silica was used as a source of silica. The influence of synthesis time, molar ratios of $CTAOH/SiO_2$ in dry gel and the water content at the bottom of autoclave on the quality and formation of mesophases has been investigated.

Keeping synthesis temperature and $CTAOH/SiO_2$ molar ratio fixed, Si-MCM-41 with improved hydrothermal stability was obtained by steam-assisted dry gel conversion route.

Transesterification of sunflower oil with alcohol

The novelty of the heteropolyacid on clay (K-10) for the transesterification of vegetable oil with lower and higher alcohols was studied.

based base catalyst in the transesterification of sunflower oil with methanol in a heterogeneous manner was also investigated. Catalyst preparation variables such as, the KNO_3 loading amount and calcination temperature were optimized. The catalyst prepared by loading of 5wt% KNO_3 on flyash followed by its calcination at 773K has exhibited maximum oil conversion of 87.5%.

Esterification of carboxylic acid with alcohol

The esterification of carboxylic acids is one of the fundamental reactions in organic synthesis. Liquid phase esterification is an important method for producing various esters.

Esterification of carboxylic acid with alcohols such as ethanol, n-propanol and iso-propanol catalyzed by dodecatungestophosphoric acid, $H_3PW_{12}O_{40}$ (DTPA), on acid treated montmorillonite clay (K10) were carried out.

Among different catalysts, 20% w/w DTPA/K10 was observed to be the optimum catalyst for all studied alcohols, with 100% selectivity towards alkyl esters.

Recycling of mother liquor (ML) produced during the hydrothermal crystallization of K-LTL zeolite

With a aim of recycling ML produced during the hydrothermal crystallization of K-LTL zeolite to synthesize different zeolites of commercial importance, systematic studies on (1) optimization of the synthesis variables such as crystallization temperature and molar SiO_2/Al_2O_3 ratio in gel to minimize the generation of chemical waste, (2) establishing of the cause and effect relationship between composition of the recycled ML and the type/quality of the zeolite phase formed by hydrothermal crystallization and (3) screening of different zeolites obtained by recycling ML for their catalytic performance in commercially important esterification of acetic acid with n-butanol reaction was undertaken.

Hydrothermal crystallization of K-LTL zeolite with minimum chemical waste was achieved at 443 K from starting molar gel composition $8K_2O : Al_2O_3 : 20SiO_2 : 200H_2O$.

After recovery of crystalline K-LTL, the mother liquor containing unutilized reagents was effectively recycled for synthesis of K-LTL, K-W, Na-P and Na-A type zeolites. The cause and effect relationship was established between composition of the starting gel and the type of the zeolitic phase formed. Under identical reaction conditions, the K-LTL and KW obtained from recycled ML exhibited n-butanol conversion of 85 % in esterification of acetic acid with n-butanol.

Na-A has shown better n-butanol conversion of 88 %. Na-P was observed to be less active (80% n-butanol conversion) amongst all.

Oxyanion-induced hydrothermal crystallization of Sn-BEA molecular sieve in fluoride medium from unseeded and Al-free gel

In prior art, either Al-free seed or source of aluminum was used in initial gel to prepare Sn-BEA. Moreover, the synthesis in the conventional basic medium usually results in the formation of connectivity defects which affects the sorption, hydrophilic/hydrophobic properties and thermal stability. Earlier methods of synthesis of Sn-BEA by hydrothermal method suffer from a drawback of longer crystallization period which restrict its application on bulk scale.

In order to overcome the drawback of longer crystallization period and por quality, we have made an attempt and successfully developed a facile synthesis route for the preparation Sn- BEA by oxyanion-induced hydrothermal crystallization in fluoride medium from unseeded and Al-free gel.

Different unseeded (dealuminated or otherwise) Al-free gels will be prepared and subjected for hydrothermal crystallization using H_nX, a source of oxyanion where $3 \leq n \geq 1$ and X will be selected from ClO_4^-, SO_4^{2-}, Po_4^{3-}.

The influence of synthesis variables such as molar ratio of $TEAOH/SiO_2$, HF/SiO_2 SiO_2/SnO_2 in the gel composition, amount of HnX (oxyanion source), and type of silica source materials on the crystallization period and product quality were investigated.

Catalysis

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Hydroformylation using ionic liquids as solvents

Catalyst-product separation is major drawback of Homogeneous Catalysis. Non Aqueous Ionic Liquids [NAILs] represent a class of solvents, which are considered environmentally green. Aim of the work was to develop biphasic system for the hydroformylation of 1-octene using ionic liquids as solvents.

The kinetics of biphasic hydroformylation of 1-octene was studied using Rh/TPPTS catalyst and [bmim][PF_6] as catalyst solvent. Typical concentration-time profile is presented in Fig. 1. The concentrations of dissolved CO, H_2 and 1-octene in [bmim][PF_6] required in the kinetic modeling were evaluated from solubility data obtained experimentally at different temperatures, using pressure-drop technique for gas-liquid equilibrium and multiple headspace gas chromatography as well as thermogravimetry for liquid-liquid equilibrium.

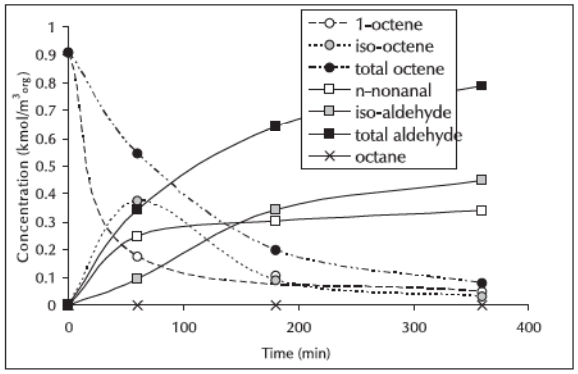

Fig. 1: Typical concentration-time profiles for hydroformylation reaction of 1-octene using [bmim][PF6]/decane biphasic system

The rate of hydroformylation was found to be first order with respect to catalyst concentration and partial order with respect to both olefin concentration (0.75) and hydrogen partial pressure (0.43). Its evolution versus CO concentration exhibited a maximum, indicating an inhibition at higher pressures. The activation energy was found to be 25.8 kcal/mol. The kinetic data were represented by a simplified rate equation derived from a classical mechanistic model, excepting the observed trend with respect to hydrogen.

A first simulation attempt of the concentration-time profiles including isomerization was also proposed. Few experiments were carried out using sulfoxantphos as a ligand to compare catalyst activity and selectivity.

It was observed that only n-aldehyde was obtained as a product and iso-aldehyde was not at all detected in this reaction. However, the activity of the catalyst was very low (~23 times) compared to the catalyst with TPPTS as a ligand.

Reaction conditions$Rh(CO)_2(acac)$: 6.97×10^{-3} kmol/m^3IL, TPPTS (without 10% impurities): 2.09×10^{-2} kmol/m^3IL (P:Rh=3:1), 1-octene: 0.973 kmol/m3org, T: 353 K, P_T: 40 bar (H_2:CO = 1:1), total liquid volume: 100×10^{-6} m^3 (organic:IL = 60:40 v/v), agitation speed : 1200 rpm.

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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. Recently there is an increasing interest to develop a catalyst for the synthesis of acrylic acid from direct oxidation of propane instead of propene due to the abundant availability of propane and hence, economic reasons.

The aim of the work was to develop new or improved mixed oxide catalysts containing alkali, alkaline or rare earth metals for the selective oxidation of propane to acrylic acid with high selectivity to acrylic acid.

Mo- and V-based mixed oxide catalysts containing alkali or alkaline earth metals have been prepared by various catalyst preparation methods at different preparation conditions. A very low selectivity to acrylic acid (< 7%) was obtained when the reaction was carried out over un-doped Mo-V-Sb-Ox catalyst. The carbon oxides (CO and CO_2) were found to be the major by-products with ≥70 % selectivity for the un-doped catalyst.

The surface properties (surface area, acidity, crystal phases) were significantly influenced by the catalyst preparation method. Among the alkaline earth doped catalysts, Mg- and Sr-doped catalysts were found to be highly active and selective for the oxidation of propane to acrylic acid. For all the catalysts, acrylic acid was obtained as a major liquid product in the reaction.

For Mg-doped catalysts, propane conversion was obtained in the range of 8-23% with 15-35% selectivity to acrylic acid. The oxidation of propane has also been carried out using Cs-doped catalysts. Among the Cs-doped catalysts prepared by different methods, a highest surface area was obtained for the catalyst prepared by co-precipitation method and its XRD pattern was totally different compared to catalysts prepared by dry-up, hydrothermal and slurry methods.

For this catalyst, CO and CO_2 were obtained as the major products with very high selectivity (~85%) to carbons oxides (CO and CO_2) with very little formation of acrylic acid. The Cs-doped catalyst, prepared by dry-up method, showed a promising catalytic performance with about 50 % selectivity to acrylic acid with reasonable propane conversion (8%).

Significant improvement in the selectivity to acrylic acid was observed when the reaction was conducted in presence of water vapor. The results clearly indicate that water is playing a very important role in improving the acrylic acid selectivity.

Catalysis

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Publications
- *Appl. Catal. A: Gen,* **2009**, 370, 16.
- *Catal. Surv. Asia,* **2009**, 13, 205.
- *Ind. Eng. Chem. Res.*, **2009**, 48, 9423, 9457

Green chemistry via catalysis

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.

Selective for liquid phase air oxidation using solid catalysts

Oxidation of organic substances is one of the most important methods for producing diverse chemicals from oil derivatives and vegetable raw materials. In the production of fine chemicals it is imperative that the reactions are selective. The traditional oxidation methods often involve the use of stoichiometric amounts of inorganic oxidants, such as chromates, which clearly cause serious effluent problems. In addition, these reactions usually require high temperatures and pressures, which consume a lot of energy and cause lower selectivities.

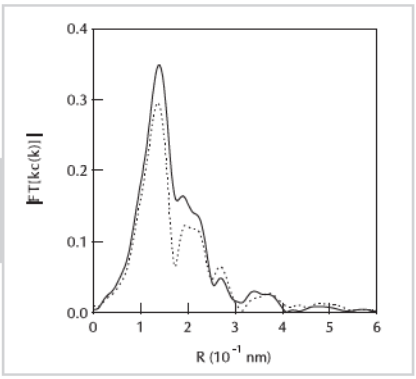

Fig. 1: Fourier transforms of k-weighted EXAFS spectra at Co K-edge for Co-salen (—) and Co(salen)-mont (-).

These drawbacks can be overcome by developing catalytic processes for oxidation. From an industrial point of view oxidation catalysis poses three challenges: a) activation of molecular oxygen, b) avoid over oxidation of the substrate, and c) overcome the lack of functionality in the feedstock. In our study, two-dimensional montmorillonite and saponite clay were chosen as a host framework for intercalation of Co-salen type complexes.

Structural parameters for Co-salen and Co(salen)-mont obtained by a curve fitting analysis of the EXAFS Fourier transforms (Fig. 1) indicate that cobalt atoms in Co(salen)-mont form two additional Co-O bonds with a bond length of 0.199 nm by the intercalation, while retaining the Co-salen structure, as shown schematically in Fig. 2. This heterogeneous catalyst was found to give a five-fold higher TON than the homogeneous cobalt salen complex for liquid phase air oxidation of *p*-cresol.

In continuation of our efforts on developing new insoluble catalysts for oxidation of phenol derivatives, we also developed for the first time synthetic saponite containing Co^{2+} in the octahedral layer as a highly efficient catalyst for liquid phase oxidation of p-cresol. This is an example of trioctahedral smectite in which the charge imbalance due to isomorphic substitutions in the structure layers is compensated by cations placed in interlamellar position.

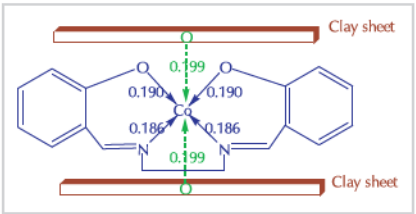

Fig. 2: Schematic representation of cosalen-mont catalyst

Therefore, Co-saponite obtained can be viewed as a nanocomposite (100nm) of Co phases over aluminosilicate support as a catalyst for oxidation reactions. The core level BE of $Co2p_{3/2}$ and $Co2p_{1/2}$ were observed at 781.9 eV and 797.6 eV respectively (Fig. 3).

In addition to these spin-orbital peaks, the satellites for $2p_{3/2}$ and $2p_{1/2}$ were also observed at 787.4 and 803.3 eV respectively, confirming that cobalt was mainly present in (II) oxidation state. The broad peak (FWHM=3.4 eV) of $Co2p_{3/2}$ (shown as inset in Fig. 3) in Co-saponite suggests the presence of octahedrally and tetrahedrally coordinated divalent cobalt species.

DRUV-visible of Co-saponite shows bands at about 495, 530, 570 and 645 nm (Fig. 3) assigned to tetrahedral Co(II) species. Band at 250nm could be due to oxygen-to-metal charge transfer (CT) transition [19]. A broad and intense band at 530 nm suggest

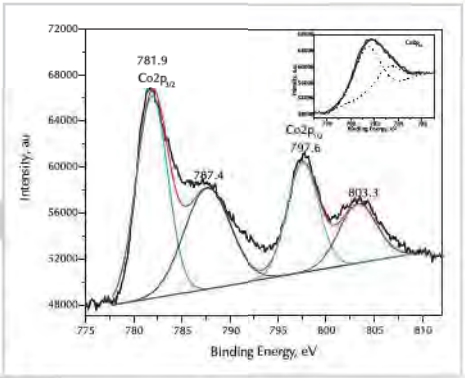

Fig. 3: Co 2p XPS spectra of Co-saponite

the presence of extra-lattice Co(II) in octahedral symmetry.

Highest conversion of 92% of p-cresol was achieved with Co-saponite catalyst at 827 kPa of oxygen pressure giving 92% selectivity to p-hydroxybenzaldehyde. Formation of benzoic acid could be significantly minimized as well as formation of non oxidation products were also completely suppressed using our catalyst.

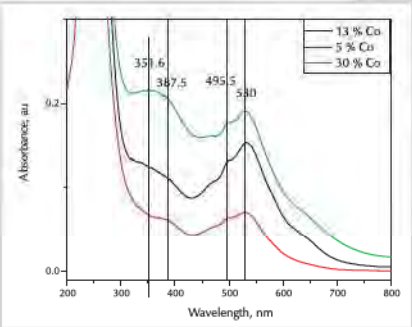

Fig. 4 : DRUV-Visible spectroscopy of Co-saponite

highest catalytic activity and selectivity. In case of hydroxyalkylation of p-cresol ,surface modified BNT (20% DTP/BNT) catalyst showed an excellent activity (95% product yield with 94% selectivity to DAM) for the hydroxyalkylation of p-cresol.

Parent DTP showed a sharp signal at -15.61 ppm that corresponds to tetrahedral co-ordination of PO_4 in the Keggin unit [(Fig. 3 a) Interestingly, 20% DTP/BNT showed broad signal which shifted towards downfield from -15.61 to -13.7 ppm after impregnation of 20% DTP on it (Fig. 3 b).

This broadening and downfield shifting of signal could be due to the strong interaction of protons of bulk DTP with surface hydroxyl groups of BNT leading to the localization of DTP protons thereby increasing their proximity to the Keggin anion because of the decrease in proton mobility. Such surface as well as acidity modification of BNT due to DTP impregnation enhanced its catalyst activity towards hydroxyalkylation of p-cresol.

Acidity tuning of various solid acid catalysts for selective hydroxyalkylation of phenol derivatives to dihydroxydiarylmethane products

For phenol hydroxyalkylation reaction, 20% DTP/SiO_2 catalyst gave the highest products yield of 34.2% and selectivity of 90.1% to bisphenol F, at 353 K and with a phenol-to-formaldehyde mole ratio of 5:1.

Ammonia TPD studies of various catalysts showed that an appropriate combination of both strong and weak acid sites of DTP/SiO_2 was mainly responsible, rather than only the stronger acidity of bulk DTP, for its

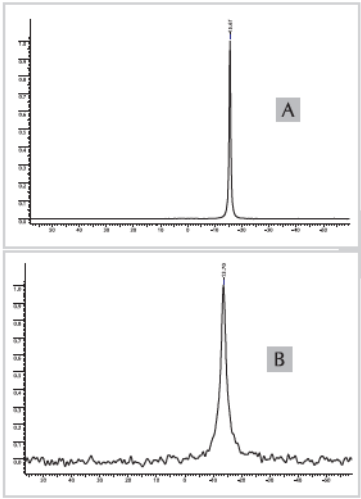

Fig. 5. ^{31}P- CPMAS NMR of (a) DTP (b) 20% DTP/BNT

Catalysis and phase behavior studies in supercritical CO_2

Hydrogenation of 4-alkylphenols was studied over a charcoal-supported rhodium catalyst in supercritical carbon dioxide ($scCO_2$) solvent, and the results were compared with those in 2-propanol. Higher cis-alkylcyclohexanols selectivities were obtained in $scCO_2$ than in 2-propanol solvent. In addition, the stereoselectivities to cis forms were improved in the presence of hydrochloric acid.

The effect of steric structure of alkyl group on the stereoselectivities is discussed based on the hydrogenation mechanism of 4-alkylphenols. To elucidate the effect of carbon dioxide pressure on the initial rate of reaction, the phase behavior of ternary (2-tert-butylphenol-carbon dioxide-hydrogen) system was separately observed with a view cell, and the calculations of vapor-liquid equilibrium and compositions in the vapor and liquid phases inside the reactor were carried out using the Peng-Robinson equation of state.

The hydrogenation behavior in the carbon dioxide solvent is discussed based on the phase behavior of the ternary system. For naphthalene hydrogenation to decalin and tetralin in sc CO_2, graphite-supported rhodium catalysts were more efficient than the rhodium supported on activated carbon catalysts because rhodium particles were found to be on the edge of graphite crystallites leading to higher hydrogen adsorption.

Catalysis

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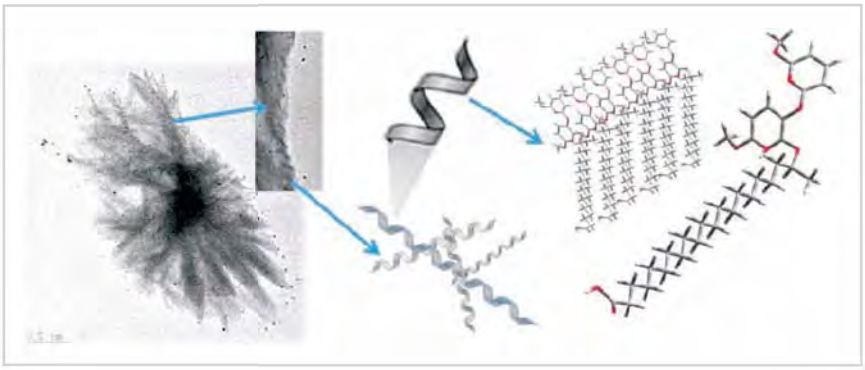
Nano Materials / Bio-inorganic hybrid materials

Bio-inorganic hybrid nano materials using some naturally derived lipids are being explored with a focus of applications in biomedical and bio-inorganic materials. Lipids prepared from natural routes are impressive in terms of their ecological and economical simplicity. Sophorolipids derived out of home-made natural recipe are being used to generate interesting bio-inorganic nano hybrids that are seemed to be more rugged and functional for different applications.

One of the successful materials is the bio-inorganic nano-whiskers. They have a huge potential to be used in biomedical applications such as an active additive for materials such as hydroxyl-apatite (HA) - silica composite. They have the best blend of biocompatibility and the inorganic functionality to improve the material property. The materials synthesis procedure has been optimized and the characterizations have been done using dynamic laser scattering (DLS), nuclear magnetic resonance spectroscopy (NMR), Transmission electron microscope (TEM) and high resolution environmental scanning electron microscope (ESEM) and optical microscope.



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Publications

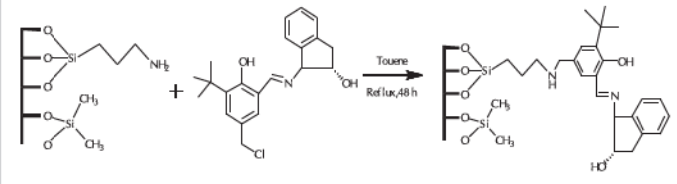
- *Appl. Catal. A*, **2010**, 372, 130
- *Catal. Lett.*, **2009**, 132, 492
- *Catal. Today*, **2009**, 141, 161
- *J. Mol. Catal. A*, **2009**, 301, 118

Asymmetric organic transformations using heterogenised chiral complexes over organo-functionalised solid mesoporous materials

The main aim of the work is to heterogenize homogeneous chiral complexes of Mn and V over mesoporous SBA-15 materials and study their catalytic application in the asymmetric epoxidation, cyclopropanation and hydrolytic kinetic resolution reactions.

The main goals are to synthesize the new chiral heterogeneous catalyst in a step by step manner. The mesoporous SBA-15 is synthesized in the first step of the reaction. The next step is grafting of 3-halogeno or 3-aminopropyl trimethoxy silane, 2-(4-amino/chlorosulfonylphenyl) ethyltrimethoxy silane over mesoporous materials through Si-O-Si bonds, leading to the hybrid materials with free 'X' (X= -Cl, -Br, -I, -NH2) groups which will be used to anchor the homogeneous chiral auxiliaries. Another objective is to synthesize a series of chiral Schiff base ligands as well as the corresponding complexes for the immobilization over proposed mesoporous materials.

Fig.1: Synthesis of heterogenised (1R, 2S)-1-(N-Salicylideneamino)-2-indanol on Pr-NH2-SBA-15



Further, textural characteristics of the catalysts will be determined by FT-IR, ^{1}H, ^{13}C and ^{29}Si MAS NMR spectroscopy, high resolution transmission electron spectroscopy (HRTEM), diffuse reflectance UV-Vis spectroscopy, Raman spectroscopy, X-ray diffraction (XRD) scanning electron microscopy (SEM), nitrogen adsorption desorption isotherm.

Next objective is to screen the synthesized and characterized heterogenised chiral catalyst for various asymmetric organic reactions as described above and the activity obtained is compared with the corresponding homogeneous catalysts.

Chiral Schiff base ligands such as [(1R,2S)-1-N-salicylideneamino]-2-indanol and (S,S) (-) [N-3-t-butyl-5-chloromethyl salicylidene]-N'-[3',5'-di-t-butyl salicylidene] 1,1'-binapthyl-2,2'-diamine were successfully synthesized and supported onto modified mesoporous SBA-15 using 3-aminopropyltrimethoxysilane (3-APTMS) and 2-(aminosulfonylphenyl) ethyltrimethoxy silane as reactive surface modifier by a covalent grafting method.

The synthesized samples were primarily characterized by XRD, FT-IR, solid state NMR and elemental analysis, etc. The XRD measurements of the catalyst confirmed the structural integrity of the mesoporous hosts even after the modification and the spectroscopic characterization techniques proved the successful anchoring of the metal complexes over the modified mesoporous support. Further the heterogenised chiral complexes over functionalized mesoporous materials will be applied for asymmetric epoxidation and cyclopropanation. The catalytic activity and enantioselectivity obtained will be compared with the homogeneous homologues.

Catalysis

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Efficient solid catalyst for hydrolysis of oils and fats

Fatty acids are major components used in the preparation of a wide variety of products, such as soaps, surfactants, lubricants, plasticizers, paints, coatings, pharmaceuticals, foods, agricultural, industrial and personal care products. Biodiesel (fatty acid methyl esters, FAME) can also be produced from fatty acids by esterification with methanol.

The conventional method of manufacturing FAME biodiesel (i.e., transesterification of vegetable oils with alcohols) is suitable mainly for refined oils or oils with low contents of free fatty acids. Currently, the production of FAME biodiesel from such relatively expensive feedstocks is uneconomical.

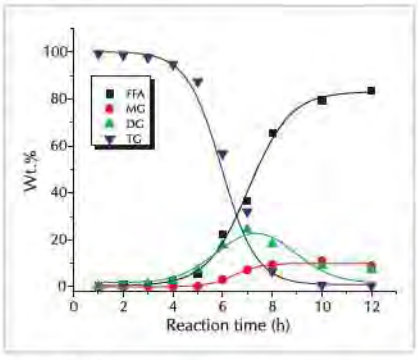
With low-cost feedstocks, like crude vegetable oils, animal fats, waste cooking oils and soap stocks which contain large amount of fatty acids, the yield of biodiesel by the transesterification route is low since fatty acids and water inhibit the reaction. An alternate, more generic process for the production of biodiesel is the hydrolysis of the waste oils/fats to fatty acids followed by their esterification to FAME.

The conventional Colgate-Emery process for the hydrolysis which works at high temperatures and pressures cannot be applied to the low cost, waste vegetable oils and animal fats especially those containing multiple / conjugated double bonds and hydroxyl groups (castor oil and fish oil, for example).

At high temperatures, these triglycerides and the fatty acids derived from them undergo undesired thermal decomposition leading to deterioration in color / odor and to a reduced yield of fatty acids. It is, therefore, desirable to have a more efficient hydrolysis process of vegetable oils which operates at moderate temperatures / pressures and produces higher yields of fatty acids and glycerine with minimum number of process steps.

Solid acid catalysts are more beneficial than homogenous catalysts due to engineering advantages and easy catalyst separation from the product stream. We have found, for the first time, that solid, hydrophobic, Lewis-acidic, double-metal cyanide (DMC) catalysts are highly efficient for the hydrolysis of various oils and fat to fatty acids at moderate conditions.

The hydrolysis of triglycerides is a three-step, consecutive, reversible reaction. In the first step, the triglyceride (TG) is converted into diglyceride (DG), which is then in the second and third steps converted sequentially into monoglyceride (MG) and glycerol (G), respectively, producing one mole of fatty acid (FA) at each step. Stoichiometrically, one mole of triglyceride requires three moles of water (oil : water molar ratio = 1 : 3) to produce three moles of fatty acids and one mole of glycerol. Excess water would drive the equilibrium towards the end-products - fatty acids and glycerol.



Several solid acid catalysts have been screened for this reaction. Fe-Zn DMC was found to be the best.

The adjacent graph shows the product composition, in the hydrolysis of soybean oil as a function of reaction time over the DMC catalyst.

DMC is highly active in the hydrolysis of a range of edible (coconut, palmolein, soybean) and non-edible (castor, jatropha, karanja, palm and rubber seed) oils and chicken fat. When 20 wt% of a partially hydrolyzed product is added to a fresh batch of reactants mixture, the conversion and FA yields have increased substantially. DMC is a recyclable catalyst.

The highly efficient activity of DMC has been attributed to its hydrophobic surface structure enabling adsorption and activation of the triglyceride molecules selectively.

Surface SCIENCE

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Publications
- *J. Phys. Chem. C.*, **2009**, 113, 7385, 9814
- *Chem. Mater.*, **2009**, 21, 2973; **2010**, 22, 565

Synthesis and characterization of novel catalytic support materials

Direct Influence of subsurface oxygen towards surface catalysis

Interactions between oxygen (O_2) and palladium (Pd) have important implications, and influence of sub-surface oxygen to oxidation reactions is not known. In our efforts to understand the above aspects, carbon monoxide (CO) oxidation reactions have been carried out with mixed molecular beam, consisting CO and O_2, on Pd(111) surfaces under a wide variety of conditions (T = 400 to 900 K, $CO:O_2$ = 7:1 to 1:10).

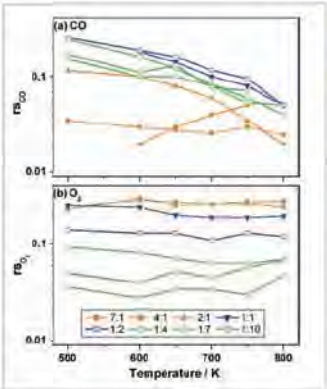

Fig. 1: Variation of reactive sticking coefficient (or adsorption capacity) of reactants with different ratio of reactants and at different temperatures, after the modification of Pd-subsurfaces with oxygen diffusion

A new aspect of the above reaction observed in the transient kinetics regime is the evidence for oxygen diffusion into Pd subsurface layers, and its direct influence towards CO oxidation at high temperatures (≥600 K). There is also a significant time delay (τ) observed between the onset of O_2 adsorption and CO-adsorption (or CO_2 production).

Interesting conclusion derived from the above studies is the necessity to fill up the sub-surface layers with oxygen atoms to threshold coverage (θO-sub), above which the reactive CO adsorption (Fig. 1) occurs on the surface and simultaneous CO_2 production begins.

Novel findings discovered is on the influence of subsurface oxygen in changing the electronic nature of top surface layers and hence oxidation catalysis. Due to oxygen filling in the sub-surface layers, an electronic de-linking occurs between oxidized surface layers and bulk, which is the driving force for oxidation at ≥600 K. An important application of the above findings is the broadening of active CO-oxidation regime to high temperatures, up to 900 K.

Synthesis of solid solution of GaN/InN in ZnO and their application in Solar light harvesting

Simple heating to high temperatures (400°C) changes colorless ZnO into pale yellow/brown color at high temperatures due to oxygen vacancies, and it return to colorless material at ambient conditions. Urea decomposition leads to ammonia production, which is essential to convert any oxide into nitride material. It is the above two facts that we utilized to introduce nitrogen into the ZnO-lattice at high temperatures under combustion conditions.

Zinc nitrate, and urea as fuel led to ZnO1-xNx ($x \leq 0.15$) under combustion conditions. Above conditions lead to the simultaneous in-situ generation of nascent nano clusters of ZnyOz ($y/z > 1$) in ammonia environment, and this is

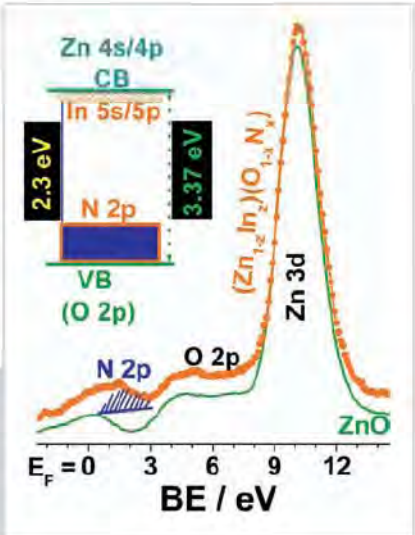

Fig. 2: Valence band photoelectron spectra recorded for the solid solution of InN in ZnO and compared to that of ZnO

the critical step to introduce N into the O - v a c a n c y positions.

In the above preparation procedure it is possible to introduce gallium nitrate and/or indium nitrate to prepare solid solutions of GaN in ZnO, InN in ZnO. By thorough characterization of these solid solutions, it has been confirmed that there are nanosize clusters of GaN or

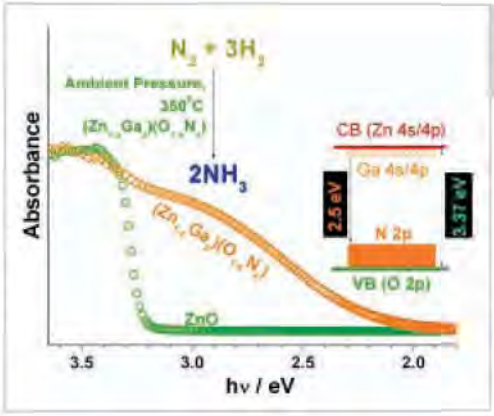

Fig.3: UV-visible absorption spectra of ZnO and GaN in ZnO shows the changes in band gap. Ammonia synthesis also could be carried out at ambient pressure

I n N distributed in ZnO. Very significant changes observed in t h e electronic structure of the above solid solution is shown in the valence band photoelectron spectra (Fig. 2) of InN in ZnO. Band gap change that occurs with the above materials is shown in Fig. 3 with the solid solution of GaN in ZnO; indeed nitrogen fixation through ammonia formation occurs with this material at atmospheric pressure.

These are being evaluated for photocatalytic activity as well as quantum dot sensitized solar cell activity, as they absorb visible light. Preliminary experiments shows good activity in the UV regime and more work is in progress.

Physical CHEMISTRY

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Publications
- *Chem. Phys. Lett.*, **2010**, 496, 143
- *J. Phys. Chem. B*, **2010**, 114, 376
- *J. Phys. Chem. A*, **2009**, 113, 13685
- *J. Solution Chem.*, **2009**, 38, 589

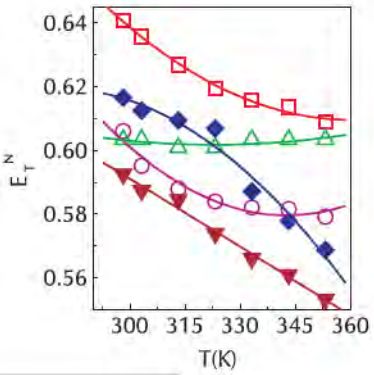
Physical chemistry of organic reactions in unusual media

Background / 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 determination of hydrophobicity at interface
- Modeling and synthesis of selected ionic liquids for electrochemical and closed fuel cycle for fast breeder technology

Work done and discussion

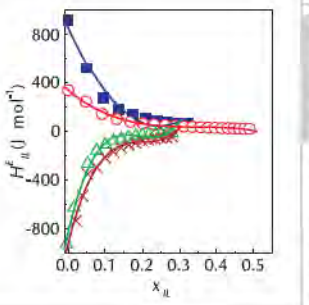
Solvent properties of ionic liquids

Accurate determination of the solvent parameters of room temperature ionic liquids as a function of temperature was achieved in the laboratory. Ambiguity in the polarity scale of ionic liquid was therefore addressed. Several polarity scales were screened and the π and ET



Temperature dependent E_T^N parameters for the pyridinium-based ionic liquids [BP][BF_4](□), [OP][BF_4] (○), [BP][NTf_2](Δ), [HP][NTf2](▽) and [OP][NTf2](◇)

parameters were considered as appropriate indicators of the polarity indices of ionic liquids. A contrast in the temperature dependence of the polarity of some ionic liquids was also observed. The similar measurements were extended to the solutions of ionic liquids to conclude that the polarity is not a linear function of composition of the mixtures.



Variations in H^E_{IL} with respect to xIL for (□) [EMIM][BF_4], (○) [BMIM][BF_4], (Δ) [HMIM][BF_4] and (×) [OMIM][BF_4] in water

Thermal effects in ionic liquids

It was noted for the first time that a reversal in thermal behaviour takes place when ionic liquids are mixed in water. This behaviour was attributed to the ion - pair and cluster formation in solution phase. The thermal effects were scanned using isothermal calorimeter in many solvents. While hydration is important in strongly hydrophilic cations like sodium, hydrophobic hydration remains a dominant force in the cations of ionic liquids. The studies have been extended to Baylis-Hillman, Wittig and Diels-Alder reactions.

Organic reactions in homo and heterogeneous conditions

Experiments were designed to delineate the role of hydrophobic interactions during homogeneous and heterogeneous organic reactions. While the organic reactions under homogeneous conditions proceeded *via* hydrophobic packing, the nature of hydrophobic packing or dangling -OH group or hydrogen bonding remains far from our understanding.

Theory and COMPUTATIONAL Science

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Computational studies, using density functional theory, of organometallic catalysis reactions

Background / objectives

Homogeneous, asymmetric hydroformylation catalysis is a powerful technique for the conversion of alkenes to aldehydes, and it has great relevance for the synthesis of drugs, perfumes and other important chemical compounds. An efficient catalytic route to asymmetric hydroformylation must show (a) high activity, (b) high regioselectivity and (c) high enantioselectivity. To date, platinum and rhodium based systems have been used as catalysts, with the rhodium systems having fewer disadvantages. The best performing rhodium catalyst systems have chiral bidentate phosphites as ligands, while the platinum catalysts have usually been used in conjunction with $SnCl_2$. However, so far, the best catalysts that have been discovered satisfy, at most, two out the three criteria mentioned from (a) to (c) above. It is proposed that a proper and complete study of the mechanistic cycle for the catalysis using theoretical methods will provide insight into the electronic and steric requirements necessary to make a good asymmetric hydroformylation catalyst.

The objective is to use computational means to provide insight and guidance at finding a catalyst that can catalyse the asymmetric hydroformylation of alkenes to aldehydes satisfying all the three criteria laid out from (a) to (c) above.

Work done and discussion

The mechanism for the hydroformylation reaction is shown in Figure 1 below. As can be seen, this is a fairly involved reaction pathway, with many intermediates and transition states, as well as a possible dormant species. Care has been taken to study all of the possible structures for the formation of all the three possible aldehyde products: the linear aldehyde as well as the R and the S products.

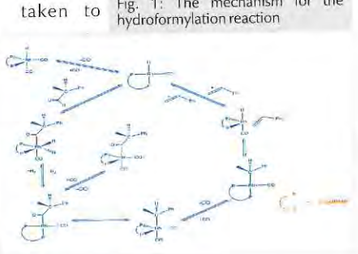

Fig. 1: The mechanism for the hydroformylation reaction

Fig.2 below shows the free energies calculated for all the three possible products. As the figure indicates, (i) the rate determining barrier for the process is the insertion of the alkene into the Rh-H bond and (ii) the linear aldehyde is the product that should be formed with the highest yield. However, it is experimentally observed that the branched S product is formed to the maximum extent, with the linear aldehyde being formed the least - in other words, we see that our computed results are *exactly* opposite to what is observed experimentally!

Fig. 2: The potential free energy surface for the rhodium hydroformylation catalysis process for the formation of the linear, R and the S products

In order to understand why this is the case, we have attempted further studies by including solvent effects by doing single point calculations with toluene modeled as the solvent. The results, shown in Fig. 3, however indicate that the relative barriers show the same trend as before. As such, the reason why computational studies give the exact opposite trend as compared to experiment is still unclear. Work is in progress in order to try and understand other possible reasons, such as inadequacies of DFT at calculating weak interactions (by trying MP2 calculations) and the possibility of reverse β-hydride elimination changing the population landscape at the rate determining step. Results for these investigations are expected in the near future.

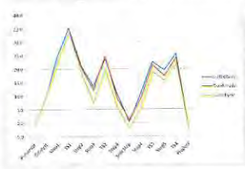

Fig. 3: The inclusion of solvent effects, done for the free energies whose gas phase potential energy surface was described in Fig. 2 above

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Publications
- *Chem. Phys. Lett*, **2010**, 484, 374, 487, 116
- *J. Phys. Chem C*, **2010**, 114, 6690
- *J. Phys. Chem A*, **2010**, 114, 2357
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Electronic structure theory

Background / objectives
- Development of novel electronic structure theories for response properties of quasi-degenerate systems
- Development of coupled-cluster based methods for vibrational properties
- Applications of computational chemistry to hydrogen storage and catalytic materials

Work done and discussion

Implementation of constrained variation approach to electric properties of quasi-degenerate systems

We have made further advances of our constrained variation approach to multi-root electronic structure theories for quasi-degenerate systems, developed by us.

We already initiated implementation of this to Fock space multi-reference coupled-cluster approach and this year, coded calculation of first hyper-polarizability using the calculated first derivative of the Lagrange multipliers. At the same, we made an implementation of this to generalized van Vleck perturbation theory at second order to calculate dipole moments of excited states and dipole surfaces of molecules, in collaboration with the group of Mark Hoffmann in University of North Dakota, USA.

Hydrogen storage materials

In continuation of our efforts on hydrogen storage materials, we have investigated the effect of light metal decoration on the stability of metal organic framework (MOF)-5 and its subsequent hydrogen storage properties. Our results of solid state calculations using VASP reveal that decoration of Mg and Be on MOF-5 does not stabilize the MOFs to any significant extent, while decoration of Al and Li on MOF-5 stabilizes the system significantly.

Furthermore, frontier molecular orbital interaction analysis suggests that there is a predominant contribution from electrostatic effects in the interaction of Li, Be, Mg decorated systems, but the main factor in the interaction of Al decorated system is orbital overlap rather than electrostatics. Hydrogen binding energies for Al decorated MOF-5 are found to lie between 10 to 14 kJ/mole, while the hydrogen binding energies for Li-decorated MOF-5 are found to lie between12 to 18 kJ/mole. Our results show that the hydrogen uptakes for Al and Li decorated MOF-5 are 3.9 wt% and 4.3wt%, respectively.

Catalytic properties of beta-zeolites

The Lewis acidic nature and reactivity of two industrially important catalysts, viz., Sn and Ti substituted beta zeolite (T-BEA) are analyzed using a unique combination of structural parameters, energetics and reactivity descriptors. To achieve this purpose, we adsorb the industrially important moieties (L) namely NH_3, H_2O, CH_3OH, CH_3CN on the active sites of T-BEA.

Our interaction energies show that adsorption of all ligand moieties is stronger at Sn center than that of Ti. In general, the order of stability of the different T-BEA adducts is $NH_3 > H_2O > CH_3OH > CH_3CN$. The ligand interaction is associated with the corresponding bond elongation and bond reduction of the adsorbed molecules on catalyst active site, which can be taken as measure of red or blue shifted frequencies.

Study of dipole moments of vibrational states of molecules using coupled-cluster method

The dipole moments of vibrational states of molecule have been formulated using coupled cluster linear response theory in bosonic representation. The study uses extended coupled-cluster type representation using different truncation schemes. Convergence studies of truncation schemes of the bosonic cluster expansion have been studied using model surface of water molecule.

Study of non-iterative density functional response approaches

A detailed comparative study of non-iterative coupled-perturbed Kohn-Sham (NIA-CPKS) response approach developed at NCL, Pune and auxiliary density perturbation theory developed in Mexico city has been made for electric polarizabilities. NIA-CPKS code has been included in demon developers' version.

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Multiscale simulation, polymers, peptide, protein, membrane, fuel cell membrane

Background / objectives
- Structural, thermodynamical and dynamical properties of liquids of simple and complex molecules by molecular dynamics simulations
- Morphology of polymers, block copolymers, polymer networks in bulk, solution on surface and in confinement from mesoscale simulation
- Conformation of biological materials like peptides, proteins and lipids etc from molecular dynamics and coarse graining simulations
- Structural, electronic and optical properties clusters, nanotubes, nanowires of metal and semiconductor materials
- Understanding the mechanism and hydrogen (other gases) adsorption and diffusion in storage materials e.g. metal organic framework, polymer composites, porous materials from molecular dynamics and grand canonical Monte Carlo simulation.
- Proton conductance mechanism in polybenzimidazole derived polymer membrane from atomistic molecular dynamics simuations.
- Force field development of new molecules for molecular dynamics simulations

Work done and discussion

We address issues which are in the interface between chemistry, physics, materials science, biology and chemical engineering. Therefore our main research areas include polymer assembles, soft nanotechnology, biological aspects of soft matter and surface/interfaces.

Molecular modeling of such materials is a challenge because of its larger length and longer time scale. So we are in continuous development mode to accommodate various phenomena of soft matters, which occur in higher length and time scales. But at the same time atomic/molecular details of any component of soft matter also important to elucidate structure property relation at atomistic scale. Therefore we are developing a multiscale molecular modeling approach, which can handle such systems from atomic scale to mesoscale and establish connections between different scale phenomena. In the following we present some problems, which we are addressing currently.

Morphology of fuel cell membrane

Self-assembly process, morphology of block co-polymers etc are large length (micrometer) and long time (microsecond) scale phenomena. To simulate such properties we apply dissipative particle dynamics (DPD) simulation method. The interaction potentials we use for it is only repulsive and related to solubility between different blocks of the systems. The solubility constants are calculated from all atomistic molecular dynamics simulations. So we connect different methods in different scales via parameter transfer. In this way we have used multiscale molecular modeling method for the simulation of phosphonic acid based fuel cell polymer electrolyte membrane.

Phosphonic acid based membranes are block co-polymers where phosphonic acid functionalized blocks are responsible for proton transport in fuel cell. We have calculated the mechanism of proton transport in such system and showed that protons are transferred via hydrogen bond network formed by the phosphonic acid blocks. The morphologies of such block copolymers, which are dependent on the composition and topology of different blocks of the copolymer, are calculated by DPD method. The morphology of grafted block copolymer consists of polystyrene backbone and heptylphosphonic acid side-chain depicted in fig. 1.

PcrA Protein and it domain motion

PcrA, standing for Plasmid copy reduced, is a helicase that catalyses the unwinding from a free 3' end of double stranded plasmid DNA using ATP. PcrA contains all of the signature helicase motifs and, consequently, is also related to the vast number of RNA helicases that have been identified in eukaryotes.

We are exploiting the site directed spin-labeling (SDSL) technique with molecular dynamics for determining the structural features along with domain motion of PcrA's (3PJR, 2PJR, 1QHH, 1PJR). By incorporating, at least, two spin-labeled side chains; distance between elements of secondary structure can be determined. The range of distances measured will provide a useful ruler for determining the spatial arrangement of known elements of secondary structure in a protein. These distances are characterized by PELDOR (Pulsed electron spin resonance spectroscopy) experimentally by our collaborator in St Andrews University, Scotland. In our study, MTSSL [3-(methanesulfonylthiomethyl)-2,2,5,5-tetramethylpyrrolidin-1-yloxy)], the spin-label, was used to modify the cysteine residues. Rationalization of the distances and their distributions with the experimental data (shown in the fig. 2) are carried out by molecular dynamics simulations.

DPPC bilayer and water interface

We have used atomistic molecular dynamics to simulate 1,2-dipalmitoylphosphocholine (DPPC) water interface (fig. 3) as a mimic of biological membrane-water interface and have observed, on the contrary to the simulations reported in literature, that water penetrates deep into the DPPC bilayer with the help of head group of DPPC molecule. The partial density profile plot of water has proved the entry of water deep into the bilayer (fig. 4). A two-dimensional density map (fig. 5) of water in the system shows the distribution of water at interface. We have also observed that water forms bridging hydrogen bonds with various atoms present at the head group region of DPPC.

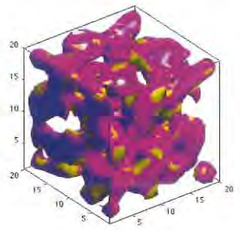


Fig. 1: Different morphologies of phosphonic acid based block co-polymers

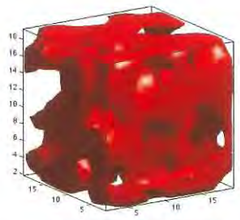


Fig. 2: Comparison between histograms derived from experiment and simulation

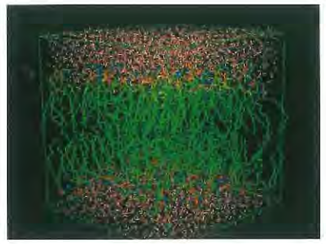
Hydrogen storage in metal organic framework

Hydrogen storage materials for fuels cells became an important research topic due to the increasing demand of clean and efficient alternatives of fossil fuels. Metal-organic frameworks (MOFs) in this regard have attracted great deal of attention because of their topologies and potential applications such as hydrogen storage. In order to build MOF based materials with high gas storage capacity it is essential to have a molecular level understanding of interactions between gas molecules and the porous framework.

In our group, we are trying to predict gas adsorption capability of different MOF materials using ab-initio quantum chemical calculation and grand canonical Monte Carlo (GCMC) simulation.
We are performing calculation on gas adsorption of a reported fluorinated F-MOF-4 (fig. 6) and Mg-MOF with different ligands. Fluorinated MOFs supposed to have more gas adsorption capability than their non-fluorinated counterparts (-CF_3 groups replaced by -CH_3). We have done ab-initio quantum chemical calculation on clusters cut from F-MOF-4 and its non-fluorinated hypothetically generated counterparts. The adsorption energy for H_2 molecules on these clusters shows that the non-fluorinated counterpart adsorbs in a localized manner. Whereas adsorption energies at different positions of F-MOF-4 cluster shows H_2 molecules can bind in different sites on the cluster.

Currently we are focusing on the H_2 molecule adsorption behavior of lightweight MOFs i.e. Mg-MOFs. They are different from the conventional MOFs from the point of view of synthetic difficulty and weight.

Fig. 3: DPPC bilayer - water interface



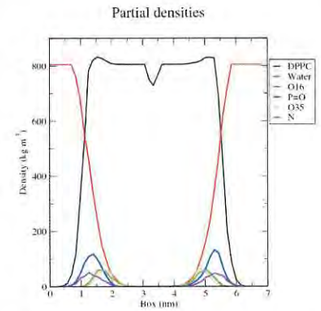


Fig. 4: Partial density of water and different constituents of DPPC

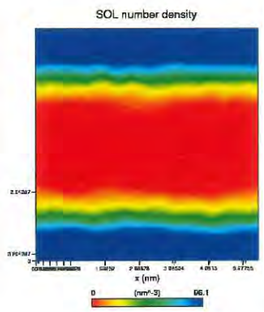


Fig. 5: 2-D density map of water in DPPC bilayer

Fig.6: Structure of F-MOF 4, highlighted region is the cluster model we considered for ab-initio calculation

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Early conformational and dynamical propensities of the helical amyloid β-peptide

In an attempt to understand the early events in the pathway to aggregation, we have considered the structural dynamics of the helical form of the Amyloid beta peptide in water. This 42-residue peptide is a product of the enzymatic cleavage of a large, transmembrane precursor protein.

The precursor itself has a largely helical structure, while the diseased form of the peptide is always associated with insoluble plaques in the beta-sheet form. Therefore, the conformational changes that lead the peptide to the diseased state plausibly begin with a helical conformation.

An in-depth understanding of the early conformational changes might help in the design of small molecules that will trap the conformations in the non-diseased states.

We have performed a 120 ns MD simulation of the helical Ab peptide (starting with the structure in TFE proposed by Tomaselly et al.) at 300K and 1 atm pressure, using the CHARMM22 force field, with the NAMD2.7 simulation package. Shown in Fig.1 is the Radius of gyration (Rg) of the peptide over the simulation trajectory.

The peptide conformation evolves over the simulation time, showing a marked decrease in compactness from 40 to 100 ns. To understand the conformational differences and the unfolding propensities of the two helices along the trajectory, we select equilibrated snapshots from 16 to 18 ns ('t1': plots in black line), 56 to 58 ns ('t2': plots in red line), and from 104 to 106 ns ('t3': plots in green line).

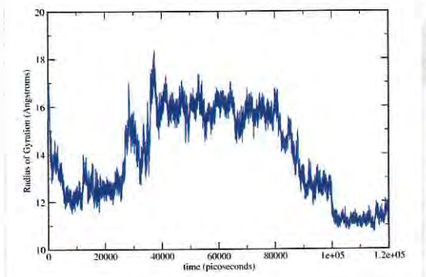

Fig. 1: The Radius of gyration of the peptide over 120 ns

Conformational propensities

The initial structure of the peptide can be divides into five segments, starting from the N-terminus. Residues 1-7 (random coil), residues 8 - 25 (helix 1), residues 26 - 27 (turn), residues 28 - 38 (helix 2), residues 39 - 42 (random coil).

The pathway to the amyloidogenic, beta sheet form should proceed as *helical form→ unstructured coil → sheet*. In an attempt to unravel the unfolding propensities of the two helices, we have calculated the mean squared fluctuations (MSFs) of the residues over the trajectory segments t1, t2 and t3.

The data (Fig.2) clearly shows that the overall loss and subsequent gain in compactness (from 40 to 100 ns, and from 100 - 120 ns) is predominantly brought about by structural changes of the longer first helix. The second helix (residue 28 - 38), on the other hand, shows a decrease in structural fluctuations during t2, when compared with t1.

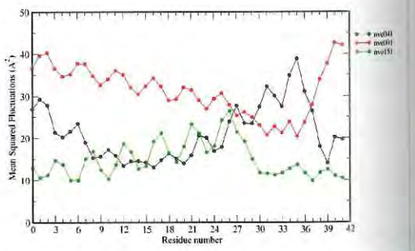

Fig. 2: Mean Squared Fluctuations of the peptide residues along trajectory segments t1, t2 and t3.

Solvent structural arrangement and dynamics

It is well known that protein structural dynamics is intimately coupled with that of the surrounding solvent. In order to distinguish the conformational propensities, we have calculated the radial distribution function of the solvent (water) hydrogen atoms around the oxygen atoms of the C=O groups of the backbone.

This data is depicted in Fig. 3 for the trajectory segments t1, t2 and t3. As seen in the figure, the first solvation layer is roughly 5 times dense around the second helix as compared to the first helix. Thus, the second helix is to interact more strongly with the solvent water molecules.

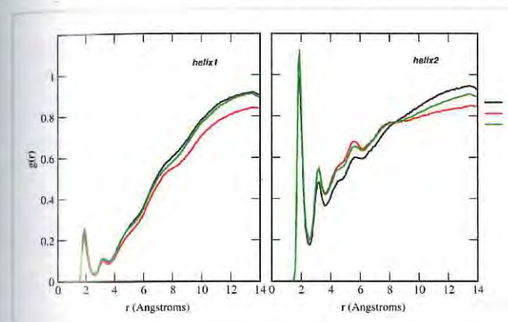

Fig. 3: Radial Distribution Functions of water oxygens around backbone C=O for helixes 1 and 2.

This implies that the second helix, closer to the C-terminus, is more likely to be unstructured compared to the first helix.

Fig. 4 shows the residence time correlation functions of water molecules within 4 Angstroms of the heavy atoms of the two helices, for trajectory segments t1, t2 and t3. The functions decay marginally more rapidly for the second helix, depicting the greater extent of unfolding for it as compared to the first helix.

We have used the replica exchange molecular dynamics (REMD) technique for enhanced sampling of the peptide's conformational space. While there is no distinct change to beta sheet conformers, we do find a greater propensity of the second helix to unfold and to go to the sheet region of the Ramachandran space (results not shown in this report).

It is to be noted that the final beta-sheet form of the peptide has a disordered N-terminus which encompasses part of the helix 1.

Thus, our MD results suggest that the sheet formation is not rate limited by the unfolding of the helical part near the N-terminus, but rather, the formation of beta-sheet takes precedence over the attainment of the unstructured N-terminus. It may therefore be helpful to design pathway blockers aimed at the C-terminus.

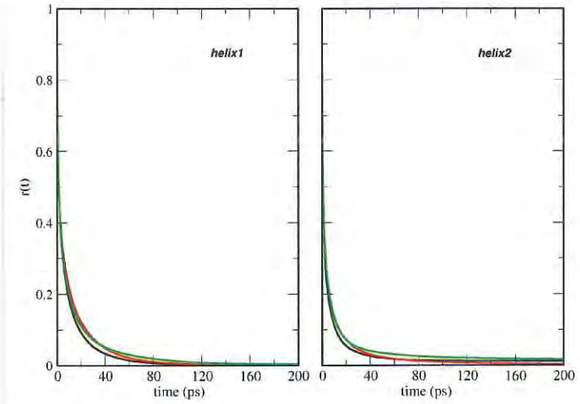

Fig. 4: Residence time correlation functions of water molecules within the first solvation layer for helices 1 and 2.

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Development of insect tolerance in plants

Helicoverpa armigera is a highly devastating and polyphagus insect pest of over 250 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. Overwhelming success of Bt cotton for controlling pest infestation increase hope of more environment-friendly solutions in near future. 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.

Identification and characterization of novel CanPI genes

We have demonstrated that bitter gourd *(Momordica charantia L.)* seeds contain several squash-type serine proteinase inhibitors (PIs), which inhibit the digestive proteinases of the polyphagous insect pest Helicoverpa armigera. In the present work isolation of a DNA sequence encoding the mature peptide of a trypsin inhibitor McTI-II, its cloning and expression as a recombinant protein using *Pichia pastoris* have been reported. Recombinant McTI-II inhibited bovine trypsin at 1:1 molar ratio, as expected, but did not inhibit chymotrypsin or elastase. McTI-II also strongly inhibited trypsin-like proteinases (81% inhibition) as well as the total proteolytic activity of digestive proteinases (70% inhibition) from the midgut of *H. armigera* larvae. The insect larvae fed with McTI-II-incorporated artificial diet suffered over 70% reduction in the average larval weight after 12 days of feeding (Fig 1). Moreover, ingestion of McTI-II resulted in 23% mortality in the larval population. The strong antimetabolic activity of McTI-II toward H. armigera indicates its probable use in developing insect tolerance in susceptible plants.

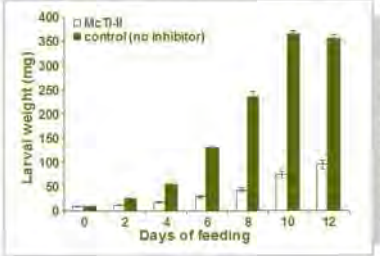
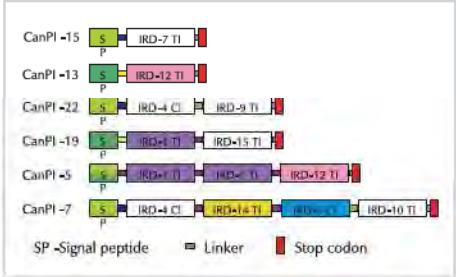


Fig 1: Effect of McTI-II ingestion on the growth of H. armigera larvae.
Recombinant McTI-II (20 µg/g) was incorporated in the larval diet. Larvae were weighed every 48 hours. Each value represents the average weight of 60 larvae. Error bars indicate the standard error.

In our previous studies we observed that diverse Pin-II PIs from *Capsicum annuum* differentially influence *H. armigera* growth and development. Furthermore, *C. annuum* upon *S. litura* and aphid attack showed strong up regulation of multi-IRD PIs. *C. annuum* have characteristic *CanPI* expression pattern in various tissues. For example, in stem 1- and 2-IRD CanPIs exhibited higher expression while predominance of 2-IRD in leaves. On the other *hand* 3- and 4-IRD *CanPIs* showed higher expression in fruits. These results indicate significance of *CanPIs* for their defensive and endogenous role which still remains poorly understood. Our aim is to identify and characterize better candidate *CanPI* gene for

Fig. 2: 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



H. armigera control. In the following study, we attempt to address the questions (i) what is the fate of rCanPIs in insect gut? (ii) What is the insect's response to the ingested CanPIs? (iii) Whether this reaction is different for different CanPIs? We selected six *CanPI* genes on the basis of sequence variation, specificity and number of IRDs and characterized them with specific reference to their (i) processing by HGP (ii) stability in proteolytic environment and (iii) inhibitory activity against HGP. Using, IF-MALDI-TOF-MS, enzyme assays and PI activity gels, interaction of rCanPIs with HGP was analyzed. Since these studies are based on product(s) of particular PI gene(s), it leads to identification of potential PI(s) or IRD(s) effective against constitutive and induced insect gut proteases.

Six diverse representative *Capsicum annuum* protease inhibitor genes viz. CanPI-5, -7, -13, -15, -19, and 22 comprising 1 to 4-inhibitory repeat domains (IRDs), were cloned and expressed in *Pichia pastoris* (Fig. 2). The recombinant proteins were evaluated for their interactions with bovine trypsin, chymotrypsin, and *H. armigera* gut proteases (HGP) using electrophoretic (native and denaturing) and mass spectrometric (MALDI-TOF-MS in combination with intensity fading assays) techniques (Fig. 3).

These techniques allowed us qualitative and semi-quantitative analysis of multiple and processed IRDs of purified rCanPI proteins. rCanPIs showed over 90% trypsin inhibition, varying chymotrypsin inhibition depending on number of respective IRDs and over 60% inhibition of total HGP. rCanPI-15 that has only one IRD showed exceptionally low inhibition of these proteases.

Interaction studies of rCanPIs with proteases using intensity fading (IF)-MALDI-TOF-MS revealed gradual processing of multi-IRD rCanPIs into single IRD forms by action of HGP at the linker region, unlike their interactions with trypsin and chymotrypsin. IF-MALDI-TOF-MS assay showed that CanPI-13 and -15, possessing single IRD and expressed predominantly in stem tissue are degraded by HGP; indicating their function other than defense. *In vitro* and *in vivo* studies on rCanPI-5 and -7 showed maximum inhibition of HGP isoforms and their processed IRDs were also found to be stable in presence of HGP.

Even single aa variations in IRDs were found to change the HGP specificity like in the case of HGP-8 inhibited only by IRD-12.

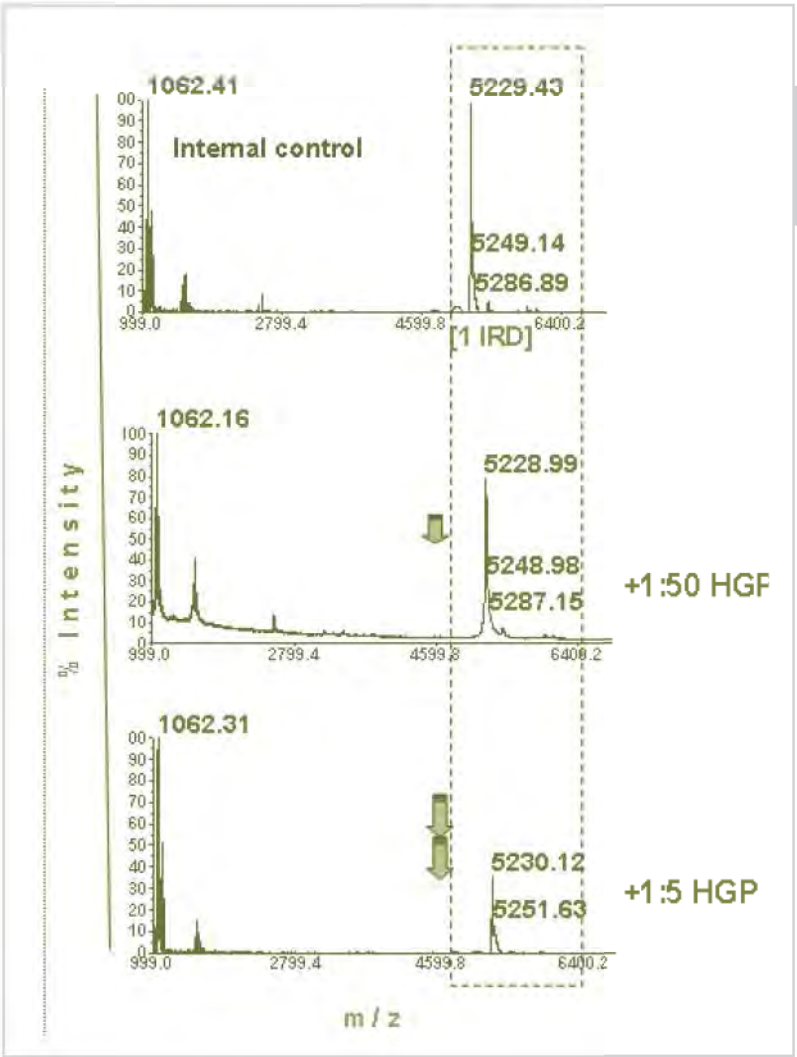


Fig 3: IF–MALDI-TOF-MS analysis of rCanPI-15. The decrease in the relative intensity of rCanPI-15 (6 kDa) upon addition of target protease, HGP was evident. The internal control (1062 Da) has been used as reference for relative quantification.

Presence of active PI in insect gut might be responsible for changed HGP profile. rCanPI-5 and -7 enhanced HGP-7, reduced HGP-4, -5, -10 expression and new protease isoforms were induced. These results signify isoform complexity in plant PIs and insect proteases.

Chickpea transformation with PI genes

We have attempted a chickpea transformation using *CanPI-7* and *NaTPI* genes with *Agrobacterium tumefaciens*. The putative chickpea tissues are in process of characterization using different molecular approaches. We are also studying the changes in *H. armigera* digestive and other metabolic enzymes upon feeding on recombinant PI proteins as well as various host plants by analyzing specific gene expression and unbiased proteomic approach.

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- *Tree Genetics and Genomes*, **2010**, 6, 13
- *Genetica*, **2010**,138,197
- *J Sci. Food Agri.*, **2009**, 89, 2071

Molecular genetic approaches for plant improvement

A) Molecular marker technology approach in wheat quality and rust resistance breeding

The present program 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 leaf and stem rust as well as water stress conditions.

i) BMQ analysis using mixograph approach

Besides the direct methods for evaluation of BMQ, the indirect methods like mixograph, farinograph, extensigraph are also exploited to understand BMQ. Mixograph is routinely used to test and evaluate the quality of wheat, more particularly to provide general information on the mixing properties (dough development time and tolerance to mixing). Application of mixograph can be further enhanced by QTL mapping for mixograph traits. Mixing tests were conducted using a computerized 10 g Mixograph (National Mfg. Co., Lincoln, Nebraska, U.S.A.) at ARI, Pune.

The complete RIL population (with 5 repeating checks) of HI977x HD2329 was analysed for the mixogram patterns. For mixograph traits, an average of all traits was calculated based on six data sets with three locations. Based on the nature of curves the overall dough strength of HI977 was observed to be comparatively higher than Hd2329.

Trangressive segregants were identified for all the mixograph traits with wide range, suggesting that both the parents carry both favourable and unfavourable alleles. These traits were selected for QTL mapping and interval mapping of all the traits for all the six experimental data sets was performed using the framework map established.

ii) Identification of molecular markers closely linked to stem rust resistance genes

Molecular markers tightly linked with stem rust resistance genes, which are not yet heavily deployed in commercial wheat cultivars, are needed for wheat improvement to assist in combating the threat to global wheat production and food security posed by the recent emergence of the highly virulent stem rust pathogen, Ug99.

A double haploid mapping population developed from the cross Diamondbird/Janz was evaluated for variation in stem rust response in 8 field trials, conducted in Cobbitty, Australia (3), Wellington, Nilgiri Hills, India (3) and Njoro, Kenya (2), at the adult plant stage, using *Puccinia graminis* f.sp. *tritici* pathotypes predominant in the respective locations. One hundred and seventy one double-haploid lines were genotyped using DArT (Triticarte Pty. Ltd. Australia) markers.

Following preliminary linkage and QTL analysis, chromosomes of interest associated with resistance were targeted with SSR markers. For this purpose, a high-throughput semi-automated SSR genotyping system using a fluorescence-based DNA fragment analyser (MegaBACE 1000) was implemented.

A genetic linkage map, consisting of 403 marker loci (355 DArT and 48 SSR) and spanning 2,122 cM, was constructed using JoinMap 4.0 software. All chromosomes, except 4D, were represented in the linkage map. A framework map consisting of 262 informative markers and covering 2,085 cM was used for subsequent QTL analysis using QGene 4.0 software.

A joint analysis, in which individual trait data from each of the three locations (Kenya, Australia and India) were treated as correlated, confirmed QTL detected by composite interval mapping and indicated the involvement of chromosomes 2B (Australia, Kenya), 3B (Australia, India), 3D (Australia, India) and 7A (Australia). Several other putative QTL regions explained additional variation in stem rust response in this population.

B) Mango flavor biogenesis

Mango (*Mangifera indica*), popularly known as 'The King of Fruits', is one of the oldest cultivated tropical fruits. India is the largest mango producer and contributes 37% of total 30.5 million tons of global mango production. Presently, India harbours more than 1000 mango cultivars and represents the largest mango germ pool in the world. Among this vast

diversity of mango cultivars Alphonso represents highly delicious and most flavored mango cultivar. However, we lack the valuable information about the chemistry of flavor formation in mango and the locality dependant variation observed in Alphonso flavor.

The myriad of volatiles found in Alphonso mango are biosynthesized by complicated network of metabolic pathways. These volatile markers help to determine agronomically important stages of fruit life (fruit-setting, harvesting maturity and ripening climacteric). However, we poised a need to find out more and precise markers to understand the process of development and ripening. Fruit's transcriptome can be a good source of such markers. Therefore, we isolated 18 genes related to the physiology and biochemistry of the fruit and profiled their expression in developing and ripening fruits, flowers and leaves of mango using relative quantitation PCR.

In most of the tissues, genes related to primary metabolism, abiotic stress, ethylene response and protein turnover showed high expression as compared to that of the genes related to flavour production. Most of the genes showed their least expression on the second day of harvest, suggesting that harvesting signals significantly affect the fruit metabolism. Changes in the expression profiles clearly marked the important stages in the fruit life.

C) Fatty acid pathway analysis in Linseed

Linseed/Flax (*Linum usitatissimum L.*) is an important oil seed crop having high nutritional as well as industrial value. It is the richest and the cheapest agricultural source of α-linolenic acid (ALA), which is an omega-3 fatty acid. We have planned to understand and characterize the pathway of omega 3 fatty acid synthesis in linseed.

Expression analysis of the desaturase genes (Δ9, Δ12 and Δ15), which encode the 3 key enzymes of the biosynthetic pathway of PUFA, from 5 low and 5 high ALA containing Indian linseed cultivars during seed development has been initiated.

Expression patterns of Δ15 desaturase gene (FAD3) and Δ12 desaturase gene (FAD2) in variety NL97 (High ALA) showed considerable expression at the flower stage but barely detectable levels at 4 and 8 DAF. There was several fold increase in the expression at 12 DAF reaching maximum at 22DAF. Expression levels decreased at the later stage (30DAF), while at 48DAF there was almost negligible expression. Δ9 desaturase gene (SAD) gene expression in the developing bolls did not show as much expression as seen for Δ15 and Δ12 desaturase genes.

There was expression at the flower stage which decreased at 4DAF and increased at 8, 12 and 16 DAF. At 48 DAF there was no expression of the SAD gene observed. Fatty acid profile of the developing seeds of variety NL97, determined by gas chromatographic analysis, corresponded well with the expression levels of desaturase genes in developing seed stages. Similar study will be extended for the remaining nine flax varieties and a comparative study will be done.

D) DNA barcoding of *Dalbergia* species

The Western Ghats (WG) in India are well known for their rich and unique assemblage of flora and fauna, and are amongst the 25 biodiversity hotspots identified in the world. Dalbergia is an important member of the WG flora; valued for decorative and often fragrant wood (rosewood, African blackwood, sisu) and is rich in aromatic oils. There is taxonomic confusion with respect to several *Dalbergia* species.

Hence, the size of the Dalbergia genus remains disputed. Although DNA barcoding is well established in animals, a universally accepted barcode is still lacking in plants. Hence, the main objective of this study is to develop a unique barcode for quick, accurate and reliable species identification using the Dalbergia genus as a model system.

Leaf samples from fifteen accessions each, belonging to six validated Dalbergia species (*melanoxylon, candenatensis, rubiginosa, latifolia, volubilis* and *paniculata*) were collected from various locations in WG were used for DNA barcoding.

A total of 37 primer pairs specific to several chloroplast genes (*matK, rpoC, rpoB, rbcL, accD, ndhJ, ycf5* and *trnH-psbA*) as well as the nuclear genes were evaluated on the samples. We are currently targeting the DNA sequences corresponding to *matK, rpoc, rpoB, rbcl trnH-psbA* and nuclear ITS. Based on the preliminary sequence data, the resolution of the species differentiation using the *rpoC, rpoB* and *matK* genes individually was 66.66%. Further work is in progress to achieve 100% species resolution and develop a successful barcode using other important genes either individually or in combination.

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Chickpea improvement through biotechnological approaches

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. India is a major producer of chickpea and contributes 65% of the world's production.

It is the most important legume in the Indian subcontinent in terms of the area under cultivation (6.7 mha), production (5.6 mt) and consumption. However, the chickpea productivity is very low (~850 Kg/ha) in its intensively cultivated areas, mainly due to low yield potential and susceptibility of the present day cultivars to biotic and abiotic stresses.

Fusarium wilt is a widespread and serious chickpea disease caused by the soil borne fungus *F oxysporum* f.sp. *ciceri* (Foc). In this program it is attempted to analyse chickpea-*F oxysporum* interactions and to map the chickpea genetic loci contributing to *Foc* resistance.

Molecular mapping of wilt resistance genes in chickpea

We evaluated an F_9 recombinant inbred line population of chickpea for resistance to three Foc races (1, 2 and 3) in pot culture experiments and identified flanking and tightly linked DNA markers for all the three resistance genes.

The inheritance of resistance to late wilt caused by Foc races 1 and 4 was studied in a set of ninety three RILs derived from an F_9 RIL population of a cross between the wilt resistant parent Vijay and late wilting parent ICC-4958. The SSR markers TS72 and TA02x flanked the Foc1 late wilt resistant gene at 2 cM interval on LG-4, while the Foc4 late wilt resistant gene was identified at a distal end of the same LG.

The later was flanked by two RAPD markers $UBC43_{550}$ and $UBC173_{600}$ with 3 and 10 cM distance, along with an SSR marker NCPGR51 co-locating with the Foc4 late wilt gene. The two resistance genes were 19 cM apart, with seven markers between them.

The segregation ratio of 1:1 for resistance: susceptible confirmed the monogenic inheritance of both the genes in this population.

Molecular analysis of chickpea-Fusarium interactions

Serial Analysis of Gene Expression (SAGE) is an effective approach to identify plant defense genes and involves transcriptome profiling of plant-pathogen interactions. The technique generates a large number of short (10-17 bp) tags, from a unique location in transcripts of expressed genes, which can potentially identify 4^{10} to 4^{17} unique transcripts.

The frequency of each SAGE tag directly reflects the transcript abundance. Hence, SAGE results in an accurate picture of gene expression at both qualitative and quantitative levels. This study, therefore aims to use SAGE to perform a large-scale analysis of the chickpea-fusarium interactions, to identify the resistance genes, to elucidate the mechanism of resistance and to isolate the cDNAs of resistance genes for possible development of wilt-resistant chickpea.

We selected a wilt-resistant and a wilt-susceptible chickpea cultivar and infected them separately with three Foc races under controlled conditions in greenhouse. Root and shoot tissues were separately collected at eleven time-points starting from 0 hr to 28 days. Development of SAGE library of infected resistant cultivar has been completed and sequence analysis is in progress. Another SAGE library of control resistant cultivar is being prepared.

Gene expression profiling during chickpea-Fusarium oxysporum interactions

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. In this study, semiquantitative RT-PCR analysis of defense 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.

Race specific response of Foc

The response of fungal virulence related genes, namely *Fgb1*, *Gas1*, *Chs7* and *Fow1*, in *Foc 1*, 2 and 4 inoculated JG62 and Digvijay from 2-13 dai was determined (Fig. 1). In case of race 1

inoculated JG62, all the four pathogenesis related genes showed higher level of expression in comparison to Digvijay. Gas1 and Chs7 showed variable response in both, JG62 and Digvijay inoculated with race 2. Fgb1 and Fow1 showed higher expression in Foc 2 inoculated JG62 as compared to Digvijay, throughout the course of infection.

A similar finding was observed in case of race 4 inoculated JG62 and Digvijay. However, race specific response in Chs7 gene expression was observed, expression being higher in Foc 4 inoculated Digvijay initially, as compared to that in Jg62.

Chickpea defense response to *Foc races*

Defense response of susceptible and resistant chickpea cultivars, JG62 and Digvijay towards, Foc race 1, 2 and 4 from 2-13 dai was studied (Fig. 2). It was observed that race 1 inoculated, resistant cultivar, Digvijay showed higher expression of defense related genes namely, *GroES2, 60srp, BetvI, CHS* and *IFR*, as compared to susceptible cultivar JG62, throughout the study.

In case of race 2 inoculated plants, expression of *CHS* gene was higher in Digvijay as compared to *JG62* throughout the course of disease development, indicating its importance in defense against race 2. However, *GroES2* and *BetvI* showed low expression initially at 2 dai in Digvijay as compared to JG62, which enhanced at 6 and 9 dai where the expression of these two genes was higher in the resistant cultivar as compared to the susceptible cultivar JG62. Since 60srp and IFR showed variation in their expression, the role of these genes is difficult to explain. In case of race 4 inoculated cultivars, BetvI showed higher expression in the resistant cultivar Digvijay throughout from 2-13 dai when compared to JG62. While 60srp, CHS and IFR showed low expression in Digvijay as compared to JG62 initially at 2 dai which reversed at 6 and 9 dai.

GroES2 showed variation in expression making its role difficult to understand with respect to race specificity.

Fungal pathogenesis related genes																								
	2 dai						6 dai						9 dai						13 dai					
GENE	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4
Fgb1	3.2	2.8	3.1	1.9	3	2	4.5	1.9	3.9	1.9	4.5	2	6.5	5.5	6.5	3	7.8	4.5	7	4.9	6.9	1.9	6.6	1.8
Gas1	3	2.8	2.8	2.7	2.9	2	4	2	0.9	1.9	3.3	1.9	2	1	2.5	0.9	3.4	2	1	0.5	0.65	0.25	3.7	0.5
Chs7	1.5	1	0.75	0	0.5	0.75	2.75	2	1.9	2.3	2.2	0.65	3.5	0.7	3	2.5	2.7	0.7	2.7	0.5	2.9	1.8	3	0.7
Fow1	5.5	5	5.5	5	5.9	5.5	5.5	3	4.9	2.8	5.8	2.5	6.5	3.5	6.3	3.8	6.1	2.8	7.8	3.8	7.5	5.5	8	2

Fig. 1: Response of fungal virulence related genes, namely *Fgb1, Gas1, Chs7* and *Fow1*, in *Foc* 1, 2 and 4 inoculated JG62 and Digvijay from 2-13 dai

Plant defense related genes																								
	2 dai						6 dai						9 dai						13 dai					
GENE	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4	JG1	DV1	JG2	DV2	JG4	DV4
GroES2	1.8	4	1.8	1.5	1.9	0	1.2	2	1	1	0.8	0.9	0.8	1	0.4	0.5	0.7	0.7	0	0	0	0	0	0
60srp	2.7	3.7	3.1	3.3	3.3	3.2	1.3	1.4	1.3	1.49	1.4	3.2	1	1.1	1.25	1.1	1.1	3.3	0	0	0	0	0	1.49
BetvI	2.5	3.25	2.9	2.8	3	3.2	2	2.3	1.8	2	2.4	2.6	1.9	2.3	1.9	2	2.4	2.6	1.3	1.7	1.5	1.75	0.9	1.7
CHS	1.7	2.5	2.2	2.5	2.25	0.95	1.2	2.5	1	4	0.8	3.2	0	2.4	0.9	1.9	0.4	1.6	0	2.1	0.4	0.7	0	0
IFR	1	1.8	2	2	1.3	0.9	0.8	1.3	1.3	1.2	1	4	0	1.15	0.3	0.45	0	1.45	0	0	0	0	0	0.35

Fig.2: Defense response of susceptible and resistant chickpea cultivars, JG62 and Digvijay, towards *Foc* race 1, 2 and 4

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Engineering disease resistance in economically important crops

Under this project studies are being carried out on different aspects essential for engineering disease resistance in economically important crops in ginger and onion using antimicrobial peptide strategy (AMP).

The work has already been carried out on isolation, identification of disease causing organisms of ginger and onion using biochemical tests and 16s rRNA gene analysis. Studies revealed that in ginger *Pseudomonas, Xanthomonas, Staphylococcus* are bacterial and *Aspergillus niger, Rhizopus stolonifer, Botrytis alli* are fungal pathogens, where as in onion *Pseudomonas*, *Bacillus*, *Staphylococcus*, *E. Coli*, are bacterial and *Aspergillus niger*, *Rhizopus stolonifer* are main fungal pathogens.

AMPs are the important component of natural defense of most living organisms against invading pathogens exhibiting broad spectrum anti microbial activity against fungi as well as bacteria and most are non-toxic to plant and mammalian cells.

Besides these natural AMPs, synthetic AMPs have also been synthesized. These are unique candidate target peptides which are about half of the size of natural counter parts and are more stable and active at low concentration without the concomitant toxicity to host tissues. They show reduced degradation by proteases.

In the current year, work was carried out on designing of novel synthetic AMPs and testing for AMP action towards above mentioned organisms.

Based on the literature survey, the AMP was designed as neutral amino acids at N and C terminal along with alternate hydrophobic and hydrophilic residues in the peptide.

Growth curve of above mentioned pathogens was studied individually. The sensitivity assay was carried out using three synthetic AMPs D4E1 (17 amino acid), hexa peptide (6 amino acid) and newly synthesized neo peptide (9 amino acid). It was found that during log phase of the microbial growth the AMPs are more active in their action because the cells are actively dividing during log phase.

The inhibitory concentration of D4E1, neo peptide and hexa peptide ranged from 10-15 μM, 15-45 μM and 30-60 μM, for bacterial pathogens respectively. For fungal pathogens, the inhibitory concentrations ranged from 20-30μM, 40-60 μM and 50-70 μM respectively. Thus, D4E1 is required in less amount as compared to neo peptide followed by hexa peptide.

It was concluded that more than the amino acid content of the peptide the size of the peptide is of significance for AMP activity. Larger size peptides form pore in cell wall and kill the cell. But as the size of peptide reduces, it needs cluster of peptides for the same action resulting in the increased amount of peptide required for killing the organisms.

Fig. 1: Growth of Pseudomonas solanacearum completely inhibited at 20 μM concentration of neopeptide

Toxicity of the D4E1, neo and hexa AMP on 9 day old chick embryo was also checked. The peptide is nontoxic as the chick embryo was found alive after 3 days of incubation.

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Chemical ecology of insects

A study on host-parasitoid interactions with special reference to the Uzi fly and *Antheraea assama*

Plant volatiles are known to have numerous functions including attracting herbivores and/or natural enemies besides attracting pollinators. There has been increasing evidence suggesting the role of induced plant defenses serving tritrophic interactions. Parasites have been shown to respond to volatiles emanating from both undamaged plants and plants that have been fed upon by insects. Based on the high detectability and reliability of herbivore induced plant volatiles, parasitoids are able to use these cues to locate their hosts from a distance.

One of the major problems encountered by silkworm farmers is the uzi fly, *Exorista sorbillans* - a tachinid dipteran endoparasitoid which causes 20-40% loss in the Muga silk industry. Control of this fly is mechanical by the use of nets and fly screens at all entry points. Beside, certain chemicals and specific biological control agents have also been tried with limited success.

With a view to identify volatile organic chemical(s) emanating from plants fed upon by the larvae of the muga silkworm, *Antheraea assama* which could be used in traps/baits to control the uzi fly menance, electrophysiological studies were conducted. In general, alcohols stimulated more than the corresponding aldehydes or ketones. Also, compounds with odd number of carbon atoms gave higher responses. GC analysis of volatiles released from both damaged as well as undamaged host plant, some revealed some interesting differences.

There are both qualitative and quantitative differences in day and night time volatiles. Also, the volatile profiles of damaged and undamaged, som plants are different. GC-MS analysis reveals the presence of C_6 alcohols, aldehydes and their corresponding acetates besides terpenes in addition to the presence of som acids, the latter group being present in larval faeces well.

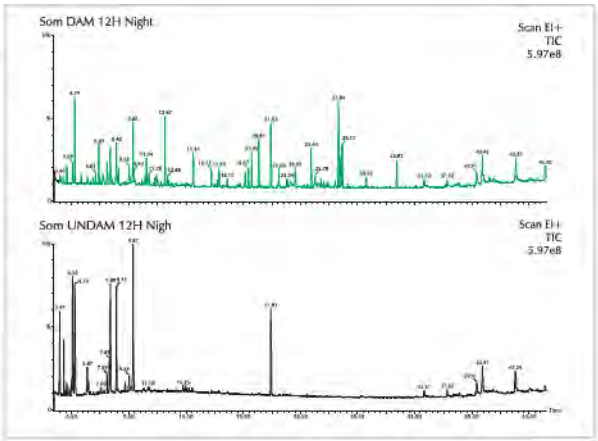
Application of regurgitant to undamaged plants resulted in volatile profiles that are quite similar to insect damaged plants. GC analysis of regurgitant suggests that they are linolenic acid/ linoleic acid based amides.

Thus, higher release of volatiles results in greater attraction for parasitoids as revealed in behavioral bioassays and may be adaptive to the plant. The seven carbon compounds may be important in host seeking behavior by the uzi flies.

Olfaction in the Malaria mosquito: Role of human skin emanations

Perception of a complex odor blend is essential for host specificity in most mosquito species. The role of human skin emanations in host seeking behavior of the malaria mosquito, *Anopheles stephensi* are being studied with the objective to characterize behaviorally relevant chemical stimuli and elucidate how these stimuli are detected and integrated in the chemosensory system.

Electroantennograms were recorded from 5-6 day old females of *A.stephensi*. Each of the 46 compounds tested evoked EAG responses. In general, the alcohols evoked the largest response followed by acids which are essential components of human skin emanations. The thresholds for aldehydes and ketones were lower.



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Fungal biotechnology

The objectives of our work are:
- To understand the biochemical and molecular mechanism of fungal morphogenesis
- To use fungus-fungus and -insect interactions for the development of biocontrol agents
- To explore the biocontrol potential of fungal enzymes and chitin synthase inhibitors in fields
- To study the fungal diversity of different environments

Fungi and fungal products as biocontrol agents

Under the Indo-Swiss Collaboration in Biotechnology (ISCB) the studies were undertaken to develop a mycoinsecticide, *Metarhizium anisopliae* for the control of *Helicoverpa armigera* on pulses in April 2000.

As the work on "proof of concept" was completed successfully the II phase of the project started with to complete the studies on large scale (field trials on hectare basis), product application (use of foliar and soil application), shelf life of the product, cost-effective production of the spores, feedback from end-user, registration of the product and its introduction in national and international market in 2004.

In the III phase now sufficient spore (5 kg) material has been produced to carry out shelf life and formulation studies, as well as field trials on hectare scale. Total 68 isolates are being maintained regularly. *In situ*, maintenance of the virulent strains of *M. anisopliae* is also being tried. In addition to biochemical and molecular studies of fungus-insect interaction the biophysical studies have been carried out using 1st and 40th sub-culture of commercial strain (M34412) of *M. anisopliae*.

The surface charges and hydrophobicity of the conidia have been studied using zeta potential measurement, sedimentation and microbial adhesion to hydrocarbons (MATH) assays. The possible role of cuticular hydrocarbons of *H. armigera* in host-fungus interaction has been reported.

The cuticle degrading enzymes of *Myrothecium verrucaria* with and without *M. ansiopliae* have used to control mealy bug and downy mildew infection in grapes. The field trials indicated that the combination of two treatments as preventive sprays successfully controlled pathogen and pest attack. The enzyme complex of *M. verrucaria* and *M. anisopliae* spores were found to be compatible with pesticides used in a farmers' practice.

The chitin, β-1,4-linked *N*-acetylglucosamine polymer, is the main structural component of the fungal cell wall. As it is absent in plants and mammals, targeting the enzyme chitin synthase (CHS) involved in the synthesis of chitin could be one of the eco-friendly strategies for the control of plant pathogenic fungi in agriculture.

Nikkomycin and polyoxin are naturally occurring nucleoside peptides, known competitive inhibitors of chitin synthase. Number of compounds have been synthesized based on nikkomycin scaffold.

It has been observed that aryl ether 1,2,3-triazolyl linked uridine compounds were active against all tested fungal strains with MIC values 0.003-0.305 µmol. Aryl ester 1,2,3-triazolyl linked uridine compounds also found to be active against all tested fungal strains with MIC of values 0.033-0.257 µmol.

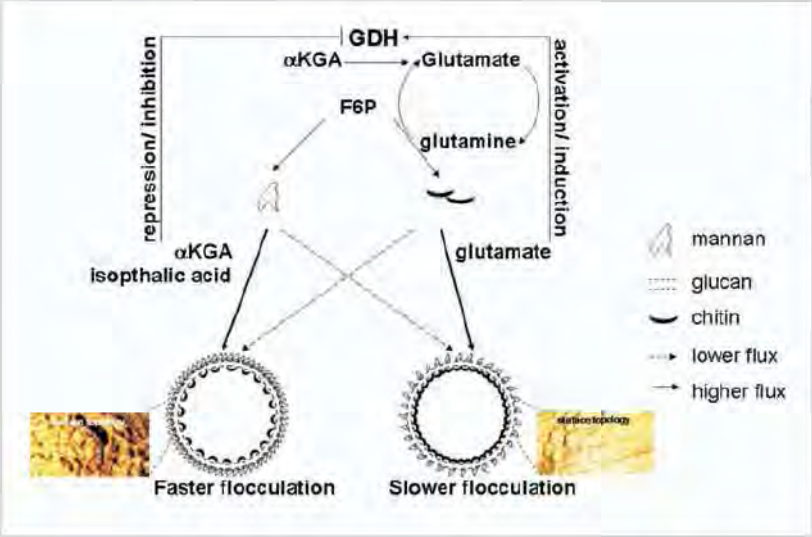
Chitin synthase activity of *B. poitrasii* cells was estimated with and without compounds (4 µg/mL) using a non-radioactive chitin synthase assay.

It was observed that four compounds inhibited 80-95% of chitin synthase activity while seven compounds exhibited 70-80% inhibition of chitin synthase activity.

Fungal diversity

In the dimorphic fungus *B poitrasii*, parent yeast (Y) and monomorphic yeast mutant (Y-5) have different surface properties which are important in adhesion, aggregation and flocculation.

The agents modulating NAD-dependent glutamate dehydrogenase (NAD-GDH) activity could be potentially used to enhance flocculation in fermentative yeasts and as therapeutic molecules for control of dimorphic fungal pathogens. The NAD- GDH has been



A model for controlling flocculation in yeasts (α-KG- α-ketoglutarate, F6P - Fructose-6-phosphate).

purified to homogeneity which is a tetramer having molecular weight 371 Kda.

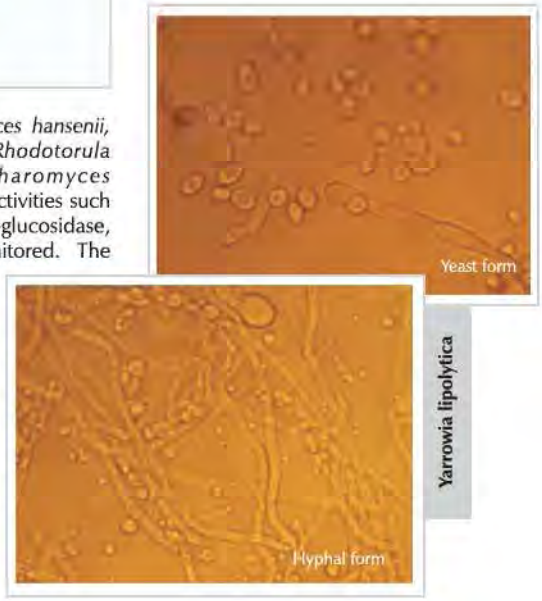
The yeast diversity was studied on the basis of morphological, colony, physiological characteristics and 5.8S-ITS sequencing of rDNA of the isolates. Six grape varieties, Bangalore blue, Zinfandel, Cabernet, Chenin Blanc, Sauvignon Blanc and Shiraz are being used in India for wine making.

For the first time, *C. azyma* was isolated from Bangalore blue and Cabernet and *Pichia manshurica* from Shiraz variety. 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.

We have also isolated seven isolates belonging to four genera from apple juice and identified as *Debaryomyces hansenii, Pichia membranefaciens, Rhodotorula mucilaginosa, and Saccharomyces cerevisiae*. Different enzyme activities such as pectinase, glucanase, β-glucosidase, during fermentation were monitored. The study indicated that natural flora present on the grapes was involved in breaking down β-glucoside bonds and gave aroma to wine.

Number of bacteria and yeast isolates from petroleum contaminated soils were studied for their potential to degrade hydrocarbons.

Three isolates from the genera *Psuedomonas, Bacillus* and *Micrococcus* and two yeast, *Yarrowia* strains demonstrate good degradation characteristics for alkanes (C9-C29). C10 and C11 alkanes, that are reported to be toxic to the growth of soil microorganisms and plants, were completely degraded. *Y. lipolytica*, a marine isolate was found to degrade alkanes in the yeast form and the morphological transition from hypha- yeast was found to be necessary for the same.



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Biophysical characterization of α-mannosidase, human eukaryotic initiation factor2 α and two plant lectins

Background / objectives

1α-Mannosidases from *Aspergillus fischeri*, *Lens esculentum* and jack bean

α-Mannosidase (α-mannoside mannohydrolase, E.C. 3.2.1.24) is an exoglycosidase which catalyzes the hydrolysis of terminal nonreducing mannose residues in mannans. N-linked glycosylation is a posttranslational modification found in eukaryotes.

In various tumor cell lines such as those from breast, colon, and skin cancer, the distribution of the cell surface N-linked sugars is altered. Enzymes of this glycosylation pathway are therefore potential targets for the development of inhibitors for cancer treatments.

Human eukaryotic initiation factor 2α and heme regulated eukaryotic initiation factor 2α kinase

In eukaryotes, interaction of various protein factors along with mRNA and ribosome in a specific manner brings about the translation initiation. The eukaryotic translation initiation factor 2 (eIF2) is one such GTP binding protein that plays a major role in initiating translation. It is a heterotrimer composed of α (36 kDa), β (38 kDa) and γ(52 kDa) subunits that tend to associate throughout the initiation cycle.

The phosphorylation / dephosphorylation of a conserved serine residue (Ser51) in the α-subunit is one of the major regulatory mechanisms of translation initiation in eukaryotes.

Moringa oleifera and Aracea lectin

Molecular recognition of carbohydrates by proteins is of prime importance in many biological processes, such as viral, bacterial, mycoplasmal and parasitic infections, targeting of cells and soluble components, fertilization, cancer metastasis and growth and differentiation. ACL, a 13 KDa protein isolated from the tubers of *Ariesaema curvatum* was found to possess mitogenic potential for human blood lymphocytes.

Alkaline protease from *Nocardiopsis* sp. Actinomycet

Proteases are used in the food industry for protein liquefaction, milk clotting and as meat tenderizers.

Work done and discussion

α-Mannosidase from *A. Fischeri*

As an initial step towards using α-mannosidase as a target against anticancer drugs, inhibition studies of a model enzyme, class II -mannosidase from *A. fischeri* in presence of polyhydroxy piperidine derived glycosidase inhibitors, metal ions and amino acid specific reagents were carried out to reveal the sensitivity of the enzyme.

Three of the derivatives showed competitive inhibition (K_i =45, 48 and 235μM) and the binding of the inhibitors to the enzyme was entropically driven. Among the metal ions checked, Cu^{++} (K_i = 21nm) and Se^{++} ions (K_i =32 μM) showed noncompetitive and Co^{++} (K_i= 1.195 mM) showed competitive inhibition of the enzyme activity with insignificant change in the secondary structure of the protein.

The above studies exhibit the potential of the enzyme in studying anticancer drugs. Treatment of the enzyme with group specific reagents showed the presence of carboxylate, Arg and Cys at the active site. Substrate protection studies and kinetics of the modified enzyme confirmed the above results. Trp and His at the active site were observed to be in proximity.

Human eukaryotic initiation factor 2α and heme regulated eukaryotic initiation factor 2α kinase

The α-subunit of the human eukaryotic initiation factor 2 (heIF2α), a GTP binding protein, plays a major role in the initiation of protein synthesis. During various cytoplasmic stresses, eIF2α gets phosphorylated by eIF2α specific kinases resulting in inhibition of protein synthesis. The cloned and over expressed heIF2α, a protein with a single tryptophan (trp) residue was examined for its conformational characteristics using steady-state and time-resolved tryptophan fluorescence, circular dichroism (CD) and hydrophobic dye binding.

The steady state fluorescence spectrum, fluorescence lifetimes (τ_1 =1.13 ns and τ_2 = 4.74 ns) and solute quenching studies revealed trp conformers to be present in hydrophobic and differential polar environment at any given time. Estimation of the α-helix and β-sheet content showed: i) more compact structure at

pH 2.0, ii) distorted α-helix and β rearranged α-sheet in presence of 4 M guanidine hydrochloride and iii) retention of more than 50% ordered structure at 95°C. Hydrophobic dye binding to the protein with loosened tertiary structure was observed at pH 2.0 indicating existence of molten globule like structure. These observations indicate the inherent structural stability of the protein under various denaturing conditions.

Lentil and Jack bean α-mannosidase

Several seeds belonging to the family leguminosae were screened for the α-mannosidase enzyme activity and it was found that seeds of the plant Lens esculentus (Lentil) showed maximum enzyme activity. Soaked seeds showed 3 times more activity than the dry seeds. The time of soaking and the time and pH of extraction were optimized for maximum enzyme activity as 21 h and 3 h at pH 8.8, respectively. *Lens esculentus* (Lentil) contains two electrophoretically separable α-mannosidases, LAM 1 and LAM 2 which were purified to electrophoretic homogeneity by fractionation with ammonium sulphate followed by cation exchange chromatography on CM-Sepharose and alkaline PAGE, pH 8.8.

The optimum pH and temperature for both LAM 1 and LAM 2 was found to be pH 5.0 and 55°C respectively. Both LAM 1 and LAM 2 were found to be thermotolerant as LAM 1 retained about 65% activity at 60°C for around 2.5 hours and LAM 2 retained about 98% activity at 60°C for around 1.5 hours. The kinetics of LAM 1 and LAM 2 using pNP-α- mannopyranoiside as substrate yielded Km as 3.72mM and Vmax as 0.9056 U/mg/min for LAM 1 and Km as 3.92mM and Vmax as 0.6403 U/mg/min for LAM 2. LAM 2 activity was inhibited by about 75% when incubated with 5mM and 10mM EDTA for 2 hours. Incubation with 500mM mannose for 30 minutes also led to about 65% inhibition of LAM 2 activity. LAM 2 upon incubation with anionic detergent, SDS (1%) for 30 minutes led to almost complete loss of activity whereas incubation with cationic detergents, Tween 20 (1%) and Triton X-100 (1%) for 30 minutes led to activation of enzyme activity by about 50%.

Moringa oleifera* and *Aracea lectin

Denaturation studies are being carried out on these proteins.

Alkaline protease from *Nocardiopsis* sp.

Work on this protein was taken up and standardization of production and purification of the enzyme is in progress.

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Publication
- *J. Industrial Microbiol. Biotechnol.*, **2009**, 36, 373

Studies on novel highly acidic phytase from Aspergillus niger: Up-scaling, characterization and its application in poultry feed

Phytase is one of the important industrial animal feed enzyme especially for poultry. Among fungi the strain of *Aspergillus niger* produce large amount of extracellular phytase and show more acid tolerance than bacteria and yeast.

We have already reported production of two different phytases (Phy I and II) by *A. niger* NCIM 563 under submerged fermentation conditions

- Strain improvement of *Aspergillus niger* NCIM 563 for phytase production
- Up scaling of phytase production by submerged fermentation from shake flask to 14 L fermenter scale
- Formulation of phytase in liquid and powder form
- Thermostabilization of phytase

Isolation of mutants

More than 1200 mutants were isolated using combination of physical (UV) and chemical (EMS) mutagenesis on plates containing 0.5% calcium phytate. Mutants were selected on the basis of small compact colony with large zone of hydrolysis on calcium phytate plate as compared to parent strain. All the positive mutants were quantified for phytase production using rice bran-glucose-salt medium in shake flask condition.

Mutants N-1 and N-79 were found to be superior to parent strain as they produce 80 IU/ml and 100 IU/ml phytase activities on 10.5th day as compared to 68 IU/ml of phytase activity by parent on 11th day.

Up-scaling of phytase production (Fermenter studies)

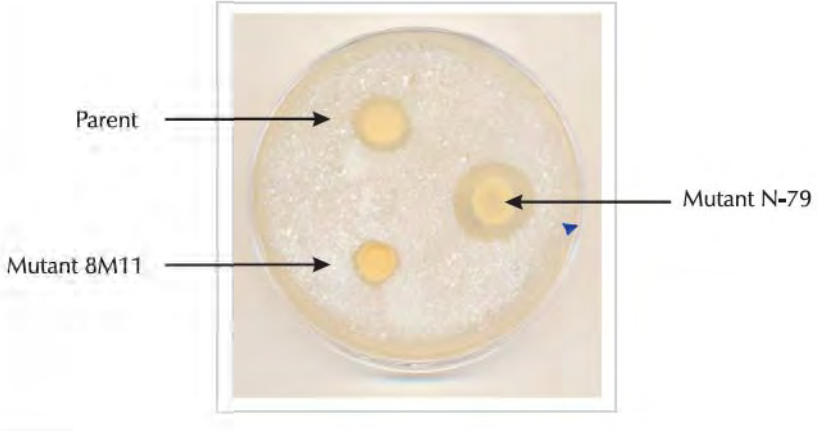
After optimizing the production of phytase under shake flask conditions it was further optimized in 3L and 14L (New Brunswick, USA) fermenter with working volume of 1.8 and 10L, respectively.

Three-liter fermenter

The production pattern of phytase by *A niger* NCIM 563 studied using a laboratory-scale fermenter (New Brunswick, USA) of 3L capacity with a working volume of 1.8L. The fermenter was run with aeration of 0.2 vvm and agitation (300 to 500 rpm), respectively. The pH of the fermenter was not controlled but was monitored. Initial pH of the medium was around 5.5, which decreased to pH 1.8 to 2.0 at the end of fermentation.

Effect of various agitation speeds on phytase production indicated that maximum phytase activity of 41 IU/ml was obtained on 7-8th day at 400 rpm. Similarly effect of various conc. of glucose in fermentation medium indicates that maximum phytase activity of 51 IU/ml was produced on 8th day of fermentation when glucose conc. in the medium was 4%.

Mutants of Aspergillus niger displaying increased zone ofhydrolysis on calcium phytate agar plates



Fourteen-liter fermenter

From 3-Lit fermenter the process was further up-scaled to 14-Lit fermenter using 1% rice bran and glucose (3.5 to 5%) supplemented with salts with aeration and agitation at 0.2 vvm and 400 rpm, respectively. Maximum phytase activity of 68 IU/ml and 66 IU/ml was obtained at glucose conc. (4%) and (3.5 %), respectively on the 10th day of fermentation.

Further optimization of agitation speed (400 rpm to 550 rpm) in 1% rice bran-3.5% glucose-salt medium indicate that maximum phytase activity of 80 IU/ml was obtained on 10th day of fermentation at 550 rpm.

Stability of phytase in liquid and solid conditions

Phytase is applied in mash feed and pelleted feed. So stability of phytase enzyme in liquid form was evaluated. Effect of various additives in the liquid enzyme indicates that enzyme preparation can be stabilized in liquid form before mixing into carrier for its easy application.

Phytase retains total activity without any contamination in presence of 50% methanol, ethanol, chloroform and acetone at room temperature and 8-10ºC. Effect of various reagents indicates that fermented broth retains its total activity at room temperature by addition of penicillin and bavistin (0.1%), formalin (0.2%), sodium chloride (10%) and glycine (1M). Addition of skimmed milk (8-12%) to phytase enzyme solution was found useful to retain the phytase activity at 70°C.

Release of inorganic phosphorus from poultry feed ingredients

In poultry, the feed supplied is generally digested within 2 h so to determine efficacy of phytase in poultry feed various feed ingredients were treated with phytase at 39°C for 2 h to simulate the condition of poultry stomach and the amount of Pi released was evaluated. From most of the feed ingredients 4.46 to 12.9 mg/g inorganic phosphorus was found to be released.

Bioformulation for application in poultry feed

Among various carriers evaluated wheat bran and rice bran were found to retain total phytase activity in dry free flowing form. However calcium carbonate and silica gel powders were found to loose phytase activity very rapidly. Thus concentrated liquid phytase solution can be mixed with either wheat bran or rice bran and dried at 50°C for 2 h to remove the moisture and can be subsequently mixed with poultry feed as source of phytase. This method is more suitable and cost effective than the existing commercial phytase which is generally available in granular or powder form.

Purification of phytase

A niger NCIM 563 produced two different extracellular phytases (Phy I and Phy II) under submerged fermentation conditions at 30°C in medium containing dextrin-glucose-sodium nitrate-salts were purified to homogeneity. The molecular mass of Phy I and II as determined by SDS-PAGE and gel filtration were 66 kDa, 264 kDa and 150 kDa, 148 kDa respectively, indicating that Phy I consists of four identical subunits and Phy II is a monomer.

The pI of Phy I and II was 3.55 and 3.91, respectively. Phy I was highly acidic with optimum pH of 2.5 and was stable over broad pH range (1.5-9.0) while Phy II showed pH optimum of 5.0 with stability in the range of pH 3.5-9.0. The Phy I exhibited very broad substrate specificity while Phy II was more specific for sodium phytate. Similarly Phy II was strongly inhibited by Ag^{+}, Hg^{2+} (1 mM) metal ions and Phy I was partially inhibited.

Peptide analysis by Mass Spectrometry (MS) MALDI-TOF also indicated that both the proteins were totally different. The *Km* for Phy I and II for sodium phytate was 2.01 and 0.145 mM while Vmax was 5018 and 1671 umoles min^{-1} mg^{-1}, respectively. The N-terminal amino acid sequences of Phy I and Phy II were FSYGAAIPQQ and GVDERFPYTG, respectively. Phy II showed no homology with Phy I and any other known phytases from literature suggesting its unique nature. This, according to us, is the first report of two distinct novel phytases from *A niger*.

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Publications
- *Biochim. Biophys. Acta.*, **2010**, 1800, 526
- *Entomol. Res.*, **2010**, 40, 113
- *Biores. Technol.*, **2010**, 101, 5366

Hydrolytic enzymes and their inhibitors

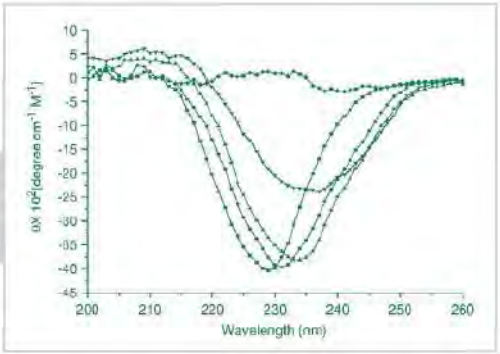
Aspartic protease inhibitor

A novel bifunctional Aspartic Protease Inhibitor (API) isolated from *Bacillus licheniformis* inhibits acid protease from *Aspergillus saitoi* and chitinase A (ChiA) from *Serratia marcescens*. Chitinase inhibitors have chemotherapeutic potential as fungicides, pesticides and antiasthmatics.

The majority of chitinase inhibitors reported are natural products like argifin, argifin linear fragments, argadin, allosamidin and disulfide-cyclized peptides. The binding affinity of API with ChiA and type of inhibition was determined by the inhibition kinetic assays. Fluorescence and CD spectroscopic analysis and chemical modification of API with different affinity reagents elucidated the mechanism of binding of API with ChiA.

The peptide has an amino acid sequence N-Ile1-Cys2-Glu3-Ala4-Glu5-His6-Lys7-Trp8-Gly9-Asp10-Tyr11-Leu12-Asp13-C. The ChiA-API kinetic interactions reveal noncompetitive, irreversible and tight binding nature of API with I_{50}=600 nM and K_i=510 nM in the presence of chromogenic substrate pnitrophenyl- N, N'-diacetyl-β-chitobioside[p-NP-(GlcNAc)2].

The inhibition progress curves show a two-step slow tight binding inhibition mechanism with the rate constant $k_5=8.7\pm1\times10^{-3}$ s^{-1} and $k_6=7.3\pm0.6\times10^{-5}$ s^{-1}. CD-spectra and tryptophanyl fluorescence analysis of ChiA incubated with increasing API concentrations confirms conformational changes in enzyme structure which may be due to irreversible denaturation of enzyme upon binding of API. Chemical modifications by WRK abolished the anti-chitinase activity of API and revealed the involvement of carboxyl groups in the enzyme inactivation.



Effect on the secondary structure of ChiA upon binding of API. Far-UV circulardichroism spectra of the unliganded ChiA and its complexes with the API are shown

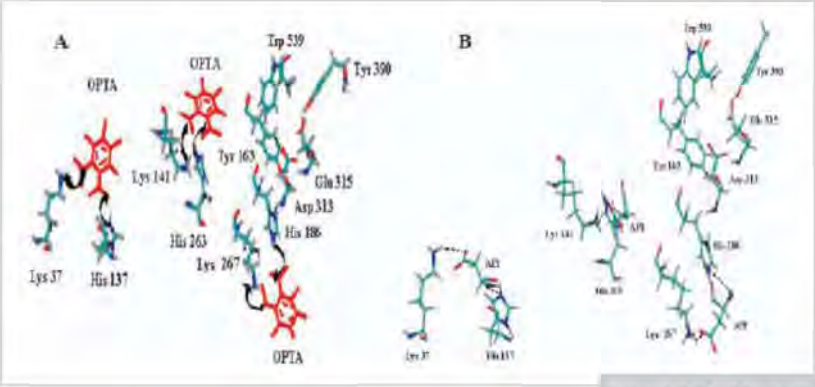
Abolished isoindole fluorescence of OPTA-labeled ChiA demonstrates the irreversible denaturation of ChiA upon incubation with API for prolonged time and distortion of active site of the enzyme. The data provide useful information that could lead to the generation of drug-like, natural product-based chitinase inhibitors.

Biofuel from hemicellulose prevalent alternative feedstocks

In collation to first generation bioethanol from starch and molasses, the development of second generation bioethanol from lignocellulosic biomass serves many advantages from both energetic and environmental point of views. However a logical approach is to develop processes for producing ethanol from alternative feedstocks while waiting for the lignocellulosic biomass ethanol technology to be ready for commercialization. A hemicellulose based feedstock such as wheat bran and tamarind kernel powder which can be readily hydrolyzed to value added products is foreseen to be significant from this aspect.

The potential of enzymatic hydrolysis of hemicellulose from agricultural by-product, wheat bran using a thermostable hemicellulase from an alkalothermophilic *Thermomonospora sp* and subsequent fermentation with a thermotolerant pentose fermenting yeast is investigated. In addition to WB, oat spelt xylan (OSX) is also studied as a model system under the consonant experimental conditions.

The study also focuses for the first time the effect of biosurfactant, sophorolipid on the increased hydrolysis of hemicellulosic substrates and simultaneous saccharification and fermentation (SSF) in which hemicellulose is used together with thermotolerant yeast. A hydrolysis of 62% and 50% for OSX (Oat



Hypothetical schematic representation of the model depicting the probable mechanism of API binding to ChiA using chemoaffinity labeled o-pthaldehyde (OPTA)

Spelt Xylan) and WBH (Wheat bran hemicellulose) were obtained in 36 h and 48 h using Accellerase™ 1000 at 50°C wherein thermostable xylanase from alkalothermophilic *Thermomonospora sp* yielded 67% (OSX) in 3h and 58% (WBH) in 24h at 60°C, favouring a reduction in process time and enzyme dosage.

The rate of hydrolysis with thermostable xylanase was increased by 20% with the addition of nonionic surfactant tween 80 or biosurfactant sophorolipid. The simultaneous saccharification and fermentation (SSF) of OSX and WBH using thermostable xylanase and *D. hansenii* in batch cultures produced 9.1g/L and 9.5g/L of ethanol respectively and had a shorter overall process time than the separate hydrolysis and fermentation (SHF). The immobilized yeast cells in Ca-alginate matrix produced ethanol with a yield of 0.46g/g from hemicellulosic hydrolysates and were reused six times with 100% fermentation efficiency.

The hydrolysis and ethanol production from tamarind kernel powder (TKP), a rich source of galactoxyloglucan (GXG) was investigated for the first time using xyloglucanase and thermotolerant *D.hansenii*. The acid hydrolysis of TKP with 2 N H_2SO_4 at 120°C for 30mins yielded an overall saccharification of 94% based on the total available carbohydrate content and further fermentation at 40°C with thermotolerant *D. hansenii* produced an ethanol yield of 0.35g/g.

A maximum hydrolysis of 55% and 78% for GXG was obtained in 48h at 50°C using *Thermomonospora* xyloglucanase (TXy) and accellerase™ 1000 respectively. The synergistic effect of β-galactosidase and xyloglucanase was demonstrated by the exogenous addition of β-galactosidase to TXy which improved the overall hydrolysis of GXG by 30%.

The rate of hydrolysis of GXG with TXy and accellerase was increased by 15-20% in the presence of chemical surfactants (tween 80 and toluene) or protein additive (BSA). The fermentation of enzymatic hydrolysates of GXG by TXy and accellerase with free cells at 40°C produced an ethanol yield of 0.39g/g and 0.41g/g whereas with immobilized cells produced 0.45g/g and 0.43g/g respectively with a theoretical conversion efficiencies of 78%-88%.

The immobilized yeast cells were reused six times at 40°C with 100% fermentation efficiency.

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Publications

- *J. Phys. Chem.* **2009**, 113, 3478
- *Extremophile.*, **2009**, 13, 363
- *Food Res. Int.*, **2009**, 42, 516
- *New J. Chem.* **2009**, 33, 646

Structure, characterization, synthesis and reaction studies of biochemical systems

Bile salt hydrolases

A thermophilic microorganism producing bile salt hydrolase was isolated from hot water springs, Pali, Maharashtra, India. This microorganism was identified as *Brevibacillus sp* by 16S rDNA sequencing. Bile salt hydrolase (BSH) was purified to homogeneity from this thermophilic source using Q sepharose chromatography and its enzymatic properties were characterized. The subunit molecular mass of the purified enzyme was estimated to be 28 kDa by SDS- PAGE and, 28.2 kDa by MALDI-TOF analysis. The native molecular mass was estimated to be 56 kDa by gel filtration chromatography, indicating the protein to be a homodimer. The pH and temperature optimum for the enzyme catalysis were 9.0 and 60 °C, respectively. BSH from *Brevibacillus sp*. hydrolyzed all of the six major human bile salts, the enzyme preferred glycine conjugated substrates with apparent K_M and k_{cat} values of 3.08 μM and 6.32 x 10^2 s^{-1}, respectively, for glycodeoxycholic acid. The NH_2-terminal sequence of the purified enzyme was determined and it did not show any homology with other bacterial bile salt hydrolases.

Ntn Hydrolase family enzymes

Bile salt hydrolase (BSH; EC.3.5.1.24) is a member of Ntn hydrolase structural super family of proteins. This enzyme plays an important role in cholesterol catabolism and involved in reducing serum cholesterol levels. We have isolated a thermophile producing bile salt hydrolase intracellularly. The thermophilic bacterium was identified to be *Brevibacillus borstelensis* by 16S rDNA sequencing.

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. Physiochemical characterization of the immobilized enzyme indicated that the structure of the support material is stable after immobilization. In application studies, 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

Biosynthesis of novel sophorolipids (Biosurfactant)

Preparations of new sophorolipid (SL) analogues with different functionalities have wide application in pharmaceutical and industrial application. We have synthesized and tested the Sophorolipid and their methyl ester products for their antimicrobial properties against both gram positive and gram negative bacteria.. This product showed good antimicrobial activity against *Bacillus subtilis* at concentrations 5, 10 and 15 mg/ml respectively.

Surface functionalisation of nanoparticles and their biological applications

The most challenging part of research in the nanoscience & nanotechnology field is the cost effective and environmentally safe procedures for synthesizing the desired nanomaterials. For the first time, we report in situ synthesis and functionalisation of gold nanoparticles (AuNPs) using β-lactam antibiotics like cephalexin, 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 synthesis provides a good system to capture AuNPs during its synthesis by the cephalexin using optical methods like Dynamic Light Scattering (DLS), Surface Plasmon Resonance (SPR) using UV-Vis light spectroscopy and Transmission Electron Microscopy (TEM)[3]. Unique bimodal distribution is observed at different temperatures (15 °C, 25 °C & 35 °C) using DLS.

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. The spectroscopic evidence of solubilising curcumin in water in a temperature-dependent manner is shown. The mechanism involved is elaborated. The as-synthesized AuNPs are characterized. These nanoparticles show anti-oxidant activity, which can be used in bio-nanomedicine.

Biotransformation of non-edible oil in to biofuels

Biodiesel is renewable, biodegradable, and nontoxic fuel as compared to the petroleum due to its total combustion property. Transesterification of oils yield alkyl esters of long chain fatty acids which is a best alternative for fossil fuel. In 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.

Sophorolipids are biosurfactants produced by yeasts which comprise of one sophorose molecule linked to a fatty acid. The membrane components of mammalian cells-glycosphingolipids and gangliosides which are similar in structure to sophorolipids are known to modulate cell growth, adhesion and trans membrane signaling. They also have some role in oncogenesis and differentiation. Sophorolipids have been reported to induce differentiation in number of leukemic cell lines.

We have explored the effects of sophorolipids on LN229 cells- a cancerous cell line of neural origin which we are reporting for the first time. When LN229 cells were exposed to pure acidic form of oleic acid sophorolipid, long thread like extensions were seen arising from ends of the cells and they got aligned which can be regarded as indication of neural network formation. Cell death was observed at higher concentrations. The morphological changes suggest that sophorolipids are potential differential inducers. 10μg/ml SLOAC 2 (40X magnification) elongated cells and formation of bundles is there.

We also tried to produce sophorolipids using different fatty acids precursors. As an attempt to reduce the cost for sophorolipid production non edible oils pongamia oil and jatropha oil have also been tried out as precursors. Satisfactory yield was obtained with both the oils. They also displayed good emulsification and surface tension lowering activity.

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Publications
- *Appl Biochem Biotechnol* **2009**, 157, 463
- *Photochem. Photobiol. B: Biol* **2009**, 97,109

Penicillin acylases and related NTN hydrolases

Work done and discussion

Penicillin acylases and related Ntn hydrolases

6-aminopenicillanic acid (6-APA) is a key intermediate in the manufacture of semi-synthetic penicillins such as ampicillin, amoxicillin etc. Semisynthetic lactam antibiotics account for about 65% of the total antibiotic market. 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-APA and the corresponding organic acid side chain. Penicillin acylases selectively hydrolyze the amide bond at the side chain of the penicillin moiety keeping the beta lactam amide bond intact. Conventionally process involving penicillin G acylase (PGA) dominates pharmaceutical industry over penicillin V acylase(PVA) though the penicillin V acylase has many advantages over penicillin G acylase.

Screening was carried out to obtain new microorganisms producing penicillin V acylase with unusual characteristics. A bacterial isolate identified as Bacillus cereus is reported by us for first time to produce PVA. Fermentation conditions were standardized for optimal production of PVA from the potential producer *Erwinia aroideae* (DSMZ 30186) and enhancement in cell-bound activity is achieved through permeabilization using various solvents. The physicochemical properties of the organic solvents used for permeabilization were correlated with the change in activity.

Penicillin V acylase from *Rhodotorula aurantiaca* (*Ra*-PVA) has been purified to homogeneity and characterized extensively. This is the first report of smallest active monomeric PVA. Modification of the enzyme with amino acid specific reagents indicated presence of serine and tryptophan residues at or near the active centre of PVA. Microenvironment of the tryptophan residues in active and denatured Ra-PVA was studied using various quenchers and fluorescence spectrophotometry. The tryptophan residues of Ra-PVA were found to be largely buried in the core of protein matrix and surface tryptophans were found to have predominantly more electro-positively charged amino acids around them, however differentially accessible for ionic quenchers. This *Ra*-PVA is the first penicillin V acylase of the kind which has active serine at N terminal end of enzyme instead of cystine.

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Publication
- *Mycol. Res.*, **2009**, 113, 290

Induction of siRNA-mediated resistance to papaya ringspot virus-P in Carica papaya

Papaya (*Carica papaya*) is of major economic importance to India, since country is one of the leading papaya producers in the world. The fruit production is severely affected by the Papaya Ring Spot Virus-P (PRSV-P). Conventional control measures for PRSV-P so far have had only limited success worldwide.

Recently, major efforts have been directed to improve the crop through genetic engineering. RNA silencing, also termed as post-transcriptional gene silencing (PTGS) is a conserved eukaryotic gene inactivation system that plays regulatory roles in antiviral responses and is an effective strategy to develop resistance against viruses.

Thus, the present work was carried out with the objective of developing transgenic papaya having resistance against PRSV-P by using siRNA post-transcriptional gene silencing method.

Work done and discussion

Work on isolation of RNA from PRSV infected leaf of Papaya plant was carried out by following Trizol method. cDNA was synthesized from RNA by reverse transcriptase enzyme. PRSV cp (coat protein), HC-Pro and rp (replicase) genes were amplified and isolated by PCR method.

CP gene was amplified by using forward primer CP-D1:5' (ATGGTNTGGTGYATNGARAAYGG) 3' and Reverse primer CP-R1: 5'(GTTGCGCATACCCAGGAGAG) 3', generating a 900bp amplicon. HC-Pro gene was amplified by using forward primer HPF1: 5' (AATGACGTGGCTGAAAAATTC TG) 3' and Reverse primer HPR1: 5'(GCCGACAATGTAGTGCTTCATTT) 3', and a 1.4 kb amplicon was generated.

RP gene was amplified by using forward primer RPF2: 5' (AGTGGAAGTCGATGGCTCTTTGC) 3' and Reverse primer RPR3: 5'(CCCCATGACTCTATCATTGC) 3', and a 1.5 kb amplicon was generated.

Amplified genes were cloned into pGEMT vector. Cloned vector transformed into *Epicurian Coli* XL 10 competent cells by Heat-Shock method. After Blue-White colony screening, individual white colonies were selected. PCR and restriction digestion was performed on each to confirm transformation. Plasmid was isolated from the colonies showing positive results for further transformation work and sequence analysis. Multiple sequence analysis of the cp, HC-Pro, and rp amplicons with BLAST and CLUSTALW showed 97%, 89%, 90% nucleotide sequence similarity respectively as per other reported PRSV-P strain.

Work on cp, HC-Pro and rp genes cloning into siRNA binary vector having sense and antisense cassette of cp and rp genes is in progress. These cloned vectors will be mobilized into *Agrobacterium by* freeze-thaw method and the construct will be used for development of transgenic papaya.

The regeneration potential of immature zygotic embryos of five papaya cultivars, cv. Pusa Nanha, CO2, CO6, Poona Local and Red Lady) was studied. Plant growth regulators (PGRs) such as 2,4-D, 2,4,5-T and Picloram at the concentrations of 2, 3 and 1 mg/L respectively, were incorporated in the Murashige and Skoog's (MS) medium to study their influence on induction of somatic embryogenesis (SE) in the five papaya cultivars.

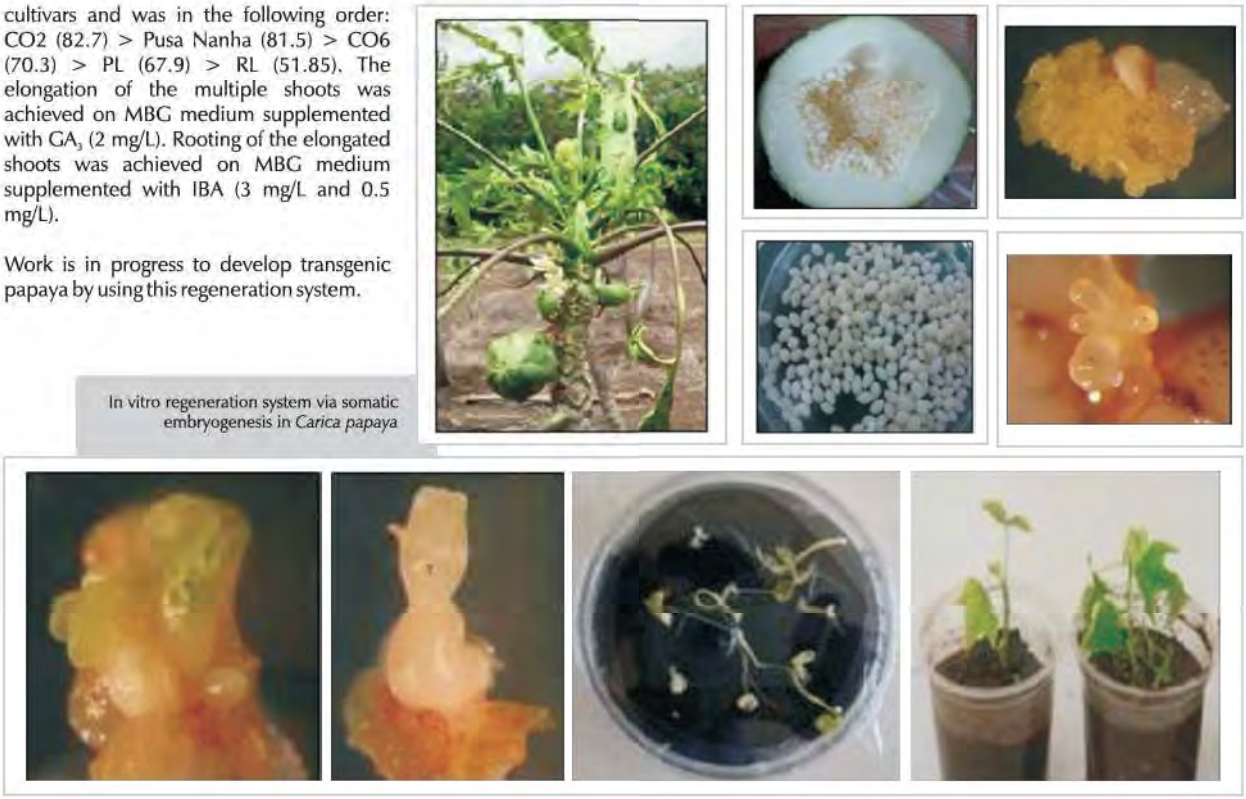
All the three growth regulators tested, induced somatic embryos in the immature zygotic embryos, though its response varied among the five cultivars. Type of PGR, its concentration and photoperiod had influence on the percentage of SE response.

The somatic embryogenesis response observed was in the following order: Pusa Nanha (40.5%) > CO2 (40.2%) > CO6 (26.2%) > PL (22.9%) > RL (13.8%). Explants incubated under total dark condition showed higher SE responses compared to incubation under 16h photoperiod. Maturation of somatic embryos was achieved on MS medium supplemented with ABA (0.1 mg/L). The matured somatic embryos germinated upon transfer to MS medium with GA^3 (1 mg/L).

Also, multiple shoot regeneration was achieved on MS salts with B5 vitamins (MBG) medium supplemented with BAP (1 mg/L) + NAA (0.1 mg/L). The percentage of organogenesis response however, varied among the five

cultivars and was in the following order: CO2 (82.7) > Pusa Nanha (81.5) > CO6 (70.3) > PL (67.9) > RL (51.85). The elongation of the multiple shoots was achieved on MBG medium supplemented with GA_3 (2 mg/L). Rooting of the elongated shoots was achieved on MBG medium supplemented with IBA (3 mg/L and 0.5 mg/L).

Work is in progress to develop transgenic papaya by using this regeneration system.



In vitro regeneration system via somatic embryogenesis in *Carica papaya*

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Publications

- *Adv Fun Mater*, **2010**, 20
- *Physiol. Mol. Biol. Plants*, **2009**,15, 311
- *Extremophiles*, **2009**, 13, 363

Metabolic engineering of phenylpropanoid pathway in plants

Leucaena leucocephala, a leguminous tree species is mainly used as pulpwood and also as a forage crop. The presence of lignin which constitutes 20-30% of wood is considered an undesirable factor in paper making as it not only limits accessibility to cellulose, but also reduces paper quality. It also limits the digestibility in a fodder crop. Thus there is a lot of economic interest in engineering the lignin content and composition in this tree species. Currently the biosynthetic pathway of lignin has been well defined in various plants including few tree species. 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 lignin biosynthetic pathway 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.

Three different Cinnamate-4-Hydroxylase (C4H) genes (cDNA clone) from *L. leucocephala* have been cloned and characterized. The nucleotide sequences of isolated C4H genes from Leucaena show about 90% similarity, while the deduced amino acid sequences show more than 95% similarity with the previously reported C4H genes from other plants.

These genes have been expressed in *E. Coli* and recombinant proteins are being purified for expression studies. At the same time, for the study of down-regulation of C4H gene expression in genetically engineered *Leucaena* and tobacco plants, recombinant binary vector (pCAMBIA 1301 containing partial C4H fragment in Antisense orientation) has been transfected into *Leucaena* and tobacco through *Agrobacterium tumefaciens* (strain GV2260) mediated transformation and the plants are currently growing in vitro.

Our understanding on the transcriptional regulation of lignin biosynthetic pathway is still limited. This phenomenon is largely mediated through proteins that interact directly or indirectly with specific DNA sequences (cis elements) in the promoter region of genes. Among the different classes of transcription factors (TFs) directly or indirectly implicated in lignification, R2R3-MYBs are strong candidates for the regulation of phenylpropanoid enzymes which are known to bind to AC elements, found on promoters of most of the monolignol biosynthetic genes. With an objective to understand the transcriptional control of the phenylpropanoid pathway in lignin biosynthesis, partial promoter sequences were isolated for CCoAOMT (508bp, GenBank:GU132437) and C4H(196bp) genes, using the approach of TAIL PCR. *Insilico* analysis of these two as well as a partial CCR promoter helped us identify motifs for MYB-binding domains.

Based on this fact as well as reported studies, two novel R2R3 type MYB genes (GenBank: GU901208 and GenBank: GU901209) were isolated and cloned based on degenerate primer based approach from xylem cDNA pool of the plant, followed by rapid amplification of cDNA ends (RACE).

Biological Sciences

Both the genes were found to have the highly conserved 50-52 amino acid repeat sequence responsible for DNA binding. A Southern analysis using the 50-52 amino acid repeat encoding gene fragment was used as probe, which showed multiple bands in the autoradiogram (Fig1).

A phylogenetic tree was constructed for the two MYB genes to understand their evolutionary relationships with the reported R2R3 MYBs. One of the genes, Ll_MYB_SSM (GU901209) formed a close subgroup with AmMYB308, which is known to regulate the lignin biosynthetic pathway (Fig. 2).

Understanding the transcriptional control of lignin biosynthesis during wood formation will have important implications in tree biotechnology. It will be possible to use one or a few transcription factors to down- or up-regulate the entire lignin biosynthetic pathway and thereby alter lignin content in wood based on our needs.

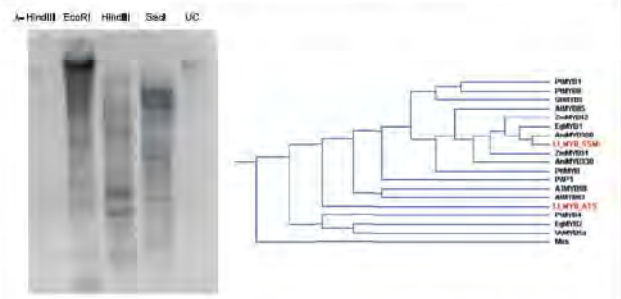

Fig. 1

Fig. 2

Cellulose biosynthesis

Paper is one of the basic needs of modern life and wood is the main raw material for the production of pulp and paper. The major constituents of wood are cellulose, hemicelluloses, and lignin. Removal of lignin and hemicelluloses from wood yields Pulp. Pulp consists of cellulose, which is a simple polymer of unbranched β-1,4-linked glucan chains, which coalesce to form microfibrils. It is the major component of wood and thus paper.

The polymerization of glucose residues into a β-1,4-linked backbone is catalyzed by the enzyme Cellulose Synthase (Ces A), which utilizes UDP-glucose as the substrate. Cellulose biosynthesis has not been studied so far in *Leucaena sp.* Study of these Cellulose Synthase (Ces A) genes will help in understanding the biosynthesis of cellulose in *Leucaena sp.* and its manipulation by genetic engineering to meet the needs of pulp and paper industry. With the aim of understanding cellulose biosynthesis and their genetic manipulation we have isolated this gene from *Leucaena* plant. After sequencing of 8 Full-length clones, In silico study have shown two different Ces A genes designated as a Ll7Ces A (Accession No. FJ871987) and Ll8Ces A (Accession No. Gq267555).

Southern blot analysis was done and it was found that Ces A gene is a multigene family.

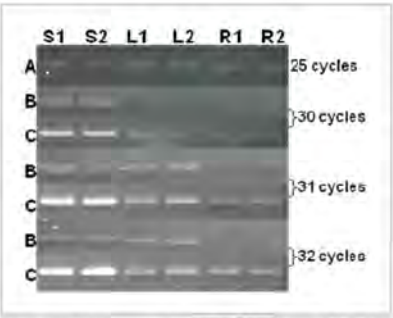

Fig. 4: Semi quantitative PCR of two Ll-CesA genes: S1, S2, L1, L2, R1, R2 shoot, leaf and root in duplicate respectively; A, 5.8S rRNA internal control; B, Ll-*7CesA;* C, *Ll-8CesA*

Fig. 3: Southern Blot

Differential expression of these two Ces A genes was done by using semi-quantitative and quantitative Real-time PCR (QRT-PCR) and cDNA as a template. It was found that *Ll7Ces* A gene expressed more in stem (1.75 fold more) than leaves and not in root and *Ll8Ces* A gene expressing more in stem than leaf and root (In leaf 1.89 fold and in stem 6.12 fold more than root).

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Publications
- *Seed Sci. Biotechnol*, **2009**, 3, 54
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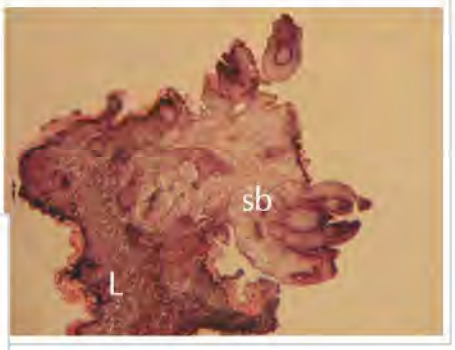
Tissue culture studies

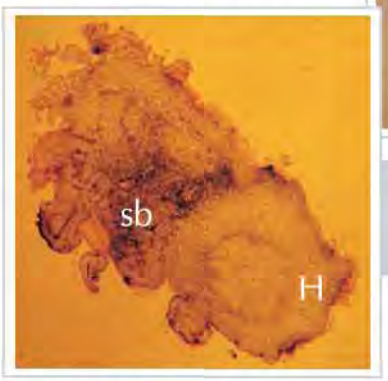
Tissue culture studies in oil producing plants

Our objectives are to develop tissue culture protocols for rapid propagation using seedling / mature explants and standardization of protocols for de novo organogenesis / embryogenesis, useful for genetic transformation.

Jatropha

Histological studies were carried out in order to determine the origin of *de novo* organogenesis in *Jatropha curcas*. In case of leaf explants cultured on BAP containing media, shoot buds were initiated through direct morphogenesis while in hypocotyl explants, large meristematic masses were formed from which shoot bud initiation was observed.





Histology confirming *de novo* organogenesis of shoot buds (sb) from leaf (L) and hypocotyl (H) explants of Jatropha seedlings cultured in BAP containing media

Semecarpus anacardium

The work carried out includes,
- Isolation of DNA from hairy roots induced in various explants and confirmation of presence of *rolA*, *rolB* and *rolC* genes in the roots.
- Chemical analysis of the ethyl acetate extracts of different parts of *Semecarpus anacardium* plant showed the presence of amentoflavone in the leaves.
- Molecular characterization using ISSR markers was carried out for the variation among the populations from various locations.

Biophysical characterization of cadmium and lead toxicity in *Gladiolus* and *Nerine*

Cadmium (Cd) and Lead (Pb) are two major land contaminating heavy metals in India posing significant health and environmental hazard. Geophytic floricultural plants form appropriate phytoremediation crop due to their perennial self sustainability, ornamental utility, larger underground biomass productivity and frequent above-ground biomass harvestibility.

Cd and Pb at low (T1), medium (T2) and high (T3) concentrations were applied in sand hydroponic culture to the propagules of *Gladiolus* and *Nerine* to evaluate their individual effects on sprouting, growth and leaf photometric properties.

- Except for *Gladiolus* in high Cd level, both plants were successfully established and grew in all heavy metal toxicity regimes.
- Aerial growth rates and root development suggested efficient competency in presence of heavy metals. Pb had a positive influence on the aerial growth rate and biomass of nerines whereas Cd favored shoot-leaf growth in gladioli.
- Relative dry weights were affected by Cd and Pb in both the plants in a dose dependent manner.
- Machine vision analysis revealed that the reflection intensities and distribution of plant pigments varied significantly in Cd and Pb treated plants of gladioli and nerines, respectively. However, variations in the visible range leaf reflectance patterns were not metal specific.

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Dehydration of glycerol to acrolein

Background / objectives

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. Main objective of the work was to develop catalyst for dehydration of glycerol to acrolein with high activity and selectivity.

Various Bronsted acidic ionic liquids were prepared starting from aromatic amines like 2-picoline, 3-picoline, 4-picoline, pyridine, and 3,4-Lutidine with 1,3-propane sultone and 1, 4-butane sultone by following the literature procedure.

Silica supported catalysts (20% loading of ionic liquid) were prepared from these ionic liquids and tested for dehydration of glycerol to acrolein. All the catalysts prepared were active for the reaction and acrolein was obtained as major product in the reactions (conversion of glycerol was observed in a range of 35-90% with selectivity to acrolein in a range of 29-58%). Catalyst C-1 prepared from triphenyl (3-sulfopropyl) phosphonium 4-methylbenzenesulfonate showed good activity and selectivity at 4 h reaction time. Effect of various reaction conditions on the activity and selectivity was investigated for catalyst C-1. The conversion of glycerol decreased with increase in glycerol concentration.

Higher temperature (325°C) resulted in significantly lower conversion as well as selectivity to acrolein. Thus optimum results were obtained at 275°C. Activity of the catalysts decreased with time for all the catalysts. GC-MS analysis indicated decomposition of ionic liquids based on imidazole, pyridine and picoline under reaction conditions. In order to account for the loss of acrolein because of volatility, two additional traps cooled to -7°C were used to collect acrolein escaping product container cooled with ice. The use of two additional traps led to acrolein selectivity in a range of 59-68% for good catalysts.

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- *Biotechnol. Lett.*, **2010**, 32, 517
- *Green Chem.*, **2010**, 12, 1106
- *Mater Sci Engg*, **2010**, B168, 193

Production of polymer grade lactic acid in a 300TPA pilot plant

Background / objectives
- To isolate identify and improve D-lactic acid producing cultures
- To study the rheology of PLA produced from lactic acid

Work done and discussion

Fermentation

Fermentative production of lactic acid offers great advantage in producing optically pure L- or D-lactic acid depending upon the strains selected for fermentation. The optical purity of lactic acid is crucial factor in the physical properties of polylactic acid (PLA). Recently, stereo-complexing of PLLA and poly D-lactic acid (PDLA) was found to increase the melting point of resultant complex, thus presenting an attractive solution to heat sensitivity of PLA.

NCL is investigating D-lactic acid fermentation with a view to obtaining improved strains capable of producing D-lactic acid with enhanced productivities. *Lactobacillus lactis* NCIM 2368 is homo-fermentative D-lactic acid producing strain selected through screening protocol. Work is in progress for improving the D-lactic acid yields

Polymer processing

Polylactic acid (PLA) was reactively extruded with 2, 5-dimethyl-2,5-di-(t-butyl peroxide) in a Haake batch mixer. Based on the mixing temperature and the relative contents of peroxide, branching, crosslinking, and chain scission can occur separately or simultaneously. Molecular weight was determined by gel permeation chromatography.

The rheology of linear and branched poly (lactic acid) was investigated in shear and uniaxial extensional modes and a multi-mode differential constitutive equation, PTT, was fit to the experimental data. Time sweep experiments were performed on these samples at different temperatures to test the melt stability. Strain sweep experiments were carried out to determine the linear viscoelastic (LVE) regime, and frequency sweep experiments were performed to determine the relaxation spectrum and flow activation energy. Enhanced shear thinning behavior was noticed for branched samples compared to the linear polymers in step shear experiment. Finally, uniaxial extensional viscosity measurements were performed on the linear and branched PLA resins, and the latter showed characteristic strain hardening response.

Branched PLA had higher molecular weight, higher zero-shear viscosity, longer relaxation time, higher flow activation energy, enhanced strain hardening and shear thinning behaviors as compared to linear PLA. These rheological features are beneficial for melt processing operations such as thermoforming and film blowing, which are used for packaging applications

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- *Catal Lett*, **2010**, 135, 141

Conversion of bioglycerol to 1,3 / 1,2 -propanediol

Glycerol is the one of the main building blocks of the biodisele industry obtained by transesterification of vegetable oils. For every 9kg of biodiesel product, about 1 kg of glycerol is obtained as the by-product. Selective catalytic hydrogenolysis of glycerol represents a low cost and green route for 1,2-propanediol(PDO) which is a major commodity chemical used in various sectors.

During hydrogenolysis of glycerol, acetol is an intermediate formed which is also an important intermediate in hydrogen production by catalytic steam reforming, pyruvaldehyde synthesis through oxidation and starting material in various organic transformations. Therefore, selective hydrogenolysis of glycerol to 1,2-propanediol/1,3-propanediol, development of a suitable catalysts and process is of great interest.

Catalyst and bench scale process development at NCL

Our group has developed and evaluated 36 different copper based and noble metal based catalysts with a focus on overcoming the known limitations of poor conversion selectivity and catalyst life reported in the literature as well as to have the freedom to operate for the best catalyst. Among these catalysts the best catalyst (NMT005) gave a maximum glycerol conversion of 42% with 89% selectivity to 1,2-propanediol at 220°C; H_2 pressure of 1000 psi in 5h in a batch reactor.

For 2g catalyst loading, highest conversion of 81% was achieved with 98% selectivity to 1,2-PDO and catalyst showed excellent activity for highest glycerol concentration of 80%. Compared with BASF patented copper catalysts, our NMT005 catalyst showed higher activity and stability for aqueous glycerol feed. The suitability of our catalyst was confirmed by evaluating of a sample of bioglycerol with 76% assay, obtained from the biodiesel producer, which showed 43 % conversion in 5h in a batch operation.

Catalyst life testing of NMT 005 catalyst in a continuous operation

NCL catalyst (NMT005) showed even better performance and stability up to 800 h for continuous hydrogenolysis of glycerol (Fig. 1), with an average glycerol conversion of 65% and selectivity of > 91% to 1,2-propylene glycol. The catalyst life was found to be three times higher than the targeted catalyst stability of 250 h. For the evaluation in a continuous operation, 25 g of NMT 005 catalyst was prepared, palletized (0.25cm dia.) and charged to a fixed bed reactor consisting of a single SS tube. The operation was continued round the clock and the optimized sets of process conditions were also obtained.

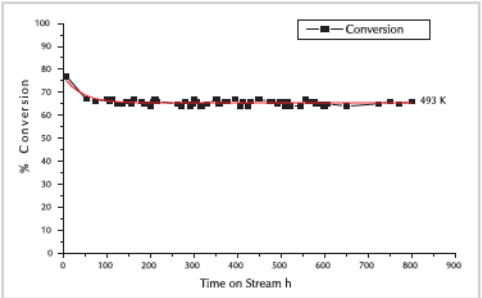

Fig. 1: Time on stream activity of NMT 005 catalyst for hydrogenolysis of glycerol

Another non chromium copper catalyst was also developed which showed a very good water tolerance giving 38% glycerol conversion with > 92% 1,2-PDO selectivity at 220oC, H2 pressure 1000 psi and reaction time 5 h. This catalyst also showed an excellent on stream activity of 400 h in a continuous operation (Fig. 2) giving an average glycerol conversion of 67% with 1,2-PG selectivity of > 90%.

NCL catalyst performance was compared with the reported literature (Table 1) which revealed that NCL catalyst showed a better performance

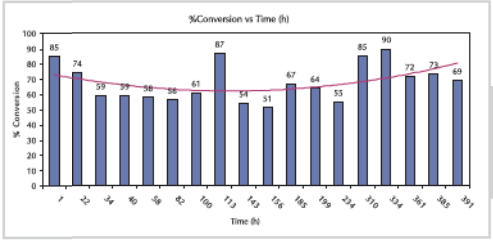

Fig. 2: Time on stream activity of non chromium Cu-Al catalyst

Table 1: Comparison of NCL catalyst with literature data

Catalyst	Substrate	Added base	Temp°C	Pressure (psi)	t/t Feed PG
Ni+Re/C+NaOH	Glycerol	NaOH	230	1300	0.55
7% Ni+1%Re/C	Glycerol	NaOH	230	1300	0.65
Homogeneous Nobel Metal	Glycerol	-	250	1000	0.717
NCL catalyst	Glycerol	-	220	750	0.60
NCL catalyst	Glycerol	-	220	600	0.75

Non chromium nano catalyst for selective hydrogenolysis of glycerol to 1,2-PG

NCL also developed highly efficient non-chromium nano (Cu: Al) catalysts by the reduction of cubic spinel-type phases, and do not require any promoter for the glycerol hydrogenolysis. Fig. 3 shows TEM image of the activated Cu: Al nano catalyst as an aggregation of the metal particles the size of which was estimated to be ~10 nm (Fig. 3 a). Fig. 3(b) shows the diffraction planes (110), (111), (311), (204) which correspond to acicular CuO nano particles.

As per the expectation, our non chromium Cu: Al nano catalyst (7-11 nm, Fig. 3) exhibited > two fold activity as compared to the bulk Cu-Cr catalyst (>25 nm) with the highest selectivity of 91% to 1,2-PDO for aqueous phase hydrogenolysis of glycerol in a very short reaction time of 5 h.

The catalyst was characterized for its physico-chemical properties based on which the observed activity results have been discussed. Effect of various reaction parameters on conversion of glycerol and selectivity to 1,2-PDO has also been reported for the nanostructured Cu: Al catalyst.

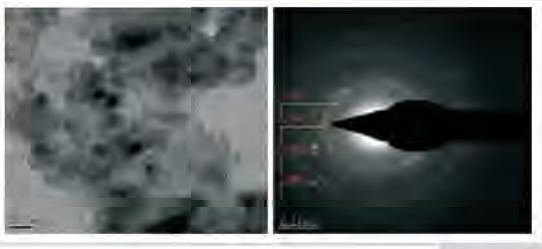

Fig 3: TEM of activated Cu:Al nano catalyst

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Conversion of cellulose and hemi-cellulose in to sugars and ethanol

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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 like 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 hemi-cellulosic fractions in to fermentable sugars by powerful cellulases and hemicellulase and their subsequent fermentation to ethanol by yeasts.

Penicillium strain isolated at NCL secretes complete cellulase and is selected as one of the lead enzymes. Preliminary studies on enzymatic hydrolysis of steam exploded bagasse and ethanol production by thermotolerant yeast at bench level resulted in maximum conversion of 63.9% (total cellulose hydrolysed) with a reducing sugar of 7.1% was obtained which was converted to ethanol (27g/L) with 75% efficiency.

Scale-up of enzymatic hydrolysis of steam exploded bagasse at 1kg level and ethanol production

Based on the earlier bench scale experiments, hydrolysis of steam exploded bagasse (SEB) the hydrolysis is scaled up to 1Kg level at 15% substrate concentration using *Penicillium cellulase* and finally conversion of sugar to ethanol by *S. cerevisiae*. Around 62.3% hydrolysis having 9.8% reducing sugar in the hydrolysate (by DNS method as glucose equivalents) was obtained in 24 h. The hydrolysate was used for ethanol production by *S. cerevesiae* which gave 3.7% (w/v) ethanol with 70% efficiency. Further Pilot scale studies are in progress.

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Conversion of cellulose and hemicellulose into sugars and ethanol

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- *Bioresources*, **2009**, 4,1669
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Ethanol is becoming a major commodity chemical because it is one of the important alternatives to petroleum based fuels. Ethanol is industrially produced mainly in Brazil from sugar cane and in USA from maize starch. In India, it is mainly produced from molasses which is the by-product of sugar industry. Despite its current success, the global impact of this manufacturing model is restricted by limits on the availability of the raw materials on one hand and maturity of the yeast fermentation technologies on other hand. If it is considered as an alternative to petroleum based fuels, we have to produce ethanol from renewable raw materials. Agricultural residues consisting of cellulose, hemicellulose and lignin are abundantly available in India. Pre-treatment of such biomass to produce an "open-structure" which can facilitate bacterial and enzyme interaction is a key method to facilitate the utilization of this biomass resource for producing fuels like ethanol.

In our laboratory experiments, we have generated several bagasse samples with decreasing content of lignin, which were used to produce cellulase with high productivities. These bagasse samples were also evaluated as a source for the production of sugars (glucose, xylose, arabinose) using enzymes that were produced by treating delignified bagasse samples with a mutant of *Penicillium janthinellum* NCIM 1171 obtained in our own laboratory. Our initial experiments gave very promising results in which we were able convert bagasse derived cellulose to lactic acid in high yield.

In order to develop a back-up to the development of enzyme technology for hydrolyzing biomass, we are also developing acid hydrolysis methods that would utilize cheap mineral acids which are not susceptible to presence of trace toxins that are inevitable present in biomass as well as pretreated biomass.

At NCL the following work was carried out
- Carried out acid hydrolysis of plain and pretreated sugarcane bagasse to produce sugars; the residual sugars are further hydrolyzed by low levels of enzymes.
- produced pretreated bagasse samples for use by various investigators (project participants from different institutions in India)
- Characterization / composition made by steam explosion and acid treatments.
- Preparation of bagasse hemicellulose
- Produced fully hydrolyzed hemicelluloses

Mutants were evaluated for cellulase production in Solid State Fermentation (SSF) and it was found that all mutants produced enhanced levels (3-5 fold) of FPA, CMCase, and xylanase than the parent strain during growth on wheat bran and pure cellulose. Mutants EMS-UV-8 and EU-2D-21 produced higher levels (150 IU/g DS & 155 IU/g DS respectively) of β-glucosidase. Steam Exploded Bagasse (SEB) also proved to be suitable substrate for cellulase production by mutant strains. Mutant EU-2D-21 produced highest FPA (70 IU/ g carbon source), CMCase (3710 IU/g carbon source), β-glucosidase (155 IU/g carbon source) when grown on 1g of pure cellulose and 4 g of wheat bran. Mutants EU1, EU2D14 and EU2D16 produced highest levels (approximately 4710 IU/g carbon source) of xylanase activity when grown on 2 g of SEB and 3 g of wheat bran. Only wheat bran or SEB did not give higher yields of cellulases. India is one of the largest sugar cane growing countries producing 200 million tons per year, which generate about 45 million tons of bagasse. Hence, we used SEB as the cheap source for production of cellulases which yielded cellulase activities comparable to the values obtained for pure cellulose. The comparison of cellulase activities produced by mutant EU2D21 in SSF with those reported in the literature demonstrated the superiority of the mutant to other fungal strains with respect to CMCase and β-glucosidase production.

Penicillium strain isolated at NCL secretes complete cellulase and is selected as one of the lead enzymes. Preliminary studies on enzymatic hydrolysis of steam exploded bagasse and ethanol production by thermotolerant yeast at bench level resulted in maximum conversion of 63.9% (total cellulose hydrolysed) with a reducing sugar of 7.1% was obtained which was converted to ethanol (27g/L) with 75% efficiency.

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Development of polymer electrolyte membrane fuel cell stacks for stationary applications

Objectives
- One of the major objectives this year is to initiate fabrication of PEM fuel cell stacks at NCL, in collaboration with CECRI and NPL.
- Development of new formulations for injection moldable bipolar plates.
- Up-scaling of batches of PBI membranes and comparative evaluation of in-house membranes with commercial ones.
- Casting of PBI membranes by phase inversion technique and synthesis of low viscosity PBI solutions to be used as binder in catalyst inks.
- Fabrication of larger sized MEAs out of Nafion membranes and their evaluation using H_2-O_2 as well as H_2-air.
- Incorporation of Decal process for MEA fabrication with PBI membranes.
- Single cell durability analysis

Work done and discussion

The aim of this project is to develop, in alliance with CECRI, Chennai, and NPL, New Delhi, various components necessary for fabrication of stacks. A summary of NCL activities focused on bipolar materials, membranes and electrocatalysts is given below.

Injection molded composite bipolar plates

The idea of introducing polymer-based bipolar plates with sufficient electrical and thermal conductivity was to counteract the highly acidic environment which prohibits the use of metallic bipolar plates. Additionally, these are light in weight and can be processed easily.

Molds of PP-graphite based composites (40 wt% PP and 60 wt% carbon) prepared earlier by injection molding gave inferior surface and through plane conductivities as compared to that of commercial plate (Schunk). Therefore, a new strategy had to be adopted as far as formulations and compounding methods were concerned. Micro-compounding experiments were carried out to arrive at a suitable formulation. Table 1 shows some of the results of the tests done.

It can be clearly seen from Table 1 that a dramatic decrease in resistivity takes place on increasing the carbon content (graphite + carbon black). The value for the mold containing 75 wt% carbon filler is close to the Schunk plate. Efforts are on to further increase the filler loading to ~ 80-85 wt%. Another strategy involves use of blend technique as blends have been found to show lower resistivities and percolation threshold as compared to individual components. Compounding of blends (PVDF/nylon and PES/nylon) have been carried out using compositions of 80/20, 60/40 and 40/60 at a temperature of 230 °C for PVDF and 345 °C for PES. SEM images of some of the blends are given below:

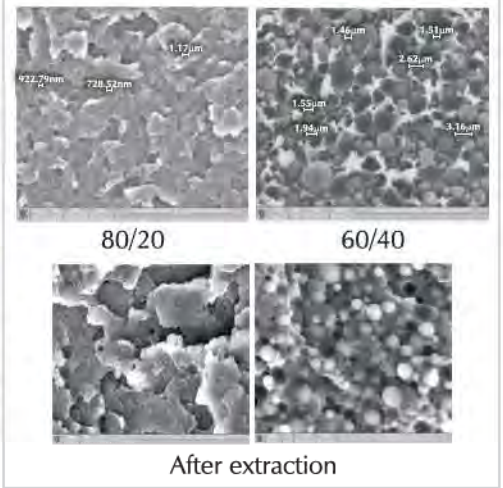

Fig. 1: SEM images of extracted PES (Gafone)/Nylon 6,12(Zytel)

Table 1. Change in resistivity values with increase in filler content

Composition	Resistivity (m ohm cm)
PP + 50 % (G+C)	4154
PP + 60 % (G+C)	432
PP + 75 % (G+C)	112
Schunk plate	19

Future plans include fine tuning of the filler content to bring down resistivity close to the

commercial value and exploration of metal injection molded bipolar plates

PBI membrane synthesis and evaluation and phase inversion technique of membrane casting

Regarding the membrane activities, failure mode analysis of PBI membranes was done by exposing them to open atmosphere for 30 days and analyzed for weight change. As can be seen in Figure 2, a sudden drop in weight was observed for the first few days owing to phosphoric acid leaching.

The weight of the exposed membranes seemed to stabilize after 10 days (240 hrs) and a negligible difference was seen at the end of 30 days. Also, an extensive comparative analysis of commercial membrane (from Celtec MEA) with in-house PBI membrane was carried out. Figure 3 shows the IR spectra of Celtec and in-house PBI-Iso membranes. It can be inferred from this graph that the Celtec PBI membrane is not so different from PBI-Iso membrane.

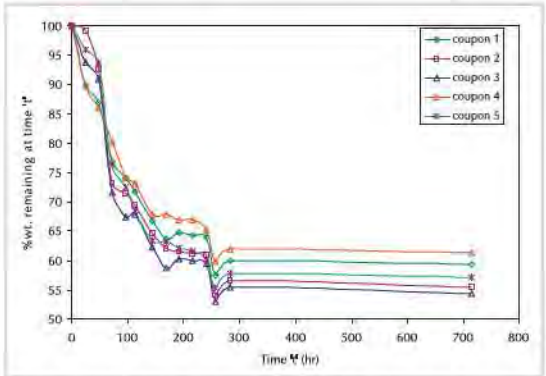

Fig. 2: Loss in weight of different coupons of membranes on exposure to open atmosphere

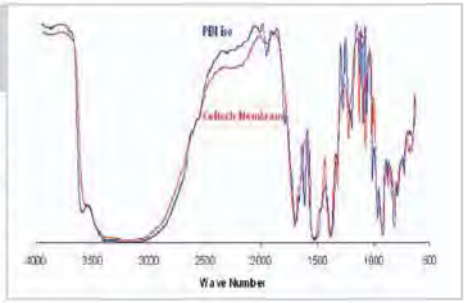

Fig. 3: IR spectra of Celtec and in-house PBI-Iso membranes

Mechanical property studies (stress-strain) also corroborate the assumption that the two membranes are quite similar.

Low viscosity PBI solutions to be used for catalyst ink preparation were made by varying monomer to acid and monomer to solvent ratios. Table 2 shows the different batches of low molecular weight PBI synthesized.

Table 2. Low molecular weight PBI prepared by varying DAB:PPA and DAB: acid ratio

Reaction code	Scale (g)	DAB : Acid ratio (g)	DAB : PPA ratio (g)	Yield (%)	Inh. Vis. (g/dl)
Bul3	10	1 : 0.5	1 : 30	-	0.89
Bul4	10	1 : 1.1	1 : 30	98	0.83
Bul5	10	1 : 1.1	1 : 50	80	0.52
Bul9	25	1 : 1.1	1 : 30	99	0.95
Bul10	25	1 : 1.1	1 : 50	85	0.66
I 24	10	1:1	1:40	97	0.95
I 25	10	1:1	1:50	96	0.76

It was found that PBI used for membrane making does not dissolve beyond 3 - 4 wt % in DMAc. Thus viscosity of the solution is too low for ink preparation. Further studies are being done for optimizing the viscosity. Phase inversion technique of membrane casting has certain advantages over the current process being employed at NCL (solution casting), the most prominent one being the number of days required to fabricate the membrane. A state diagram depicting the process is shown in figure 4.

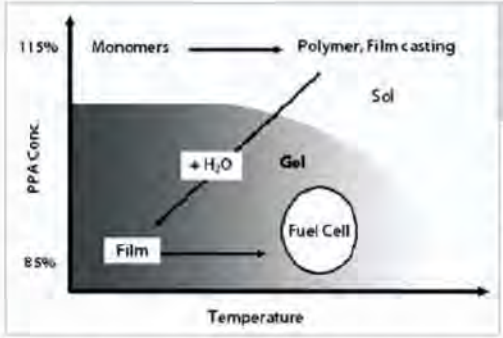

Fig. 4. State diagram illustrating the process of phase inversion.

Other benefits include higher doping levels, better consistency in properties and easier scale-up. However membranes prepared by this method give poor mechanical stability and certain other technical barriers are present which need to be overcome. Leaching issue could be solved by employing cross linking polymers and coating of MEA with a polymer.

Design and fabrication of humidity chamber and of a reactor (with jacketed vessel to maintain temperature during casting) seems to be the need of the hour for mitigating the issues related to phase inversion process. Thickness of membrane will determine the performance of a fuel cell substantially and so membranes of different thickness have been prepared and will be analyzed shortly.

MEA fabrication by decal process / brushing method and single cell evaluation

Failure mode analysis of 18 cell 350 W PBI-based stack was carried out two months after its demonstration at NCL by applying varying loads. MEAs from the failed cells (7th and13th) were pulled out and analyzed using SEM, EDAX and I-V characteristics of the MEAs were obtained. A good MEA (14th) was pulled out for comparison and polarization evaluation was carried out.

Figure 5 shows the variation in open circuit potentials in the cells 2 and 4 months after demonstration. An average loss of 27% was

observed within 2 months when the stack was stored at ambient conditions (dismantled once to remove the failed MEAs). EDAX clearly shows the presence of phosphoric acid (phosphorous and oxygen) on the membrane. Si peak is due to Si wafer which was used as a substrate to get a good SEM image.

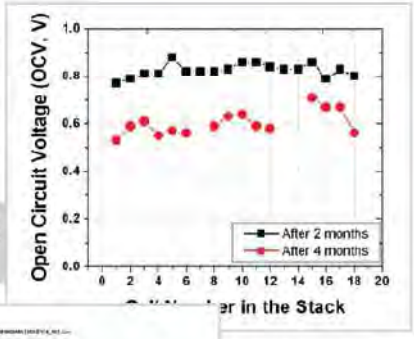

Fig. 5: Open circuit voltage variation in the cells.

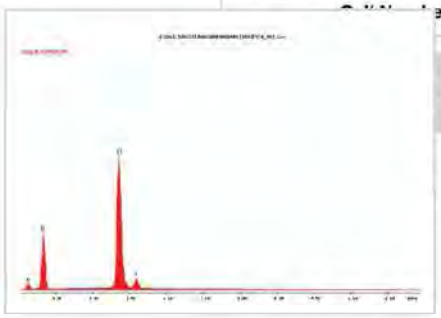

Fig. 6: EDAX of white deposits on MEA

Figures 7 and 8 show the polarization plots of MEAs (4 cm^2) from the 7th and 14th cell, respectively. MEA from the failed cell gave a better performance as compared to the 14th MEA. This method of failure mode analysis cannot be conclusive as there are several issues to be addressed such as atmospheric exposure of MEA, damage of membrane during catalyst removal, etc. A more feasible option could be single cell analysis of the entire MEA.

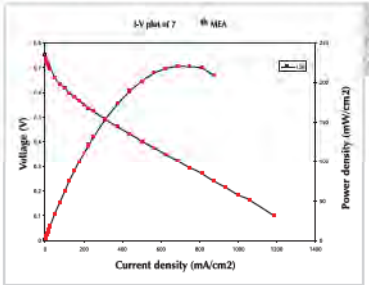

Fig. 7: Polarization plot of MEA from failed cell (7th)

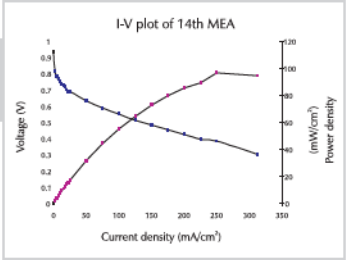

Fig. 8: Polarization plot of MEA from good cell (14th)

MEAs made by brushing method were subjected to durability tests by keeping them in open air / in desiccator for several hours/ days. Initially, a maximum power density of 870 mW/cm^2 (500mW/cm^2 @ 0.6 V) was obtained. After 6 days of storing MEA in desiccator, maximum power density dropped to 670 mW/cm^2 (~23% drop).

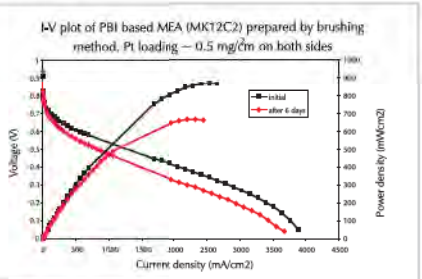

Fig.. 9: Comparative polarization plots of MEA prepared by brushing method, initial and

I-V plot of PBI based MEA (MK12C2) prepared by brushing method. Pt loading ~ 0.5 mg/cm^2 on both sides

I-V plot of PBI based MEA (MK12C2) prepared by decal method.Pt loading ~ 0.3 mg/cm^2 on both sides

MEA from the same batch of PBI membrane was prepared using decal process and tested. Hot pressing during catalyst transfer in decal process results in loss of phosphoric acid as well as mechanical stability of the membranes. Punctures were observed in the MEAs after polarization analysis.

MEAs having an active area of 50 cm^2 were prepared using both brushing and decal process. There were many roadblocks while increasing the area from 4 to 50 cm^2, such as poor contact, flooding, etc which led to a below average performance. These were overcome by adjusting the 'pinch' width between 50 and 100 μm,

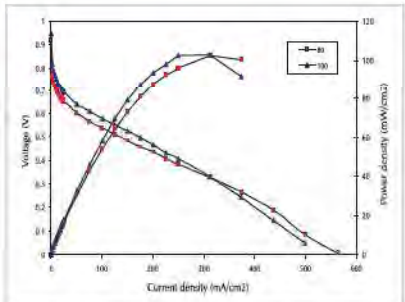

Fig.. 10: Polarization plot of MEA prepared by decal process

replacing conventional GDL by commercial one (SGL, PTFE content ~ 10%) and purging the cell with N_2 after each cycle. It was observed that MEAs having internal resistance > 50 mOhms gave a poor performance as compared to those having lesser resistance.

Figure 11 shows a comparison between MEAs prepared by decal and brushing methods. Pt loading for decal was maintained at around 0.4 mg/cm^2 on both sides. Maximum power density ~ 640 mW/cm^2 was obtained. Internal resistance was close to 23 mOhms. In case of brushing method, Pt loading was around 0.5 mg/cm^2 on both sides while a maximum power density of 560 mW/cm^2 was achieved. Internal resistance was found to be 40 mOhms.

A comparative analysis was carried out by switching the oxidant gas from pure oxygen to air. O2 and air flow rates were maintained at 0.32 slpm and 1.60 slpm, respectively. Pt loading was around 0.25 mg/cm^2 on both sides. Maximum power densities of 650 mW/cm^2 and 265 mW/cm^2 were obtained respectively. As can be seen from figure 12, a drop in performance of more than 50% occurred on changing the oxidant gas. Internal resistance was found to be close to 7 mOhms. More analysis needs to be done regarding the flooding problem.

Stack fabrication at NCL

One of the major developments in this project this year has been the decision to initiate stack fabrication at NCL. For this purpose, a team comprising of engineers from NCL was sent to CECRI for a hands-on training on stack fabrication. SOPs for fabrication of various components have been circulated and procurement of materials required has been started

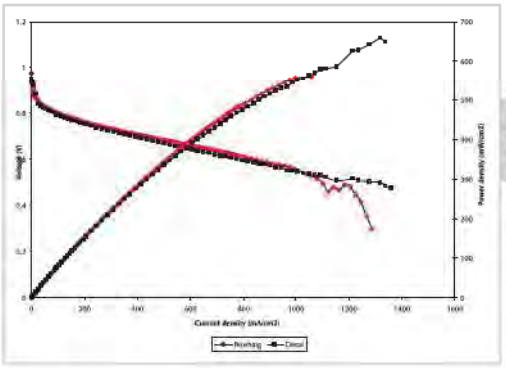

Fig.11: Comparison of larger sized MEAs (50 cm^2) prepared by decal (black) and brushing (red) methods

Conclusion

During 2009-2010, NCL in collaboration with CECRI and NPL has made tremendous progress in the development of components required for stack fabrication, which to date remains the key objective of this project. For example, new formulations have been devised for composite bipolar plates which show values enticingly close to that of the commercial plates (Schunk). Also, PBI membranes prepared by phase inversion process show some promising results and by fine tuning the doping levels and ultimately the mechanical properties, a fine method could be employed for membrane casting within a few days.

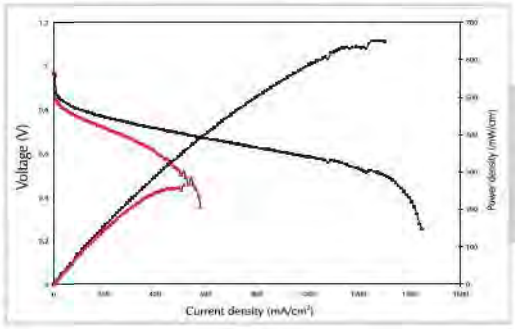

Fig. 12: Polarization evaluation of MEA prepared by decal process (N212, active area ~ 50 cm2) using pure oxygen (black) and air (red).

Decal process for larger sized MEAs (Nafion-based) has been optimized. Further studies need to be carried out to achieve better performances using both O_2 and air as oxidant gas. Further R&D needed as far as preparation and evaluation of PBI-based MEAs by decal process is concerned. Future plans include optimization of decal process employing Pt-Ru as catalyst and use of reformate gas to study the effect of CO poisoning. The decision to fabricate stacks at NCL has been taken up as a challenge and with all the participating members working hand in hand to fulfill the different requirements, one sincerely hopes that the outcome will be a fruitful one.

Joint Reserch INITIATIVES NCL-IGIB

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Chemical engineering/ modeling and analysis of biological systems

Background / objectives

Drosophila is a genus of small flies often called 'fruit flies'. In the natural habitat, embryo development does not occur under constant environmental conditions. However, existing mathematical models for pattern formation during development do not account for the effect of transient changes in the environment, though they do capture the effect of permanent changes either in the environment (e.g. temperature shift) or at the genetic level (e.g. mutations). The objective is to use mathematical modeling and analysis to assess the robustness of the biological system to such transient changes.

Work done and discussion

As part of a DST-funded project on stochastic analysis of biological networks, we are studying the effects of fluctuations either due to environmental changes, or due to stochasticity in the intracellular reactions.

In the context of Drosophila patterning, we have presented a way to analyze pattern formation in an environment with transient perturbations. We modified an existing Boolean model for the segment polarity network to incorporate temporary errors in the rules that define transitions between states. We found that the pattern was remarkably robust to transient changes, with 66% of such perturbations in one node resulting in a normal pattern.

Our simulations suggest that the network is more fragile when the perturbation results in the activation of a normally dormant gene, and is robust to temporary inactivation of normally active genes. Gene expression is known to occur in bursts, so this result is to be expected, as otherwise the natural change in gene expression levels will result in an abnormal pattern.

In nature, perturbations such as a temporary change in temperature (for instance 'heat shock') affect the entire network, and upon withdrawal of the perturbation, the pattern is reestablished.

Our model simulations captured this finding, and in addition identified the pathways involved. Simulations also revealed that if this heat shock is applied locally (i.e. only to a few cells but not the whole parasegment), the effect is lethal. Our work thus led to the nonintuitive finding that a local perturbation may be more deleterious than a global change, a prediction that is experimentally falsifiable using microfluidics or other methods.

We believe that this study is an example of the use of mathematical modeling to provide insight into the functioning of a particular biological system, to generate testable hypotheses, and to study biological robustness.

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Re-engineering discontinued drug molecules for use in novel applications and understanding drug toxicity by proteomic approaches

Many FDA approved drugs as well as several lead molecules in drug development program have to be dropped for their unsatisfactory performance in toxicity studies. This project aims to study such molecules to understand the molecular mechanism of toxicity and identify novel uses of the drug using mass spectrometric and proteomic approaches. The main aim of this proposal is to revisit such important cases and reorient their structure or biological activity for a different application.

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.

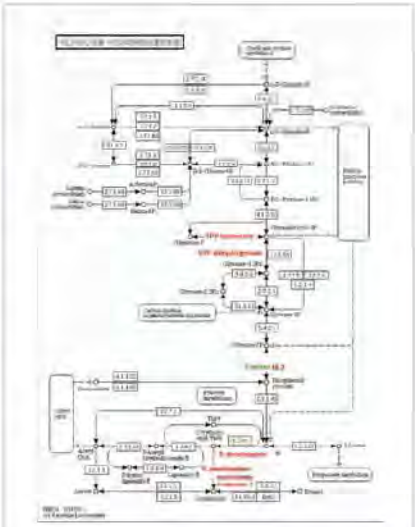
Objectives
- To identify drug interacting proteins by affinity purification and mass spectrometry
- To identify drug regulated proteins by two dimensional electrophoresis and mass spectrometry
- To study the pathway or process of drug binding or drug regulated proteins for identifying new uses
- To develop strategies of methods to study drug protein interactions

Chemical and comparative proteomic approaches reveal gatifloxacin deregulates enzymes involved in glucose metabolism

The main aim of this proposal is to revisit with drawn drug and their molecular mechanism of toxicity. One such example is gatifloxacin, the fourth generation fluoroquinolone antibacterial, was withdrawn from the US market as it shows acute hypoglycemic and chronic hyperglycemic side effects. The acute hypoglycemic effect is believed to be due to increased insulin secretion triggered by inhibition of ATP dependent potassium channel in the beta cells of pancreas. Conversely, gatifloxacin induced chronic hyperglycemic effect is due to the down regulation effect of Glucose Transporter 1(GLUT1) expression. However, the exact molecular mechanism of chronic hyperglycemic effects in human beings is not well understood. In this study we have attempted to understand the mechanism of gatifloxacin induced deregulation of glucose metabolism using yeast as a model system by combination of chemical and comparative proteomic approaches.

Differential expression studies reveal that gatifloxacin deregulates the expression of core, key regulatory enzymes of glucose metabolism, especially enzymes from the glycolysis pathway (Fig). In order to explain the mechanism of differential expression of proteins, we performed affinity chromatography and identified interacting proteins of gatifloxacin.

The sequencing of tryptic peptides of eluate by tandem mass spectrometry resulted in identification of sequences corresponding to ATP dependent helicase, GCR1, and golgin. It was interesting to find out ATP depenent RNA helicase and GCR1 as gatifloxacin binding proteins. The diffential regulation of glycolytic enzymes and dyglycemic effect of gatifloxacin in human beings could via interaction with GCR1.



Gatifloxacin regulated proteins

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Development of planar chromatography platform for proteomics

Background / objectives

Comprehensive analysis of complex biological samples such as a proteome is challenging. 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.

Existing gel-based (SDS PAGE) and column-based (HPLC) have limitations leaving scope for simpler, quicker and more efficient tools. Liquid chromatography in a planar format has several advantages and can be developed into an efficient tool for proteomics separations.

The long-term aim of this work is to develop planar chromatography platform that could enable 'high throughput' and 'minimal sample preparation' methodologies for bioanalysis including 'bottom up' proteomics and metabolomics. The methods that are being developed at NCL using materials and surface-based approaches would be put to test for the analysis of challenging biological samples.

Work done and discussion

The primary endeavor in developing newer materials in a planar format is to obtain robust surfaces on which peptide separations can be performed. Monolithic thin films are a better option than the commercially available TLC surfaces in which silica or modified silica particles of varying sizes are adhered to planar surfaces such as glass resulting in a thick film (about 250 microns).

We have attempted to synthesize structured mesoporous inorganic materials on surfaces. Robust thin films of mesoporous silica on glass surface were obtained. Preliminary characterization of these materials was performed using XRD, SEM, TEM and BET analysis. Porosity and film architecture obtained were comparable to those reported in published literature (data not shown here).

The ultimate endeavor after separation from a planar surface would be direct 'offline' analysis of the separate analytes. Laser desorption and ionization mass spectrometry (LDI MS) is a popular and an efficient tool for mass analysis of proteins and peptides. LDI MS in combination with a planar separation dimension offers a viable alternative to existing separation-cum-mass detection platforms with the added advantage of high throughput and minimal sample preparation.

The dynamic range accessed by such a system would also be substantial. Without the matrix, the 1-500 mass zone that has peaks from conventional organic matrices in MALDI TOF MS is freed up (fig. 1) as compared to a conventional matrix, 2,5-dihydroxybenzoic acid (DHB). With this method smaller molecules can now be analyzed in addition to peptides using the LDI TOF MS. Standards of several biologically relevant small molecules have been analyzed and compared with the MS using conventional MALDI TOF MS.

Figure 2 illustrates the mass spectra of amino acids L-threonine and L-glutamic acid along with commercially available peptide mass standards angiotensin, P14R, ACTH fragment and insulin chain B using titania surface supported LDI. In addition to the protonated M+H peak, sodium and potassium adducts of the analytes is also seen. Several other amino

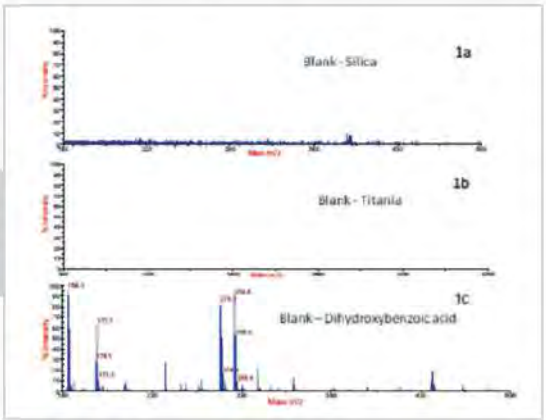

Fig. 1: LDI MS using the silica (a) and titania (b) as compared to a conventional matrix, 2, 5 dihydroxybenzoic acid (c, DHB).

acids and peptides were analyzed using this method yielding mass spectra with high mass accuracy and at sensitivity as low as pico mole quantities of the amino acids. LDI MS of -casein digest resulted in sodiated peaks for the peptides that were detected using conventional MALDI using α-CHCA as matrix. Interestingly, LDI MS of α-casein digest enables the detection of several smaller peptides that were not detected using MALDI MS (Table 1).

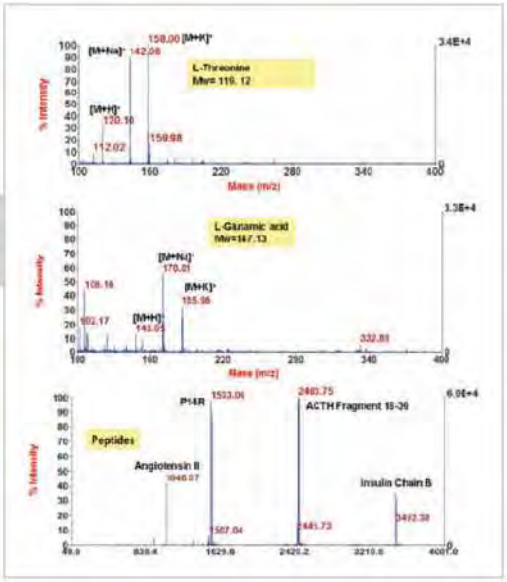

Fig 2: LDI MS of amino acids L-threonine, L-glutamic acid and peptide mass standards (proteomass MALDI MS standards), angiotensin, P14R, ACTH fragment and insulin chain B using

Table1: Comparison of peptide peaks detected using LDI-MS and MALDI-MS of ?-casein digest. LDI MS results in the detection of smaller peptides that MALDI MS failed to resolve.

Sr. No.	Peptide Sequence	LDI-MS	MALDI-MS
1	EPMIGVNQELAYFYPELFR	---	$[M+H]^+$
2	DIGSESTEDQAMEDIK	$[M+Na]^+$	---
3	HQGLPQEVLNENLLR	$[M+Na]^+$	$[M+H]^+$
4	FFVAPFPEVFGK	$[M+Na]^+$	$[M+H]^+$
5	YLGYLEQLLR	$[M+Na]^+$	$[M+H]^+$
6	EKVNELSK	---	$[M+H]^+$
7	EDVPSER	$[M+Na]^+$	$[M+H]^+$
8	VNELSK	$[M+Na]^+$	---
9	LHSMK	$[M+Na]^+$	---
10	HIQK	$[M+Na]^+$	---

LDI-MS was performed using sol-gel Titania
MALDI-MS was performed using 2-cyano-4-hydroxy cinnamic acid

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De Novo designed peptidomimetic scaffolds for disrupting protein-protein / cell membrane interactions

Background / objectives

This project is aimed at developing peptidomimetic scaffolds for disrupting protein-protein / cell membrane interactions. At NCL, our group is involved in the design, synthesis and conformational investigations, both in solid- and solution-state, of novel conformationally constrained peptidomimetic scaffolds such as reverse-turns, hairpins and helices. Scaffolds developed at NCL would be incorporated into peptide sequences at IGIB for obtaining novel biologically active lead molecules - with a particular emphasis on ACE peptides / sequences.

Work done and discussion

Development of novel reverse turn mimetic based on the Ant-Pro motif

Reverse turns, defined as sites where a peptide chain reverses its overall direction, are common motifs in protein structures. Reverse turns are generally categorized as γ-turn, β-turn, α-turn, and π-turn, which are formed by three-, four-, five-, and six-amino-acid residues, respectively. According to the folding mode and backbone dihedral angles, each of such turns can be further classified into several different sub-types. Reverse turns play an important role in globular proteins from both the structural and functional points of view. There is growing evidence that peptide-activated GPCRs (G protein-coupled receptors) recognize turn conformations as evidenced by structure-activity relationships in their native ligands, and modified peptide fragments. Being conformationally flexible, native peptide ligands for GPCRs provide limited clues to the design of nonpeptidic ligands useful for drug development, because they tend to bind in different ways to, or at different sites on, a GPCR. Therefore, there is ever-increasing demand for the development of novel conformationally rigid synthetic "turn" mimetics with possibilities for extensive periphery modification which might be useful in the reverse-turn-based pharmacophore design that has become a central topic in medicinal chemistry in recent years.

A general approach to the synthesis of peptidomimetic compounds involves the use of non-peptide building blocks, which enforce or stabilize a particular type of beta-turn, when inserted into a peptide chain. We have extensively investigated the possibility of using Ant-Pro motif which we reported recently *(Sanjayan et al: J. Am. Chem. Soc. 2008, 130, 17743.)* as a robust reverse turn mimetic. Several crystal structures have been solved to learn insights into the reverse turn formation by

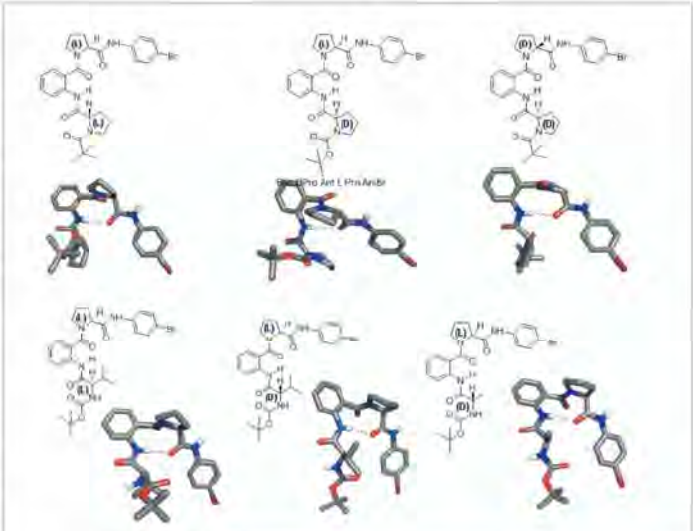

Fig. 1: Molecular and corresponding crystal structures of reverse turns featuring the robust Ant-Pro motif

Ant-Pro motif. It is being concluded based on extensive crystal structure and solution-state NMR investigations that the reverse turns formed from Ant-Pro motif are stable and insensitive to structural perturbations in and around the delicate turn segment.

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Biocatalysis and biosynthesis

Background / objectives

The attempt to create a NCL-IGIB joint research initiative is an unique endeavor where scientists from disciplines come together and exchange knowledge and expertise while working towards achieving common scientific goals. Biology and chemistry are two complementary areas of science where the insight gained from one is useful in the context of the other.

The principal goal of this joint research initiative (JRI) is to blend the knowledge and competence of biology and chemistry which form the core expertise areas of the two Institutes and to forge seamless cooperation at the interface of disciplines.

With the advent of the new era in biology in the post genome-sequencing period, it is being increasingly appreciated that fundamental discoveries in modern biology would not only require interdisciplinary cross-talk but also the right blend of knowledge generated from other disciplines like chemistry. It is, therefore, necessary to create a seamless team of scientists at the interface areas of chemistry and biology.

Institute of Genomics and Integrative Biology, Delhi (IGIB) has successfully demonstrated its research strength in the field of genomics, proteomics and bioinformatics and is emerging as a hub of cross-disciplinary research with chemists, computer scientists, doctors and engineers joining hands with biologists in generating a dynamic research environment.

On the other hand, NCL has strong expertise in synthetic organic chemistry of drug intermediates, bioorganic chemistry combinatorial synthesis and polymer chemistry. The primary objective of the proposed JRI is to build synergy between NCL and IGIB to work in the interface areas of chemistry and biology. The joint research initiative also will bring together on a common platform young scientists from both NCL and IGIB to stimulate new ideas and create new knowledge.

Researchers at the joint center would like to pursue collaboration in the following areas at the chemistry-biology frontier

1. Development of Chemchips for protein inhibitors and aptamers for diagnostics.
2. Development of peptide scaffolds: Identification, chemistry and biological applications.
3. Nanomaterials for biology : structure-function studies for potential applications in targeted delivery of therapeutics
4. Steroid-Peptide Scaffolds, Steroidal Dendrimers and Their Biological Evaluation
5. Re-engineering discontinued drug molecules for use in new and appropriate applications.
6. Design and Development of α and β Amino Acid Oligomers as Directive Back Bones for Low-/Multivalent Ligand Arrays: Probing the Protein-Protein, Protein-Carbohydrate Interactions
7. De Novo Designed Peptidomimetic Scaffolds for Disrupting Protein-Protein / Cell Membrane Interactions.
8. Biocatalysis: Screening and Utilization of Biocatalysts for the Useful Transformation to Produce Biologically Important Molecules or to Produce Chiral Intermediates
9. Planar chromatography for 'Bottom up' Proteomics
10. Pathway-scale analysis of biological processes

Screening and utilization of nitrilases, lipases, and oxido-reductases for the useful transformation to produce biologically important molecules or to produce chiral intermediates

Screening of nitrilase producers

More than 500 bacteria were isolated from various habitats using five different media. About 300 bacterial strains were screened for nitrilase activity by test tube assay. Ten nitrilase producing bacteria were isolated. Out of these, five nitrilase producers were identified by 16S rRNA gene sequencing. Identified bacteria belong to *Bacillus spp*. (3), *Clavibacter* sp. (1) and *Acinetobacter* sp. *Clavibacter* sp. and *Acinetobacter* sp. are not reported earlier for nitrilase activity. Identified cultures will be evaluated for their substrate specificity and enantio-selectivity analysis.

While screening the microorganisms for nitrilase activity, we found that several fungal strains (such as *Mucor piriformis*, THV1, A. niger, etc.) could able to carry out efficiently the hydroxylation/reduction of carbonyl group on the substrates which have multiple functional

JOINT RESERCH Initiatives NCL-IGIB

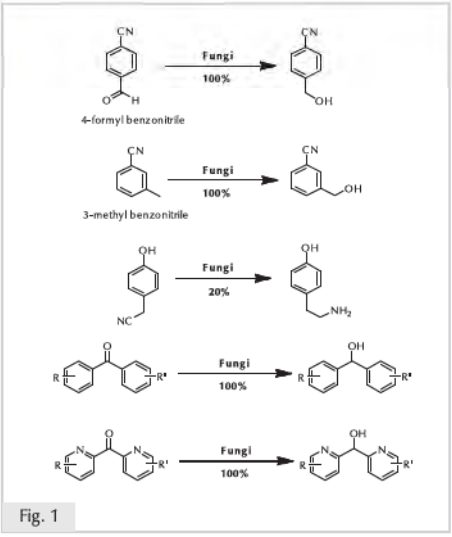


Fig. 1

groups (Fig. 1). The work is currently progressing towards the characterization of metabolites.

Cloning and expression of putative nitrilase genes

Based on literature and in-silico analysis 8 putative nitrilase genes were identified from *Mycobacterium semgmatis* genome. Primers were designed to clone and overexpress them in *E. coli* under T7 promoter with histidyl tag. All the genes were PCR amplified and cloned successfully. Cloned fragments were sequence to find out any PCR errors.

Out of the 6 genes completely sequenced, 3 had no mutation, 2 had one mutation each and 1 clone had three mutations. All the clones were transformed in expression host BL21de and expression was checked by induction with various concentrations of IPTG 7 clones. Five proteins were expressed as inclusion bodies but two proteins did not express.

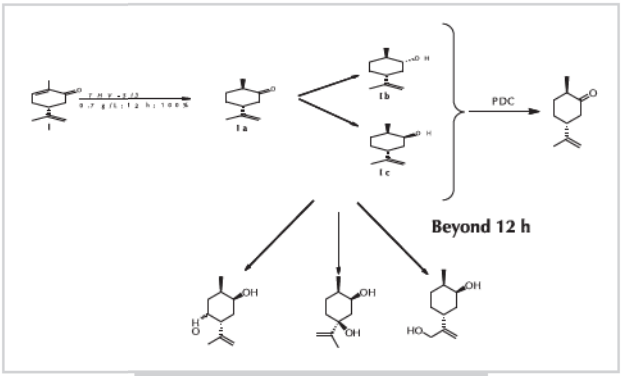
Expression is being optimized by changing various conditions to obtain soluble protein in five clones. In expression host *E. coli* C41de, small proportion of expressed protein for Msm3555 was obtained as soluble protein.

The soluble protein is being purified by Ni-NTA affinity chromatography.

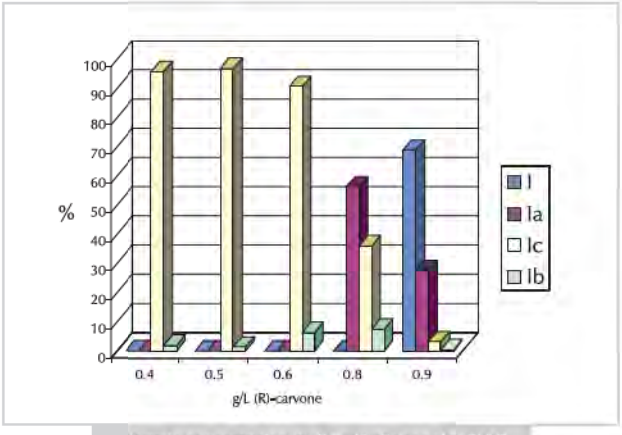
The purified enzymes will be tested for their substrate specificity and enantio-selectivity.

We have screened several microorganisms (Isolated and from culture collection) for Oxido-reductase activity. We found that several fungal str

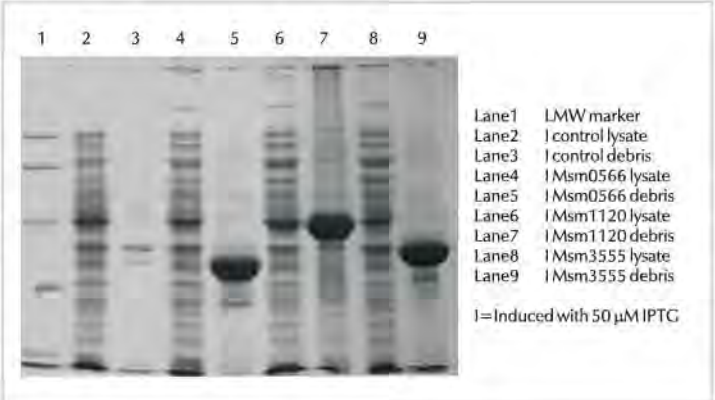
ains are capable to bring about the stereo- and regiospecific hydroxylation on isoprenoids in specific terpenoids and steroids. The soil isolated versatile fungal strains, *Mucor piriformis*, *THV-S13*, and several other fungal strains could able to reduce the double bond in carvones in stereo-specific manner with quantitative yields.



Biotransformation of (R)-Carvone by fungi



Substrate concentration studies- (*R*)-Carvone by *THV3*



Joint Research INITIATIVES NCL-IGCAR

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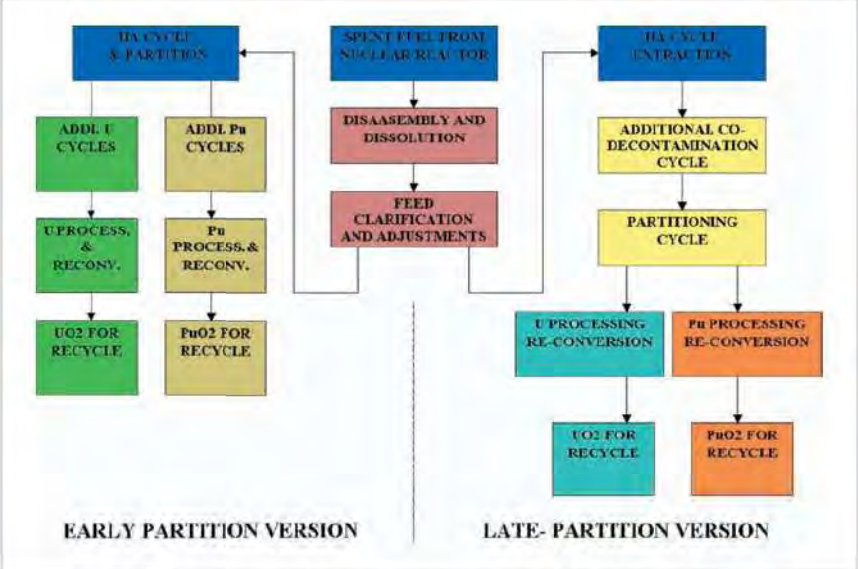
Non-ideal behaviour of aqueous ionic species in nuclear solvent extraction systems

A detailed investigation of non ideality in aqueous ionic systems of high ionic strength that is an integral part of nuclear solvent extraction has been an objective of the collaborative project. PUREX process is an efficient methodology for the nuclear solvent extraction (Scheme 1).

Thermodynamic equations based upon the specific ion - interaction theory for the mixed ionic systems of high ionic strengths were developed. The mixing of ions with symmetry and non-symmetry were decomposed into electrical and non-electrical terms.

The equations can successfully account for the vapor pressures, activity coefficients and thermal effects of the highly non-ideal solutions.



Scheme 1: A Schematic representation of PUREX Process

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Development of high temperature proton conducting solid polymer electrolyte based hydrogen sensor

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Interest in hydrogen gas sensing has rapidly increased, because hydrogen gas is renewable, abundant and efficient and unlike other alternative fuels, provides zero emission. The product of hydrogen combustion is water, making it the most environmentally friendly fuel. Hydrogen is a promising potential fuel for vehicles, so public transport fueled by hydrogen is very likely in near future. Hydrogen can also be used as a fuel in conventional combustion engine and fuel cells. However, if handled carelessly, hydrogen is dangerous for transport, storage and uses as many other fuels.

As a result, safety remains a top priority in all the aspects of hydrogen energy and sensing hydrogen leakages of storage and transportation equipment has become very essential. Although different types of sensors are currently investigated, most of them show poor response in sensing low hydrogen concentrations; therefore there is a need to develop sensor devices with very high sensitivity and selectivity towards hydrogen, especially at or near room temperature.

The objectives of this study are:

- To explore in identifying and developing new routes for synthesizing novel substituted monomers for synthesis of polymeric membranes used for hydrogen sensing in nuclear reactor applications.
- To provide a cost-effective laboratory scale process for the production of monomers and polymers such as polybenzimidazoles, ploymides and polytriazoles
- Casting, doping and evaluation of these materials for proton conductivity measurements for applications in nuclear reactor technology.
- Standardize the technology for making the membrane electrode assembly (MEA) by deposition of electrocatalysts on the characterized high temperature proton conducting electrolyte.
- Standardization of the configuration of a hydrogen sensor. using the MEA for optimal response behavior.

The proton conducting polymers

The main requirement for proton conducting polymers are: They must be chemically and thermodynamically stable and they should form a thin film. Also they should fulfill sufficient ionic conductivity with proton transport number close to unity. If proton conducting electrolytes possess all these requirements, then the advantages of proton polymeric electrolytes over other systems include preparation of thin films using these polymers with wide thermal stability.

The conductivity exceeds 10^{-5}S/cm at ambient temperatures and also they are compatible with electrode material. In view of these parameters, the more suitable conducting solid electrolyte polymers (SEP) include PVA/H_3PO_4 blend and acid doped polybenzimidazole (PBI) 1 and polytriazoles 2 (Fig. 1).

As per the objectives of the proposal, our role is to explore in identifying and developing new routes for synthesizing novel substituted monomers for the synthesis of polymeric membranes useful for hydrogen sensing in nuclear reactor applications. Thus, synthesis of PBI analogues and polytriazoles were undertaken and the polymeric membranes prepared from these monomers and supplied them to IGCAR for evaluation of these materials for proton conductivity measurements. We have carried out several experiments in this regard including few important results; the details of which are presented in this report.

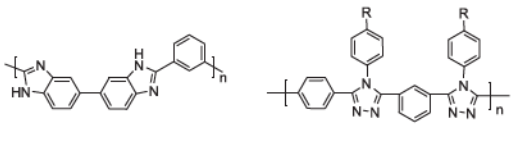


Fig 1 : PBI and Polytriazoles

Synthesis of Polybenzimidazole

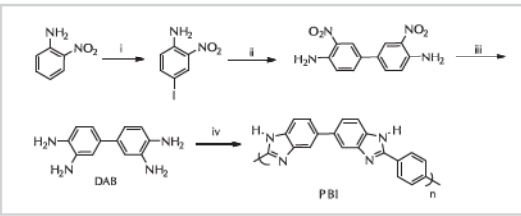
Polybenzimidazoles(PBI) are a class of linear polymers whose repeat unit contains a benzimidazole moiety. As polymer of high temperature stability, non inflammability and electrical conductance, it finds application in fuel cells, hydrogen sensors and other devices as polymer electrolyte. In order to enhance the

proton conduction and stability of polybenzimidazole, we have planned to synthesize substituted moieties of PBI, by introducing different functionalities like Br, CH_3, SO_3H, COOH etc in PBI, which will be helpful in increasing the proton transport.

In these transformations, two components consisting of diaminobenzidine (DAB), a tetramine and diacids condense to form substituted polybenzimidazole. The substituents can be introduced either in tetramine, diacid or in both of them We have prepared polybenzimidazoles using our own procedure reported recently by us. The synthetic strategy is as follows: 3,3'-DAB was condensed with terephthalic acid **(Scheme1).**

Synthesis of Diaminobenzidine

The synthesis of DAB was done with the NCL route developed by us. For the synthesis of DAB, palladium catalyzed Ullmann type of homocoupling of substituted 4-halo-2-nitroaniline has been employed as the key step. Scheme 2 shows the synthetic route envisaged for DAB molecule.



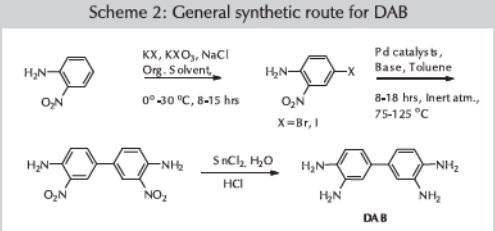
Scheme 1: Reaction conditions i KIO_3, KI, NaCl, AcOH, RT, 7 h, 98%. ii water soluble palladium complex, Et_3N, toluene, 110 °C, 89% iii $SnCl_2.2H_2O$, conc. HCl, 50 °C, 2 h, 73% iv terephthalic acid, PPA, 120 to 220 °C, 19 h.

The first step of the entire process involves regioselective mono halogenation of 2-nitroaniline using KIO_3/KX/NaCl, which is milder and not extremely exothermic. The mono iodination of 2-nitroaniline was successfully scaled up to afford multigram quantities (up to 200 g) of 4-iodo-2-nitroaniline. The mono iodination was achieved in 98% isolated yield using this method.

After the simple filtration, the palladium complex present in the toluene is once again used for the homo coupling of 4-halo-2-nitroaniline (X= I or Br) and it was found that the catalyst was quite active for the subsequent batches of coupling reaction.

The last step involved the reduction of the nitro group which was carried out using NaOH/ $SnCl_2$/conc. HCl strictly following the reported procedure. Eventually, the crude DAB was recrystallized from water and its pure form is colorless and sharply melts at 179.9 °C from DSC. Thus, the synthesized DAB had high purity of 99.65 % as determined from HPLC analysis.

Scheme 2: General synthetic route for DAB

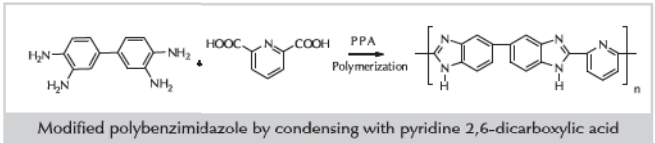


Synthesis of modified PBI

We have synthesized several analogs of PBI using our own procedure as reported recently by us. The procedure involves condensation of diaminobenzidine with different type of aromatic/ heteroaromatic dicarboxylic acids. The polymers thus obtained were cast into their corresponding films/membranes.

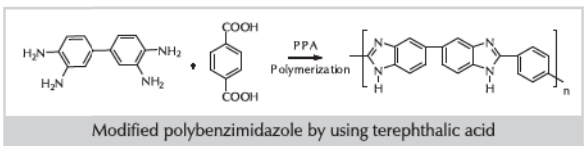
Synthesis of pyridine- based polybenzimidazole

Synthesis of terephthalic acid based polybenzimidazole



Modified polybenzimidazole by condensing with pyridine 2,6-dicarboxylic acid

Synthesis of 5-sulpho-1,3-isophthalic acid based polybe



Modified polybenzimidazole by using terephthalic acid

nzimidazole

Polymer film (PBI membrane) casting

Film samples with controlled thickness (2 mil) were obtained by casting the above dope solutions on a clean and dried glass plate using a Gardener knife. A laboratory vacuum oven set at 140°C and purged with dry air was used to remove most NMP solvent from the cast film.

Each newly cast film was dried in the oven for 20 min, cooled to room temperature for 20 min, and finally soaked in a water bath at ambient temperature. After soaking for 30 min, the films could be easily peeled off from the glass plate with the use of a razor blade.

These films were immediately analyzed, and it was found that NMP contents dropped from 13% for PBI/PA (100/0) to 4% for PBI/PA (0/100) following a linear relationship with the PA content.

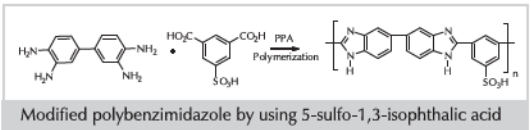
Synthesis of Vinyl triazole

The general synthetic route for a new vinyl triazole-based polymer is presented in Scheme given below. Various alkyl halides 1 were transformed into alkyl azides 2 in high yields by simple SN^2 displacement. Then, [3+2] cycloaddition reaction of alkyl azides with homopropargyl alcohol resulted in the formation of triazoles 3 in good yields.

Alcohol moiety in 3 was then transformed into the corresponding mesylates 4 and its elimination gave vinyl triazoles 5 in high yields. Further studies of polymerization of vinyl triazole were carried out although the inherent viscosity (IV) of triazole polymers was found to be in the range of 0.6 - 0.8 dL/g.

Polymerization of vinyl triazole

A single neck round bottomed flask was charged with 2-(1-octyl-1H-1, 2, 3, triazole-4-yl) (0.5 g) and AIBN (0.1g) in dry benzene (2ml) and the reaction mixture was purged with nitrogen. The reaction mixture was



Modified polybenzimidazole by using 5-sulfo-1,3-isophthalic acid

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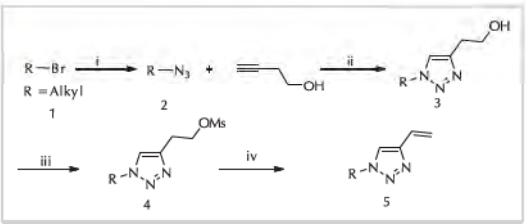
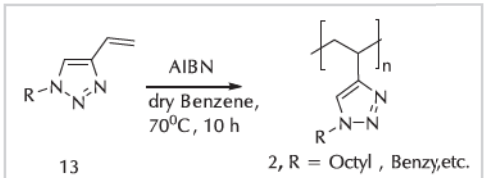


i DMF, NaN_3, 80 °C; ii Na L-ascorbate, $CuSO_4$, t-butanol; iii MsCl, Et_3N, 0 °C; iv t-BuOK, 18-crown-6, t-BuOH 50 °C.

refluxed for 10h at 70°C under nitrogen atmosphere.

The viscous mass was then poured into water to get polytriazole polymer (Scheme); Yield: 0.6 g. In the same way other PTs were prepared by taking suitable alkyl bromides



Scheme: Synthesis of polytriazole (PT)

Casting of polyvinyl triazole (PT) membrane

Polymer Polyvinyl triazole was dissolved in N, N'-dimethylacetamide (DMAc) in inert atmosphere. The reacton mixture stirred at 90 °C for 12 hrs. till we get the clear homogeneous polymer solution. The homogeneous solution obtained was subsequently used to cast the membranes.

In order to cast films, 5 wt. % polyvinyl triazole solutions in DMAc were spread onto a glass plate. The plate was next introduced inside an oven where a temperature ramp from 50 to 190 °C was programmed in order to evaporate slowly the solvents for 12 h. Once this time elapsed, the plate was immersed in DI water in order to detach the membrane from the plate. The membrane was boiled in DI water during the following 2 days in order to remove traces of solvent.

The polymeric membranes (35 numbers) made from PBI and Polytriazole were sent to IGCAR for hydrogen sensing activity studies.

Synthesis of TEHDGA and DMDOHEMA

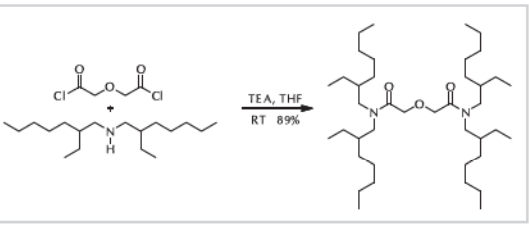
Research towards nuclear waste processing aims at separating long lived radionuclides, specially the trivalent actinide ions, An^{3+}, from trivalent lanthanide ions, Ln^{3+}, by solvent extraction.

In view of relatively long half-life of trivalent actinide elements, it is of great interest to separate them from nitric aqueous solutions in order to obviate the manipulation of effluents or waste having a high α-activity.

This separation is usually carried out by solvent extraction using neutral or acid organophosphorous compounds like tri-n-octyl phosphine oxide (TOPO) and carbamoyl methyl phosphine oxide (CMPO). However, the use of such extractants has not proved to be particularly advantageo us, because their extraction yield with respect to trivalent ions is low and their industrial use leads to numerous problems due to the necessity of using large amounts of salting agents, which increase the volume of the waste and the processing costs.

In this connection, N,N,N',N'-tetrakis-(2-ethyl-1-hexyal)-3-oxapentane-1,5-diamide (TEHGDA) and N,N'-dimethyl-N,N'-dioctylhexylethoxymalonamide (DMDOHEMA) are found to be excellent single extractants for this purpose.

To study and develop laboratory scale process for the preparation of N,N,N',N'-tetrakis-(2-ethyl-1-hexyal)-3-oxapentane-1,5-diamide (TEHGDA) and N,N'-dimethyl-N,N'-dioctylhexylethoxy malonamide (DMDOHEMA).



Scheme I) Synthesis of N,N,N'N'-tetrakis-(2-ethyl-1-hexyl)-3-oxapentane-1,5-diamide TEHGDA)

Synthesis of TEHDGA.

The tetraalkyl-diglycolamide were synthesized by reaction of diglycolyl chloride with bis (2-ethyl-1-hexyl) amine and triethylamine in tetrahydrofuran (THF). All chemicals were purchased from Aldrich and used as received, except for the triethylamine that was freshly distilled from calcium hydride before use. All water was deionized using a commercial purification system.

All glassware was oven-dried prior to use and the reaction was carried out at 23°C. A positive-pressure inert atmosphere of nitrogen was maintained with a latex balloon and the reaction mixture was stirred magnetically. Reactions on a larger scale required mechanical stirring because of the large amount of triethylammonium chloride precipitate that formed.

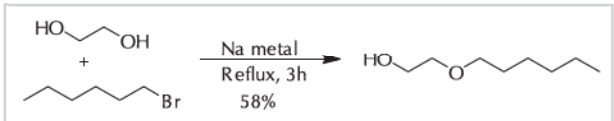
The purified final product was characterized by 1H NMR and 13CNMR and CHN analysis. The 1H NMR characterization was performed on a 200 MHz NMR spectrometer. Chemical shift values are reported relative to an internal trimethylsilane (TMS) standard.

Synthesis of DMDOHEMA

Synthesis of 2-hexyloxyethanol

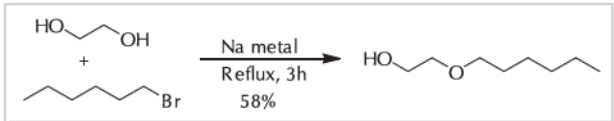
Ethylene glycol on sodium metal gives Sodium salt of glycol. The reaction mixture on reflux with hexyl bromide at 58 °C for 3 hours to give 2-hexylethanol in 53% of yield.

Synthesis of 2-hexyloxyethyl bromide



Synthesis of 2-hexyloxyethanol

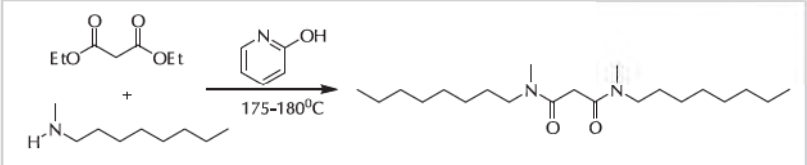
2-Hexyloxyethanol on reaction with Ph3P and CBr_4 in at 0 °C to room temperature for 12 hours gives hexyloxyethyl bromide in



Synthesis of 2-hexyloxyethylbromide

89% of yield

Synthesis of N,N'-dimethyl-N,N'-dioctyl-propane diamide



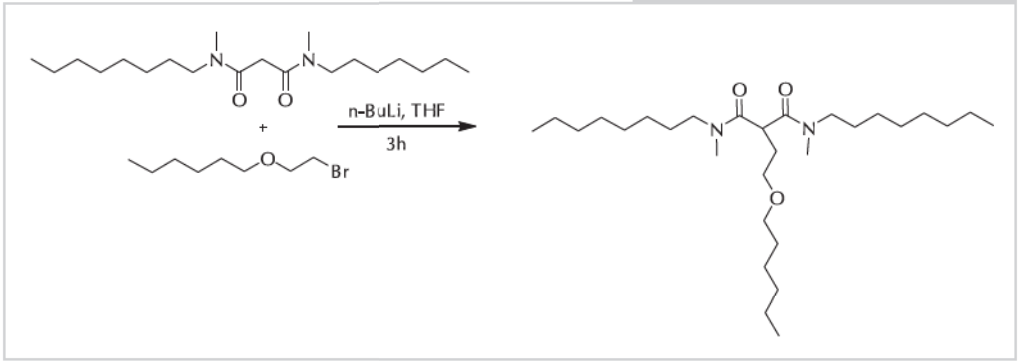
Synthesis of N, N'-dimethyl-N, N'-dioctyl-propane diamide

The reaction between diethyl malonate, 2-hydroxy-pyridine and methyl N-octyl-amine at 175°C in inert atmosphere to give N, N'-dimethyl-N, N'-dioctyl-propane diamide in 52% yield.

Step VI) Synthesis of 2-ethoxyhexyl-N,N'dimethy-N,N'-dioctyl-propane diamide

The N, N'-dimethyl-N,N'-dioctyl-propane diamide in anhydrous tetrahydrofuran reacting with n-butyl lithium prepared from 100ml anhydrous hexane. Under the same conditions a solution of hexyloxyethyl bromide was prepared from 0.1 mol of bromide and anhydrous 100ml tetrahydrofuran to give DMDOHEMA.

Synthesis of DMDOHEMA



Network PROJECTS

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Discovery and pre-clinical studies of new bioactive molecules

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Background / objectives

Plants and plant products are used for the treatment of different diseases for time immemorial. They are also used for the protection of food produce and other biomaterials such as cloth, wood etc. With the development of different modern techniques in the field of both chemistry and biology it has become essential to have a fresh look at these plants and plant products with regards to their utility and safety. Also very small fraction of plant species have been used earlier for these purposes and it is important to evaluate these un-explored flora for their utilization as drugs, pest control agents etc. Novel secondary metabolites isolated from plants can be used as lead molecules for the development of new drugs, pest control agents etc.

Different extracts prepared plants collected from one of biodiversity hotspot, Western Ghats, are assessed for wide range of biological activities which includes malaria, filarial, kala azar, anti-bacterial, anti-fungal, tuberculosis, gastric ulcer, hepatoprotective, hypertension, anti-cancer, immunomodulatory, neurological disorders and pesticidal. Bioactive leads are taken up for the isolation of active principles which is followed by product developmental work.

Work done and discussion

Under the programme for development and commercialization of Bioactive substances from plant sources extracts prepared from plants collected from Western Ghats, were 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, tuberculostattic, anti-dementia and anti-psychotic.

Development of botanical pesticides

One of the leads (NCL49) has been found to exhibit control of stored grain pests Rhizopertha dominica (lesser grain borer) and *Sitophilus oryzre* (rice weevil). This lead has been processed further for the development of a product. Developed product has shown control of both R. dominica and S. oryzre 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 has been initiated with ~750kg seed. Further larger, multi-centered field trials have been planned.

Two more leads (NCL794 and NCL2038) which have exhibited good control of *R. dominica* and *S. oryzre* are being assayed for product developmental work.

Bioassay

Plant extracts from four CSIR laboratories are evaluated for pesticidal activity. The participating laboratories include Central Salt and Marine Chemicals Research Institute, Bhavnagar; Central Institute of Medicinal and Aromatic Plants, Lucknow; North East Institute of Science and Research, Jorhat, besides NCL, Pune. The number of samples received from each lab is listed below:
NCL, Pune : 68
CSMCRI, Bhanvnagar : 35
NEISR, Jorhat : 32 and
CIMAP : 15

Samples received from the various labs are screened for their biological activities, viz., antifeedant and toxicity against the larvae of two species of lepidopteran pests - *Helicoverpa armigera* and *Spodoptera litura* and oviposition deterrent activity against the potato tuber moth, *Phthorimaea operculella*. So far, we have screened 123 samples for their biological activity against these pest insects. One of the samples received from NCL, Pune has shown toxicity against *H. armigera*. Experiments are being pursued to confirm its activity against other insects also. Further product developmental work will be undertaken on this lead.

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Publications
- *Appl. Phys. Lett.*, **2009**, 94, 182507
- *Phys. Rev. B.*, **2009**, 80, 064423

Nanostructured advanced materials/nanostructured magnetic materials

Background / objectives

Multiferroic nanocomposite multilayered films (ABO_3 type) and nanoparticls (Ferroelectric & Ferromagnetic)

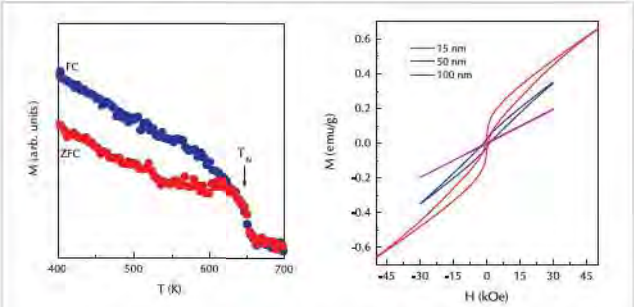
- Study of the particle size effect on the multiferroic coupling behaviour.
- Synthesis of nanostructured multifferroic ABO_3 (e.g. $BiFeO_3$, $BiMnO_3$, $GaFeO_3$) thin films for electrically switchable magnetic memory and magnetically controllable resistive switching.
- Synthesis of nanocomposite of ferrite ($CoFe_2O_4$) and ferroelectric ($BaTiO_3$) materials for magnetostrictive and magnetoelectric applications

We have studied the effect of simultaneous substitution of Bi by rare-earth ions with reduced particle size. It is observed that magnetization can be increased by this substitution and the magnetic parameters such as magnetization, coercivity and Curie temperature can be controlled by the choice of the rare-earth ion.

HRTEM and EDX (red: Bi Lα, green: Fe Kα) characterization of $BiFeO_3$ nanoparticles

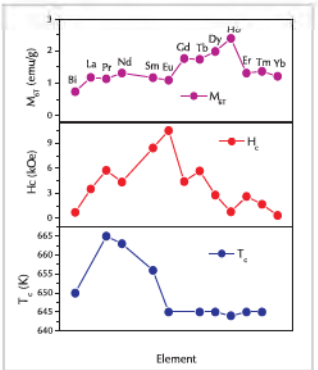
Work done and discussion

Single phase nanocrystalline $BiFeO_3$ with different particle sizes have been synthesized by soft chemical methods. The objective is to increase the magnetization and make the material ferromagnetic with decreasing particle size. The nanoparticles have been characterized thoroughly by XRD, TEM, EDX and magnetic measurements to understand the effect of particle size on phase purity and magnetic characteristics.



Magnetic characteristics of single phase $BiFeO_3$ nanoparticles of different sizes

One of the methods to make antiferromagnetic $BiFeO_3$ ferromagnetic and magnetoelectric is to do chemical substitution at the Bi or Fe site by other similar ions.



Effect of different rare-earth ions on the magnetic characteristics of nanocrystalline $BiFeO_3$

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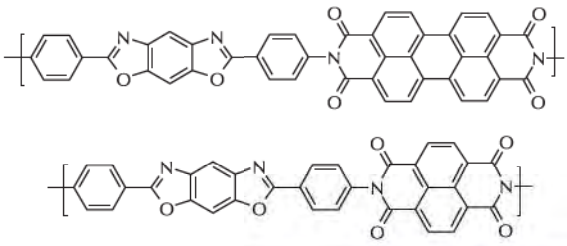
Functional organic materials for energy efficient devices

Poly(benzobisazoles) (PBO) are rigid rod polymers with extended chain conformation which have been studied extensively in the context of bullet-proof materials and fibers, but recently they have been used as electron transport materials in polymer LEDs due to their combination of n-type and other physicochemical characteristics. Materials based on Perylene and naphthalene bisimides have high charge carrier mobility and their utilization as the n type component in organic light emitting diodes (OLEDs) and solar cells have been shown to improve the performance of these devices.

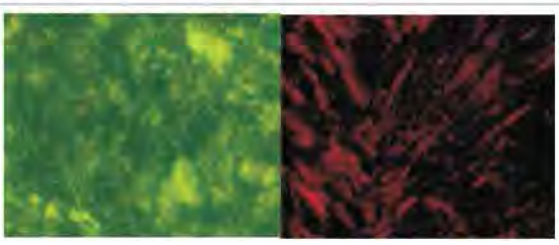


Structure of oxazoleimides based on perylene and naphthalene bisimides

Perylene and naphthalene bisimides were copolymerized with suitably designed building blocks based on benzobisoxazole with the expectation that the resulting materials will have better photoluminescence and transport properties.

These rigid aromatic materials are capable of self organization by virtue of their aromatic stacking interactions which is evidenced by their tendency to form beautiful lyotropic liquid crystalline (LC) phases.

Processing them in the LC phase gives fibres with excellent mechanical and tensile strength. These are materials with excellent thermal and thermoxidative stabilities which could be used to advantage in photovoltaic applications where most of the known conjugated polymers are plagued by thermal and oxidative instabilities.



Polarized Light Microscope (PLM) images of copolymers of naphthalene bisimide (left) and perylene bisimide (right) with benzobisoxazole in Methane sulfonic acid

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Metabolic pathway engineering for production of high-value pharmaceuticals

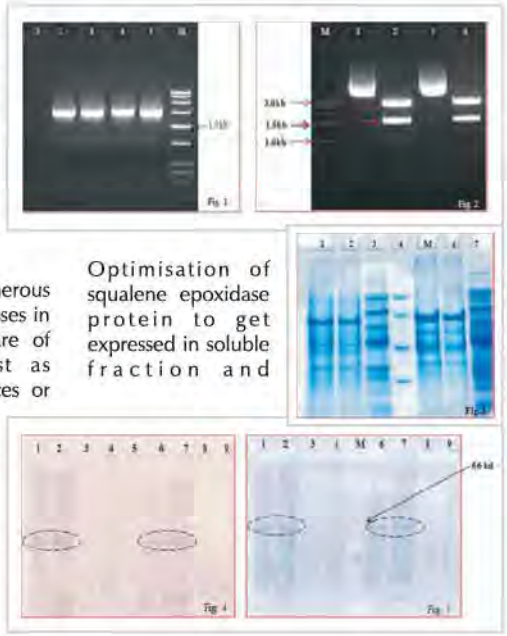
Plants are the reservoir of various bioactive compounds which are useful for mankind. They synthesize various kinds of secondary metabolites like terpenoids, carotenoids, flavonoids, phytosterols, saponins, phytoestrogens, glucosinolates and much more. These secondary metabolites carry out a number of protective functions in the human body. Plant secondary metabolites can boost the immune system, protect the body from free radicals, and kill pathogenic germs and much more. In plants several important classes of terpenoid compounds are synthesized via the mevalonate pathway.

The terpenoids sometimes referred to as isoprenoids represent the largest group of biologically active metabolites with at least 30000 chemical compounds. Plant isoprenoids are essential for the numerous physiological and developmental processes in plants and many plant isoprenoids are of considerable commercial interest as pharmaceuticals, flavours and fragrances or food colorants. Understanding the regulation of isoprenoid synthesis is therefore of immense scientific and commercial interest.

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 like 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 affordable cost.

Squalene epoxidase from *Withania somnifera*

Two full length gene sequences of squalene epoxidase (1596 bp; Fig. 1) have been isolated from *Withania somnifera* along with their respective 5' and 3' UTR regions and characterized. The above clones were cloned in pET 28a(+) bacterial expression vector and expressed in E. coli strain BL21 (DE3). The expressed protein of ~62 kd [(Fig. 3) coding region of 1.5 kb along with His tags] was confirmed by Western blotting on a PVDF membrane (Fig. 4 & Fig. 5 PVDF membrane double stained using antibody and protein) and MALDI analysis.



Optimisation of squalene epoxidase protein to get expressed in soluble fraction and attempts to get the protein expressed in eukaryotic system *Pichia pastoris* is in progress. Also, efforts are being carried out to clone sense and anti-sense constructs of SQE gene in binary plant transformation vectors to attempt genetic transformation of *Withania somnifera* using Agrobacterium and gene gun approach.

Squalene synthase genes from *Withania somnifera*

Two full length squalene synthase genes (cDNA clone): clone 1 Accession # GU181386, 1236bp, 411Aa and clone 2, Accession # GU732820, 1242bp, 414Aa , have been isolated using RT-PCR strategy. Nucleotide sequence of the cDNA shows 93% similarity with the squalene synthase reported from *Solanum tuberosum*. Both the full length clones of squalene synthase have been expressed in

E. coli BL21 (DE3). Both the proteins have been truncated from C-terminal end by deleting 24 Amino acids to get more protein expressed in soluble fraction. Maximum expression of the soluble protein was obtained at 30°C, 3 hr at an IPTG conc. of 1mM.

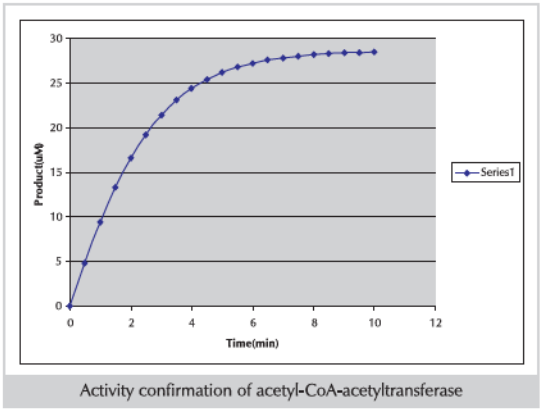
Metabolic engineering of terpenoids biosynthesis pathway in *Bacopa monniera*

Since bacosides are of immense medicinal importance and isolation of such bioactive compounds from the plant itself result in very low yield. To reduce this limitation, this work is focused on multipoint genetic manipulation of terpenoids biosynthetic pathway to facilitating the production of desirable molecules. No molecular studies are reported from this plant in context of biosynthesis of biologically active compounds.

So this present work is aimed for the development of genetically modified designer plants with high content of medicinally important compounds. For this purpose mevalonate pathway gene(s) like HMG-CoA reductase and terpenoids biosynthesis pathway gene(s) like FPP synthase, squalene synthase, α-amyrin synthase etc. are targeted.

Five full-length genes of bacoside biosynthesis pathway have been isolated and cloned from Bacopa viz. Acetyl-CoA-acetyltransferase **(FJ947159),** HMG CoA-reductase **(GU734710),** Farnesyl-pyrophosphate Synthase **(GU385740),** Squalene Synthase **(GU734711),** and α-Amyrin Synthase **(GU734709)**. Heterologous expression of all the genes in E. coli **(BL21, DE3)** has been done. Out of these five genes Acetyl-CoA-acetyltransferase has been purified and biochemically characterized.

Activity confirmation of purified recombinant acetyl-CoA-acetyltransferase also has been done by reverse reaction using acetoacetyl CoA as a substrate. The reaction mixture contained 150 mM Tris-HCl (pH-9.0), 30 μM acetoacetyl CoA, 5 mM $MgCl_2$, 100 μM CoASH and 300 ng purified recombinant enzyme. Reaction was carried out at 30 °C and decrease in absorbance at 313 nm was observed.



Activity confirmation of acetyl-CoA-acetyltransferase

Purification and biochemical characterization of other genes are in progress. Sense and anti-sense construct in pCAMBIA1301 vector of FPP-Synthase and HMG CoA-reductase are ready for Agro bacterium mediated transformation of Bacopa.

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Biotransformation of pharmaceutically important compounds using recombinant glycosyl-transferases

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.

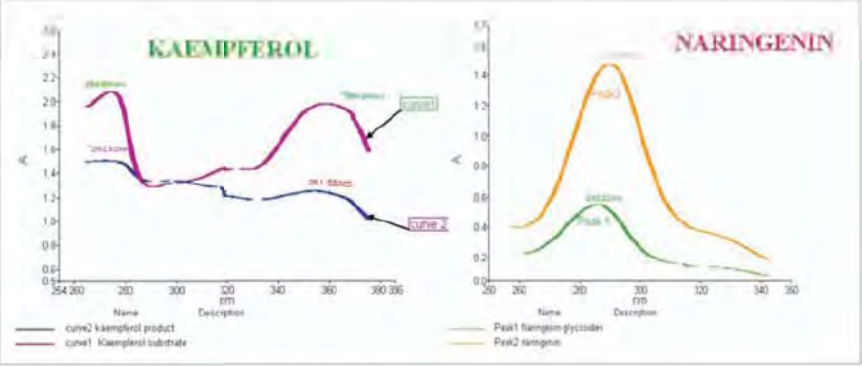
Earlier, we have isolated full length GT genes (cDNA) from *Withania somnifera* (4 genes) and *Bacopa monniera* (2 genes). These genes have been expressed in heterologous system *(E. coli)*. The purified recombinant enzymes have been used for screening various substrates to study substrate specificities.

The reaction products have been analyzed and characterized using various techniques e.g. LC-MS, HPLC and UV-VIS spectrophotometry. These genes have also been used for phylogenetic analysis to understand their functions and activities.

One of the GT gene from *Withania somnifera* (Accession no FJ654696) showed activity for various flavonoid compound as follows:

Group of flavonoids	Substrates
Isoflavones	Daidzein Genistein
Flavonols	Kaempferol Isorhamnetin
Flavonones	Naringenin Hesperitin
Flavones	3-Hydroxy flavones Apigenin Luteolin

Change in Hypsochromic shift in reaction product (Kaempferol and Naringenin) is shown in the figure below:



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Hollow fiber membranes for water purification / ultrafiltration

Development of hollow fiber (HF) ultrafiltration membranes of different MWCO was undertaken in coordination with CSMCRI, Bhavnagar while optimizing membrane preparation parameters. The major objective towards HF membrane development was their applicability for drinking water purification and waste-water treatment. Analysis of these membranes for requisite characteristics (flux, MWCO determination, pore size distribution, limiting pressure, etc.) and widening the applicability for other separation applications were planned to be investigated at NCL.

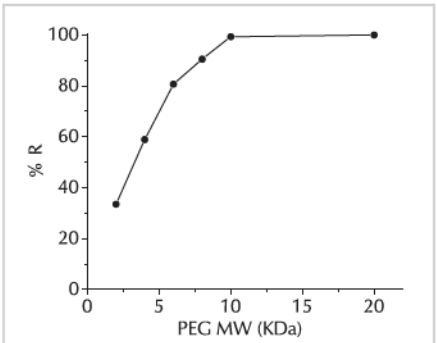

Fig. 3: Rejection analysis of PSF based hollow fiber module

Characterization of hollow fiber modules

In of wide applicability of HF membranes in water treatment, membranes with different cut-off (porosity) are required. These could be met while varying the membrane material as well as membrane preparation parameters. Hollow fiber membranes based on polysulfone (PSF), polyacrylonitrile (PAN) and blend of both were spun at CSMCRI.

The flux and rejection characteristics of these membranes were adequate to be used for water disinfection. Fig. 2 represents pore size distribution of one of the membrane type, which is narrow enough (a pre-requisite of applicability of membrane for water remediation).

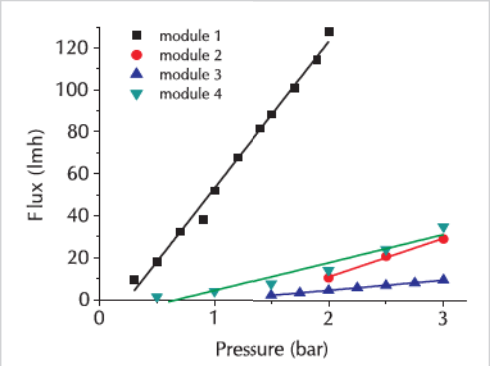

Fig. 1: Water flux of different membrane modules

Widening applicability of HF membranes

PSF was chosen as the membrane material for making thin film composite membranes by coating of thin skin of gas-selective layer on the top of HF membranes. The necessity of the HF membrane is that they should have lower MWCO.

The modules based on these membranes were analyzed for basic membrane properties such as water flux, molecular wt. cut off (MWCO), pore size distribution, compaction pressure, burst pressure, etc. Some of these elaborated below.

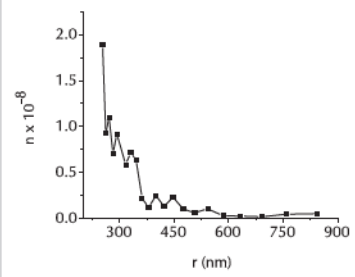

Fig. 2: Pore size distribution analysis

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Conducting polymer paints and coatings for corrosion protection and shielding of concrete structures in strategic areas

Background / objectives

Corrosion is broadly classified as oxidation of materials upon exposure to oxygen. It is easy to conceive that such oxidation can be precluded by a polymer coating with commensurate band edges. Modulation of band edges is facile in conducting polymers, hence they are the polymer of choice for corrosion protection. Although conducting polymers have been explored for corrosion protection, a design principle that would enable researchers to design new materials is lacking. Considering this, we have proposed to synthesize band edge modulated polymers and study their ability to impede corrosion.

We have also developed structure-property relationship for designing new materials. Indeed, during the course of our investigations, we will identify an efficient corrosion protection polymer material.

Work done and discussion

The probable path way of corrosion and protection of a material by polymer has been shown in Fig. 1. Conjugated polymers with HOMO energy level higher than -5.2 eV can be easily oxidized by atmospheric oxygen leading to the formation of a hole in HOMO level (Fig. 1a). This renders an opportunity for electron transfer from the material to the HOMO of the polymer and eventual corrosion of the material (Fig. 1b). Therefore, it is essential to identify a polymer with HOMO energy level lower than -5.2 eV. Such polymer is unlikely to be oxidized by atmospheric oxygen, hence electron transfer to the HOMO of the polymer from the material is hindered (Fig. 1c).

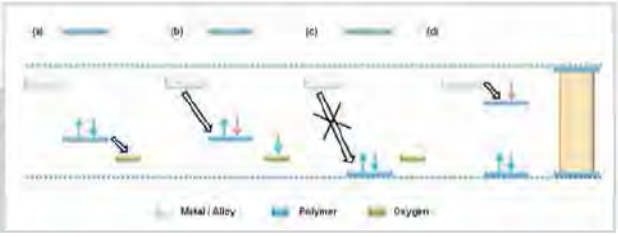

Fig. 1: Schematic presentation of possible pathways of material corrosion and protection. Band edge of ideal polymer is shown with brown band at the right end

It is also necessary that the polymer's LUMO energy levels are higher than the work function of the material to avoid electron transfer between material and polymer through the path way shown in Fig. 1d. Considering all these facts, a polymer with higher band gap and lower HOMO is desired.

To test this hypothesis, we have chosen two polymers with lower HOMO (Fig. 2a and 2b) and two polymers with higher HOMO (Fig. 2c and 2d) compared to oxygen energy level. These polymers were coated on mild steel substrate and exposed to 3.5 M NaCl, which is considered to be a highly corrosive solution.
The tafel and impedance studies indicate that the polymers do protect mild steel corrosion irrespective of the HOMO energy level of the polymer. However, we felt that such a conclusion is misleading because at the time scale of the experiment, mild steel may not be corroding. Therefore, we decided to check the polymer's corrosion protection by using rapidly oxidizing substrate, aluminum.

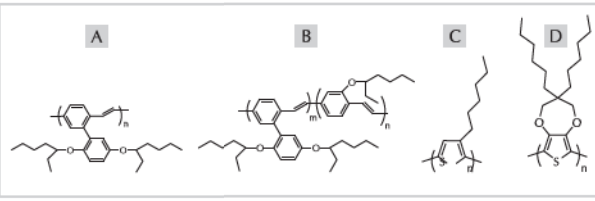

Fig. 2: Polymers used for testing the corrosion of mild steel and aluminum

The experiments were carried out by following the procedure for mild steel. We were gratified to note that the Al substrate corrodes while coated with polymers 2c and 2d. The polymers 2a and 2b having HOMO lower than oxygen protects Al oxidation. This corroborates the fact that the HOMO energy level of the polymers dictates the corrosion protection ability of a polymer.

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Identification and characterization of glycated proteins

Glycation is a series of non-enzymatic reactions between reducing sugars and amino groups of proteins leading to browning, fluorescence, and cross linking of proteins. The reaction is initiated with the reversible formation of Schiff's base, which undergoes a rearrangement reaction to form stable Amadori product.

The Amadori product further undergoes a series of reactions through dicarbonyl intermediates to form advanced glycation end products (AGEs). The formation of AGEs has been implicated in diabetic complications such as nephropathy, neuropathy, retinopathy and arthrosclerosis.

The accumulation of AGEs results in change in conformation and function of various proteins such as hemoglobin, albumin, IgG, collagen, crystalline, and metabolic enzymes. In diabetic patients, the rate of AGE accumulation and extent of protein cross linking is accelerated due to rise in blood glucose levels.

Glycated proteins and AGEs are mainly found in the plasma and 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

Objectives
- Development of method for detecting glycated proteins
- Identification and characterization of glycated proteins and AGEs inplasma
- Testing bioactive compounds for anti-glycation activity (in association with IICT)

Work done and discussion
- Established protocols for 2DE for separation of plasma proteins.
- Standardized protocols for removal of high abundant proteins.
- Established diabetic rat and mice model for studying glycation.
- Developed methods to isolate and characterize glycated proteins.
- Identified autoantibodies specific to glycated proteins
- Identified and characterized glycated proteins
- Developed a MALDI based assay for screening glycation inhibitors.
- Molecular bases of differential expression of proteins in diabetes was elucidated

Glycation induced up regulation of proteins in diabetic rat kidney

Glycation of proteins leading to formation of advanced glycation end products (AGEs) has been considered as the principal cause of diabetic nephropathy. Therefore, in this study, glycated proteins were detected by anti-AGE antibodies from kidney of streptozotocin induced diabetic rat, using two dimensional electrophoresis and western analysis. These glycated proteins include proteins from metabolic pathways, oxidative stress, cell signaling, gene regulation and immune system.

The extent of glycation was higher in diabetes compared to control, in the glycated proteins that were common to both control and diabetic kidney. Further, these glycated proteins were characterized by tandem mass spectrometry to identify different AGE modifications.

Image analysis of glycated proteins suggest that their levels were up regulated in diabetes, which could be due to formation of protease resistant protein aggregates caused by AGE modification and decreased proteolytic activity. Based on these results we conclude that glycation of proteins leads loss of biological activity, and to compensate this cells up regulate synthesis of such proteins. Eventually both the processes lead to up regulation of glycated proteins.

Autoantibodies for glycated proteins as potential biomarker for diabetic

Glycation process leads to formation of highly cross-linked irreversible compounds, called advanced glycation end products (AGEs), which have altered protein conformation and function, and elicit immune response. Earlier studies have shown that AGE proteins such as

AGE-BSA prepared in vitro are highly immunogenic in animal models such as rabbit and mouse.

The evidence that AGEs have antigenic properties has led to hypothesis that AGE can act as an antigen to elicit autoimmune response in diabetic condition. We have identified the autoantibodies for glycated serum albumin, glyceraldehyde 3 phosphate dehydrogenase, aldehyde dehydrogenase, and malate dehydrogenase in the rat plasma.

We propose that such autoantibodies will also be present in patients with diabetic complications. The titer of these autoantibodies may vary with pathophysiological condition. The lower the severity lesser will be the titer of these autoantibodies and vice versa.

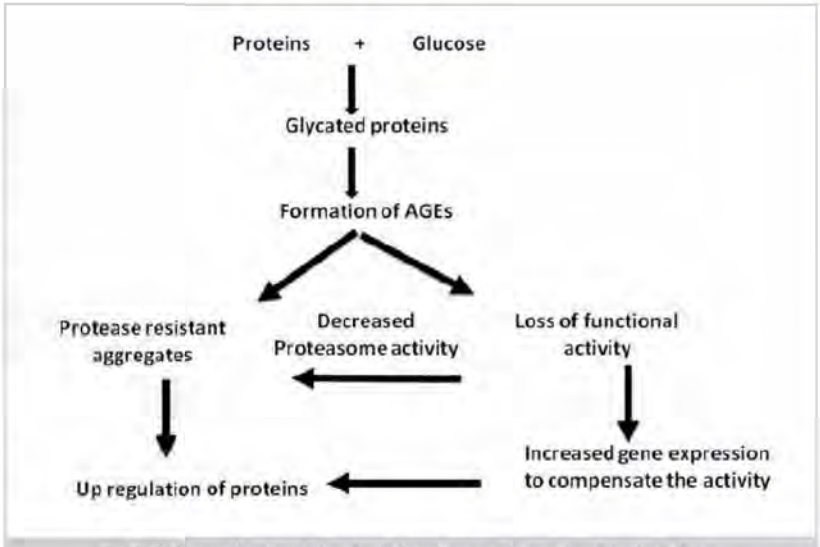

Fig. Probable mechanism of glycation induced up- regulation of proteins in diabetes

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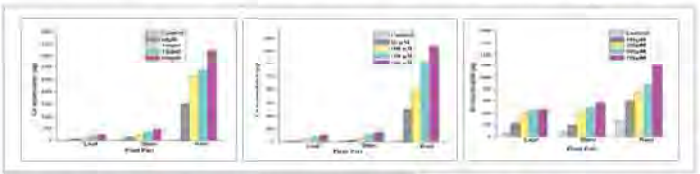
Studies on metal tolerance in plants

Under the CSIR Network Program entitled "Remediation/ eco-restoration and cleanup of contaminated ground and water resources" coordinated by NEERI, Nagpur, the NCL Project entitled "Application of biotechnological approaches in identification, characterization and development of plants useful for ecorestoration and cleanup of contaminated sites and generate useful products" is included.

The work carried out includes determination of metal tolerance in Jatropha and their suitability for different metal contaminated sites using techniques like tissue culture, Atomic Absorption Spectroscopy and protein analysis.

In vitro screening of Jatropha seeds under simulated conditions to assess tolerance towards various metals (Cd, Cu, Zn) and levels of accumulation of metals in different parts of the seedling. Growth of the seedlings reduced significantly with increase in the metal concentration of Cd and Cu in the media. The order of metal tolerance for Jatropha is Zn>Cu>Cd. This information can be useful for site specific phytoremediation.

Pattern of metal accumulation in different parts of the seedling was in the order, root>stem>leaf. Among the metals, accumulation pattern in case of roots was Cd>Cu>Zn, for stem it was Cd>Zn>Cu, while for leaves it was Zn>Cd>Cu.



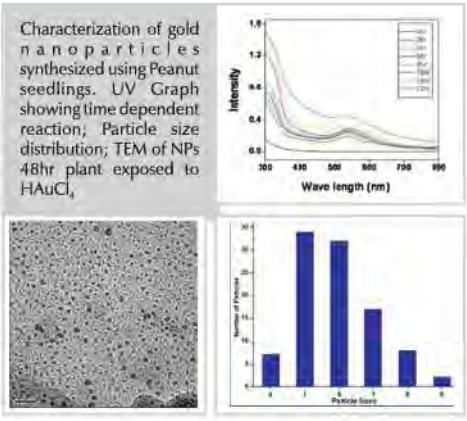
Protein profiles were also studied for the differences between the control and experimental samples of root, stem, leaves in Cd and Cu.

Induction of hairy root cultures in *Jatropha curcas* using *Agrobacterium rhizogenes*

Varying frequency to generate hairy roots from different explants of *Jatropha curcas* was noted with different strains of *Agrobacterium rhizogenes*. Among the seedling derived explants, cotyledonary leaf with petiole showed highest response for infection. Confirmation of integration of T-DNA of A. *rhizogenes* is done by PCR amplification of rolA, rolB and rolC genes with forward and reverse primers. This approach of hairy root cultures in *Jatropha curcas* will be helpful in augmenting its metal accumulation potential.

Nanoparticle formation by living plants

Biosynthesis of extracellular Au nanoparticles (NPs) by living peanut seedlings and characterization of NPs was carried out using UV and HRTEM.



Characterization of gold nanoparticles synthesized using Peanut seedlings. UV Graph showing time dependent reaction; Particle size distribution; TEM of NPs 48hr plant exposed to $HAuCl_4$

The roots of peanut seedling exposed to $HAuCl_4$ showed the pink color indicating the formation of gold nanoparticles (GNPs). Presence of intracellular particles in the epidermal layer of roots was confirmed by histology, while their characterization was carried out by HRTEM.

This study can be extended to determine the Nanoparticle producing ability of the naturally occurring metal tolerant plant species in the mine dumps and research towards Nanoparticle farming for phytoremediation of, and value addition to, metal contaminated sites.

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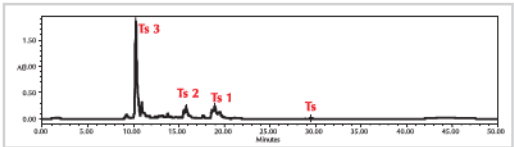
Exploration of India's rich microbial diversity

The objectives of this work are 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. At NCL we will be carrying out the following work:

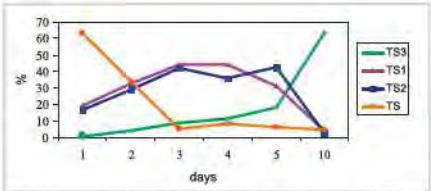
- Construction of an enzymatic tool box that would comprise well characterized biocatalysts (microorganisms or enzymes) which will be useful for different reactions such as asymmetric carbonyl reductions, asymmetric double bond reductions, stereo and regio-specific hydroxylations, and chiral resolution of esters.
- 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

We have screened microorganisms isolated from various environments and found that some of the fungal strains are able to carryout the hydroxylations at non-activated carbon atoms in xenobiotics in stereo- and region-specific manner. We have found that some of the fungal strains are able to resolve the esters into single enantiomer of corresponding alcohol in efficient way.

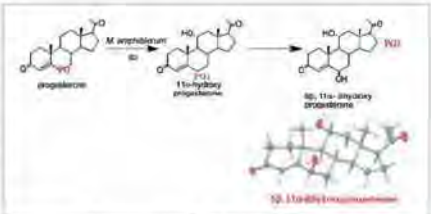
Out of the fungal strains showing desired transformations, we have selected the fungal strain *SF11* which found to carryout the hydroxylation of steroids at substrate concentrations up to 1gm/lit in quantitative yields. This transformation has been scaled up to fermentor level with 5lit of fermentation media for large scale production. This fungal strain can be used for the quantitative production of 6β ,11α-dihydroxy derivatives of testosterone, 17-methyl testosterone and 19-nor testosterone and progesterone.

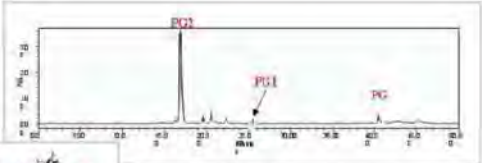


The HPLC analysis of the crude extract of testosterone after 10 days of incubation



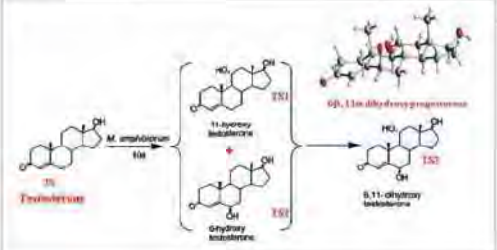
Time course study of Testosterone with *M. amphibiorum*


Progesterone by *M. amphibiorum*



The HPLC analysis of biotransformation products of progesterone after 8-days of incubation

Biotransformation of Testosterone by *M. amphibiorum*



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Publications

- *Adv. Sci. Lett.* **2010**, 3, 313
- *Chem. Commun.*, **2010**, 46, 5590
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Hydrogen energy: Overcoming materials challenges for the generation, storage and conversion of hydrogen using fuel cells

Overview of the NCL Program

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 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.

In the XIth Five Year Plan, NCL has ambitiously come up with certain research proposals with immense scientific relevance to address some of the existing issues on hydrogen economy. 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 nano tubes and metal organic frame works.

Hydrogen utilization is another area where research activities are undertaken. In this regard four programs are under progress, which include 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 and to understand mechanism for proton transport computer simulation study is on progress.. The main highlight of the work achieved during 2009-10 is briefly explained in this report.

Introduction

At present large scale industrial hydrogen production is carried out either by steam reforming or autothermal reforming of natural gas/naphtha. If hydrogen based fuel cells are used, it helps in improving the efficiencies of energy production. The full benefits can be obtained only when H_2 is produced from renewable sources such as oxygenated hydrocarbons (glycerol, sorbitol, xyletol etc.) obtained from biomass. Water Gas Shift reaction is an important component of fuel processing which not only reduces the concentration of poisonous CO but also enriches the feed with H_2 by using water. The main aim will be to develop oxide based catalysts for Water Gas Shift reaction aiming at low temperature activity and on stream durability by incorporating the noble metals in lattice points.

The success of future hydrogen is critically dependent upon the discovery of new materials that can store large amounts of hydrogen at ambient conditions. Metal-organic framework (MOF) compounds, which consist of metal-oxide clusters connected by organic linkers, are a relatively new class of nano-porous material that show promise for hydrogen storage applications because of their tunable pore size and functionality. We are developed the light weighted MOFs material which shown the good hydrogen absorption capacity. Moreover, such materials along with functionalized carbon nanotubes (F-CNTs) and metal incorporated F-CNTs also showed the good results.

As far as the hydrogen utilization concern, an important achievement is the development of a Pt dispersed carbon nano fiber (Pt-CNF) catalyst by decorating Pt along the inner and outer walls of the CNF. Understanding the high cost and its vulnerability to market fluctuations, we also initiated studies to develop low Pt system such as Pt based core-shell particles as a thrust area. If proper non-noble metal could be successfully employed as core, the resultant catalysts would naturally combine the advantages of low cost and high catalytic activity. Also, our further research is going on in the Pt-free electro-catalyst for the fuel cell application.

In case of development of electrolyte used in fuel cell, the Nafion based perflourosulfonated ionomer membranes are employed for PEMFCs due to their high and selective permeability for small cations, especially for protons. We here also demonstrate 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.

Three-dimensional structured MEA with micropatterned electrodes prepared by soft lithography can generate well defined pathways to enable reactants to more homogeneously distribute along the electrode surface and products to dissipate relatively quickly without obstructing the reactants and thereby creating a competitive environment around the active sites. The idea is to fabricate the catalyst layer on the Nafion membrane surface using a patterned PDMS master by fixing the patterned area and channel thickness to get the desired Pt loading (mg/cm^2) along the catalyst layer.

In order to supplement these materials development activities, we have also recently initiated a theoretical research programme including computer stimulation and modeling to address some of the mechanistic aspects of proton transport in polymer electrolytes.

Experimental Aspects

For the Aqueous Phase Reforming (APR) experiment, the Pt nano particle were synthesized by reducing an aqueous solution of H_2PtCl_6 by sodium borohydride. The Rh and Ni nano particles were synthesized by reducing the $RhCl_3$ and Nickel chloride hexahydrate using an hydrazine hydrate. In addition to the above nano particulates of Ni, Rh and Pt metals, we have also prepared supported metal catalysts using various Pt, Ru and Rh precursors on supports such as alumina and activated carbon. Barium cerate, Lanthanum cerate, Cu@Pt, Fe@Pt core shell Catalyst were also prepared using different chemical routes while Platinum decoration on polypyrrole coated carbon was made by pre-precipitation method.

Preparation of Nafion-functionalized multiwalled carbon nanotubes (MWCNT) composite membranes was carried out using sulfonic acid functionalized MWCNTs (s-MWCNTs)(~2 mg/mL) by a microwave treatment (100 mg) in a (1:1) mixture of 98 % H_2SO_4 (15 ml) and 70 % HNO_3 (15 ml). Appropriate amount of pre-casted Nafion membrane (570 mg; 5%) was dissolved in dimethylacetamide (DMAc) (15 mL) and mixed with a solution of (20 mg in 100 ml in appropriate amount) S-MWCNTs in DMAc. The mixture was stirred for 4 hours at 70 °C followed by 45 minutes ultrasonication before casting in an oven at 90 °C. Preparation of PDMS (polydimethyl siloxane) mold and Pt-catalyst patterns on Nafion membrane was also carried out using established procedures followed by single cell fuel cell experiments of the MEAs tested on an Arbin fuel cell test station at 60 °C cell temperature at different Relative Humidity (RH) values.

Direct solution reactions at room temperature give rise to microcrystalline precipitate in most MOFs synthesis. The hydrothermal method has been demonstrated to be a very promising technique for growing MOFs crystals. 4, 4'-(Hexafluoroisopropylidene) bis(benzoic acid) ($C_{17}H_10F_6O_4$, H_2hfbba) transition metal cations [Zn (II), Co(II) and Mn(II)] and nitrogen containing heterocyclic compounds are used for synthesisng the F-MOFs. To obtain pure crystals of F-MOFs, a strong stirring of the mixture in de- ionized water is necessary before it is transferred to an acid-digestion bomb for hydrothermal reaction. The synthesised complexes were characterised by IR, and X-ray single-crystal diffraction techniques.

Result and discussion

Aqueous phase and steam reforming of oxygenated hydro- carbons from biomass sources

The powder X-ray diffraction (XRD) pattern of Rh metal particulates shows three reflections in the 2θ range 40-100° corresponding to the 111, 200, and 220 planes of its FCC lattice, which is also confirmed by the TEM images of Rh (Figs. 1-3) showing Rh and Pt nano particles of around 4.5 nm.

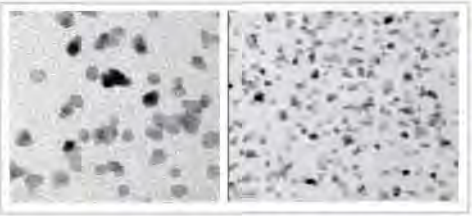

Fig. 1: Transmission electron micrographs of PVP-capped Pt nano particles

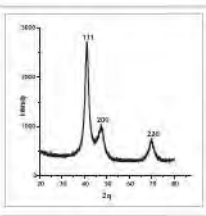

Fig. 2: (Left) XRD of Rhodium Nanoparticles Fig. 3:(Right)TEM and SAED of PVP-capped Rh Nanoparticles.

For the initial APR experiments, we have used stoichiometric solutions of glycerol: water (1:3) mixture, containing 63 wt% of glycerol, as the ultimate concentration of glycerol is expected to be much lower due to water present in the autoclave. However, for some reason, the catalysts deactivated very rapidly. We have observed increased formation of lower alkanes, particularly methane with time on stream.

It appears that the size of Pt particles grows on stream under the experimental conditions, leading to the formation of lower alkanes through hydrogenation. However, this aspect need to be probed through characterization of spent catalysts. The catalyst was re-used, without any activation the next day at increased feed flow rates. There was substantial reduction in the conversion of glycerol and in addition, there was continuous fall in the conversion with time on stream. There was also some fall in H_2 selectivity with time on stream at the higher feed flow rate of 10 ml/hour. Conversion of glycerol was initially low, but increased with time on stream reaching a value of 50%. Hydrogen selectivity was higher than 80% in the initial hours of reaction, while a substantial fall was observed with time on stream. When we inspected the spent catalyst, it was settling down much faster than the original catalyst, suggesting agglomeration of particles as the capping agents are no longer present on the nano particles.

Better catalysts for water gas shift reaction: Exploring structured and mesoporous oxides

a) Lattice incorporation of noble metals

$BaCe_{1-x}PtxO_{3-\delta}$ had already been synthesized with minimal impurities of $BaCO_3$ using citric acid method. Progressively increasing amounts of Pt were incorporated. $BaCe_{1-x}PtxO_{3-\delta}$ with Pt amounts of x = 0.02, 0.04 and 0.06 (amounting to 2, 4 and 5 wt%) were characterized by XRD to ascertain phase purity as well as the presence of Pt metal. PXRD patterns did not show the presence of Pt (Fig.4). The XPS studies which unambiguously proved that Pt exists in ionic form and the surface concentration is very low. Pt incorporated $BaCe_{0.98}Pt_{0.02}O_{3-\delta}$ was tested for WGS reaction. It showed only

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marginal activity. The Pt(IV) surface concentration is enhanced substantially (Pt(II): Pt(IV) is 1:2.5). XPS on the used catalyst shows a surface enrichment of Pt(II) (Pt(II): Pt(IV) is 1:1.12). $Ag_2Cu_2O_3$ and $AgCuO_2$ seem to be good candidates for such exploratory studies.

b) Metal and metal oxide nanoparticles encapsulated within mesoporous oxide channels : We have been highly successful in developing a novel in-situ method in achieving this in case of Pt nanoparticles in silica channels of mesoporous SBA-15 and SBA-12. We could fine tune the size and morphology of these particles by varying synthetic conditions (Fig.5) as well as template characteristics.

We could also use this method to encapsulate ~1.2 nm CeO_2 particles within SBA-12 mesochannels which are stable till 500 °C. This is an interesting observation since smallest particle reported in literature is ~ 5 nm stabilized under acidic conditions and later used in a sol gel method to be incorporated in SiO_2. In such methods, the draw back is that CeO_2 can get embedded within the SiO_2 thereby reducing the accessibility.

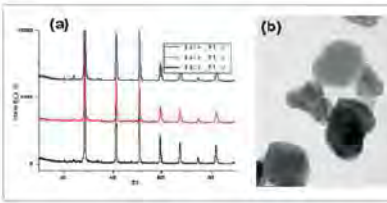


Fig. 4. PXRD patterns of $BaCe_{1-x}Pt_xO_{3-\delta}$ (x = 0.02, 0.04, 0.06) and HRTEM images of $BaCe_{0.98}Pt_{0.02}O_{3-\delta}$ showing the presence of ~100 nm particles (left) and uniformity of lattice planes (right). Inset shows the reduced FFT of BaCeO3 diffraction, (c) and (d) Pt 4f XPS data and WGS activity of fresh and recycled $BaCe_{0.98}Pt_{0.02}O_{3-\delta}$.

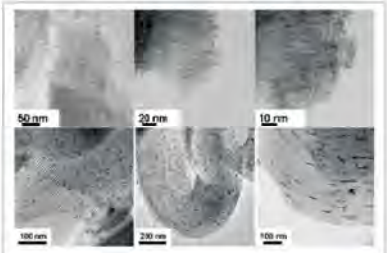


Fig. 5. HRTEM images of (left to right - top) Pt spheroids of 8 nm, Pt rugby balls, Pt nanorods in SBA-15 silica channels; (left to right - bottom) Pt spheroids of 4.5 nm in SBA-12 silica, 1.2 nm CeO_2 nanoparticles in SBA-12 channels, a closer look at the CeO_2 particles.

Studies on the synthesis, purification and functionalization of carbon nanotubes for hydrogen storage applications

Fig. 6 shows the HRTEM images of (a) pristine MWNTs, (b) PVP-capped Pd-functionalized MWNTs and (c) PVP-capped Rh-functionalized MWNTs. The micrographs of Pd- and Rh-functionalized MWNTs show numerous metal nanoparticles anchored onto the external walls of the nanotubes. The size range of these nanoparticles is about 5 - 10 nm.

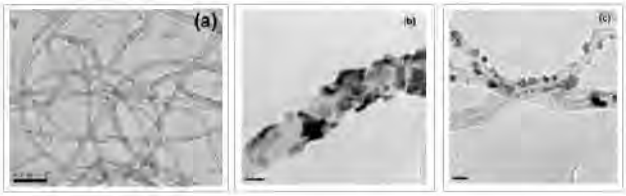


Fig. 6. HRTEM images of (a) MWNTs, (b) Pd/PVP-MWNTs and (c) Rh/PVP- MWNTs

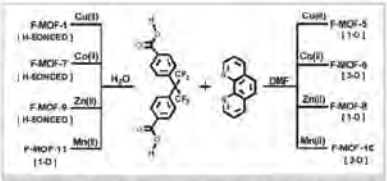
The TGA analysis indicates that systematic decreases in thermal stability as the pristine MWNTs were processed for Pd functionalization. However, in the case of Pd/PVP-MWNTs, the thermal stability is higher than COOH-MWNTs and Pd-MWNTs but, obviously lower than the pristine MWNTs. The hydrogen adsorption and desorption measurements were carried out at low temperature of 77K and pressure from low to ambient. The hydrogen storing capacity of synthesised MWCNTs was higher than that of commercial grade MWNTs. The hydrogen uptake profile for Pd functionalized MWCNTs is shown in Fig.7 along with their desorption data in Fig.8.

Design and synthesis of matel organic frameworks for hydrogen storage

a) Hydrogen Storage in Fluorinated Metal Organic Frameworks (F-MOFs)

we have synthesized several partially fluorinated MOFs, using the 4,4'-(Hexafluoroisopropylidene) bis (benzoic acid) and co-ligands as phenonthroline, 3-picolin, 2,2'-bipyridine and neocuprine along with transition metals like Co^{+2}, Cu^{+2}, Mn^{+2} and Zn^{+2}. Synthesis of F-MOF-1 to F-MOF-5 is shown in following scheme 1. Among all of these structures, we selected F-MOF-4 and F-MOF-6 for the adsorption studies as they are porous and 2 dimensional, and 3 dimensional respectively.

The permanent porosity of F-MOF-4 was confirmed by crystal structure obtained from single crystal X-ray diffraction and hydrogen adsorption isotherm for F-MOF-4 was studied at 77 k up to 1 atm pressure. The BET surface area of F-MOF-4 was found to be 196 m^2/g, which is quite low and may therefore indicate a slight constriction of the channels after solvent removal. The hydrogen adsorption isotherms for F-MOF-4 are shown in Figure 1D. While the volume of hydrogen adsorbed by F-MOF-4 is rather modest (0.6 wt% H_2), but this report once again proves that hybrid materials containing a per-fluorinated ligand can emerge as a hydrogen storage materials.



Scheme 1. Schematic diagram for the synthesis of F-MOF-6 to F-MOF-11.

The BET surface area 3 dimensional structure of F-MOF-6 was found to be 20 m^2/g. This is quite low and this may happen due to constriction of the channels after solvent removal from framework. Hydrogen adsorption isotherms for F-MOF-6 are shown in Fig.9. While the volume of hydrogen adsorbed by F-MOF-6 is rather modest (0.9 wt% H_2) at 77 K. This report once again proves metal organic frameworks

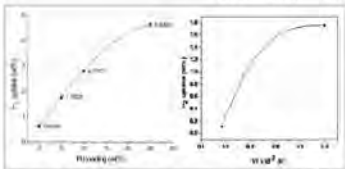


Fig.7:Hydrogen uptake profiles for Pd/PVP-MWNTs.

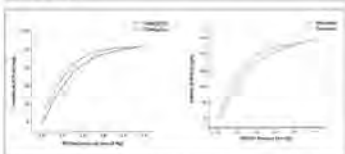


Fig. 8. Adsorption and desorption graphs for Pd-MWNTs and Pd/PVP-MWNTs

containing a per-fluorinated ligand can perform well as a hydrogen storage material.

The light weight MOFs formed by light main group metals such as Mg^{2+}, Al^{3+} and Ca^{2+}. The light weight MOFs exhibit promising hydrogen storage capacities, owing to their low framework density, high specific surface area, and tunable surface structures onto which hydrogen molecules can be adsorbed. Divalent magnesium has a number of similarities to the transition metal ions, typically used to make MOFs, in that it prefers octahedral coordination, has a comparable ionic radius. The as prepared porous Mg-MOF-1 [Mg(3,5-PDC)(H2O)] (Fig.10), by solvothermally in DMF. This chiral MOF (space group P6122) is constructed by helical assembly of Mg^{2+} ions with achiral 3,5-pyridine dicarboxylates. Open Mg metal sites show selective hydrogen (H_2) adsorption (ca.0.8 wt% at 77K) at 1 atm.

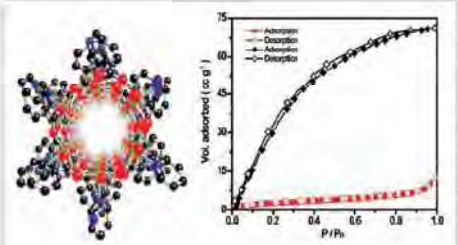


Fig. 10: A rare porous chiral Mg based MOF, Mg-MOF-1, containing open Mg metal sites was synthesized which show selective H_2 and CO_2 adsorption over N_2.

The architectural stability and permanent porosity of ZTF-1 were also confirmed by measuring the N_2 gas adsorption of the guest-free material (Fig.11a). The BET and Langmuir surface area were calculated to be 355.3 and 443.8 $m^2 g^{-1}$. Fig. 11b and 11c shows the CO_2 and H_2 adsorption isotherms for ZTF-1, which shows a disproportionately high affinity and capacity for CO_2 (5.6 mmol/g at 273K) than N_2. The CO_2 uptake at 760 Torr for ZTF-1 is 10 times higher than N_2 at 273 K.

Table 1. H_2 adsorption studies in fluorinated MOFs.

Sr. No.	Name of MOF	H2 Adsorbed wt%	Pressure
1	3a	0.87 wt%	20 bar
2	4a	0.57 wt%	20 bar
3	1	1.1 wt%	48 atm
4	3	0.23 wt%	1 atm
5	5	1.78 wt%	1 atm
6	1a	0.43 wt%	1 atm
7	F-MOF-6	0.90 wt%	1 atm
8	F-MOF-4	0.58 wt%	1 atm
9	FMOF-1	2.33 wt %	64 bar

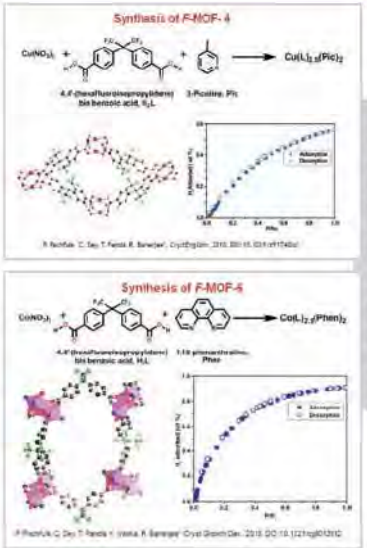


Fig. 9: Synthesis of F-MOF-4 (top) and synthesis of F-MOF-6 (bottom). Color code: Co (pink), N (blue), O (red), C (black), F (green). (d) Hydrogen adsorption isotherm of the F-MOF-6 shows an uptake of 0.9 wt % at 77 K. Filled and open symbols represent adsorption and desorption branches, respectively.

Preparation of low cost MEAs by developing low Pt and Pt-free electrocatalysts

a) Inner and outer wall Pt decoration on hollow CNF

The HRTEM image Fig. 12 (a) clearly shows the presence of ca. 6-7 nm sized Pt nanoparticles only on the inner wall of pristine carbon nanofiber; Fig. 12(b) shows the same on both the walls but with size 3 ± 0.5 nm only. Therefore, by a simple pretreatment, the available area of Pt can be doubled leading to almost half reduction in the size of the Pt nanoparticles. Almost double electrochemical active area (APt) obtained from CV and the four times higher rate constant obtained by (RDE) studies for ORR confirms the better potential of this new system. For electrochemical methanol oxidation also, the CNF based catalysts displayed excellent performance, in comparison with the conventional Pt decorated CNT catalyst.

b) Low Pt electrocatalysts based on core-shell structures

The HRTEM images of Cu@Pt/C and Fe@Pt/C particles indicteds the average particle sizes of the core-shell particle were 2-3 nm which was further confirmed from the crystalline size obtained from the XRD data. Apt area was calculated from the CV taken at 100mV/s sweep rate, which indicates that the Apt is in the order of Cu@Pt/C (125 m^2/gm-Pt)>Fe@Pt/C (115 m^2/gm-Pt)> Pt/C (94.5 m^2/gm-Pt). The positive shift for both the catalysts for oxygen reduction as compared to the Pt/C catalyst indicates that the core-shell catalysts have improved ORR activity. From the Koutecky-Levich (K-L) plots, the linearity of the graphs indicates a first order kinetics involving 4 e transfer reaction.

The fig. 13 shows, comparative polarization plots of Cu_{50}:Pt_{18}, Fe_{40}:Pt_{18} and Pt_{20} with Pt loadings of 0.1 mg-Pt cm^{-2} in the anode side and 0.3 mg-Pt cm^{-2} in the cathode side. The maximum power density of 720 $mWcm^{-2}$ and a current density of 2500 mA cm^{-2}

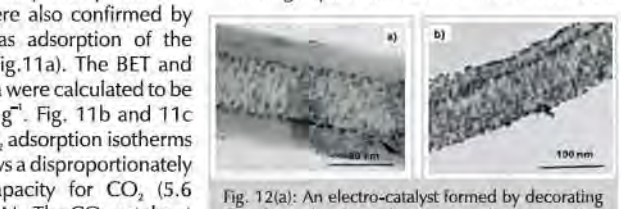


Fig. 12(a): An electro-catalyst formed by decorating Pt selectively along the inner wall of a carbon nanofiber (CNF) substrate.
Fig. 12(b): An electro-catalyst with significantly high active Pt area formed by decorating Pt along the inner and outer wall of a carbon nanofiber (CNF) substrate

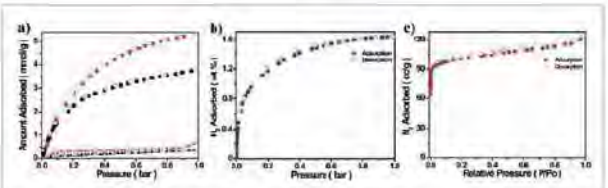


Fig. 11. Gas adsorption isotherms of ZTF-1, (a) Nitrogen adsorption isotherm (77) K. (b) Adsorption isotherms for CO_2 (circles) and N_2 (triangles) at 273 (red) and 298 K (black). (c) Hydrogen adsorption isotherms at 77K. The filled and open circles represent adsorption and desorption, respectively.

obtained for $Cu_{50}:Pt_{18}$, whereas in the case of $Fe_{40}:Pt_{18}$, these values are 580 mW cm^{-2} and 1970 mA cm^{-2}, respectively. Conversely, the Pt_{20} system displays a significantly low performance with a maximum power density of 490 mW cm^{-2} and current density of 1550 mA cm^{-2}.

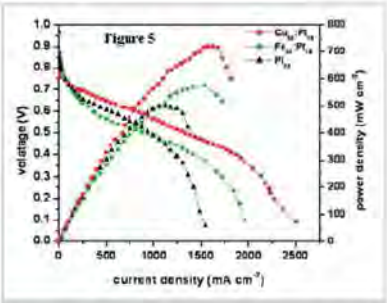


Fig. 13: Comparative polarization plot of $Cu_{50}:Pt_{18}$, $Fe_{40}:Pt_{18}$ and Pt20 with 0.1 mg-Pt cm^{-2} cathode loading and keeping constant anode loading 0.3 mg-Pt cm^{-2} of Pt20, at 70°C cell temperature by passing ultra-pure H_2 and O_2 on anode and cathode side respectively with 0.2 slpm flow rate, at 100 % relative humidity.

Inorganic-organic nano-composite electrodes and composite membranes for MEA preparation

Inorganic-organic nanocomposite electrodes

Polypyrrole (PPY) polishing of carbon helps to minimize the micropores on the surface and to increase the platinum utilization. Blocking of micropores by PPY has been confirmed by surface area and pore size analyses. Surface area analysis shows around 50% reduction in the available carbon surface area with a clear indication of covering of PPY on the carbon surface. Polypyrrole content on the surface has been confirmed by IR, TGA, TEM analyses. Morphology of the catalyst has also been studied by TEM.

The Pt particle size obtained from the TEM images was found to be 6 nm, which was further supported by XRD analysis. Compared to conventional preparation method, Pt decoration on Polypyrrole coated carbon shows enhancement in the active surface area (ESA) and oxygen reduction activity.

The platinum on polypyrrole coated carbon shows an active area of 63 m^2/gm-Pt. ESA shows significant variation with respect to the preparation method and the choice of the support materials. Pt on the composite support displays better result because around 50% of the micro pores were initially blocked using polypyrrole and in this way passage of Pt in the narrow regions could be effectively prevented.

Fig. 14 shows the single cell polarization plot for the membrane electrode assembly (MEA) based on Pt/C-PPy-Pre, Pt/C-PPy-Pol and Pt/C-Pol as cathode catalysts. Even though all the three systems display more or less similar OCV values, a significant performance enhancement in the three prominent polarization regions of activation, ohmic and mass transfer can be seen with the MEA fabricated with Pt/C-PPy.

Especially, the higher performance in the activation controlled region of the modified catalyst further confirms the improved oxygen reduction activity of this system, which has been already revealed through the RDE studies. Current densities of the catalysts at 0.6 V are 0.94, 0.78 and 0.45 A cm-2 for Pt/C-PPy-Pre, Pt/C-PPy-Pol and Pt/C-Pol, respectively. Further, the overall enhancement in the current-voltage response characteristics by the modified systems has helped this MEA to attain the highest power density of (760 mW cm-2) compared to that with the other two systems.

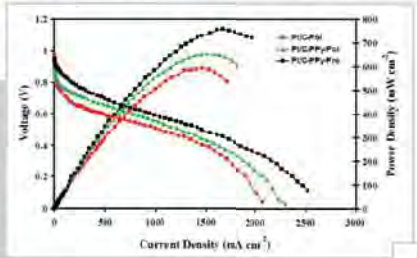


Fig. 14: I-V curves of PEMFCs with Pt/C-PPy-Pre, Pt/C-PPy-Pol and Pt/C-Pol as the cathode catalyst layers. 0.5mg cm-2 platinum in both cathode and anode, and Nafion 212 was used as polymer electrolyte membrane. Test conditions: Cell operated at 60 °C, H_2 and O_2 flow rate is 0.2 slpm and 100% humidified H_2 and O_2 at atmospheric pressure.

These results attribute that, in the modified catalyst, as more Pt particle are active to facilitate the electrode reactions, the system could respond quite well compared to the other two systems as the test station gradually drags higher current from the cell.

Inorganic-organic composite membranes

Phosphonation of CNT is successfully carried out. The presence of free phosphoric acid end on CNTs were confirmed by 31P NMR studies (Fig. 15(a). Composite of such phosphonated CNT and PBI (PBpNT) shows high proton conductivity and mechanical strength compared to the pristine PBI membrane. The proton conductivity values of the bare and composite membranes are 0.07 and 0.11 Scm-1 respectively suggesting an almost 50 % improvement. Localized phosphonate group networks might help in improving the proton conductivity better than increasing the free phosphoric acid.

Further, a comparison of the activation energy of 13.6 and 9.8 kJ mol^{-1} for the pristine and composite membranes, respectively suggests that proton transport is much facile in the latter (Fig. 15(b). Small angle X-ray scattering results reveal a 14 nm cluster formation in the composite membrane while pristine PBI membranes do not show any domains at all, mainly due to the high level of free acid present in it.

The domain formation in PBpNT membranes further signifies the role of p-CNT in forming networks for proton hopping that effectively increases the conductivity. Fuel cell polarization experiments reveal a performance enhancement of 135% in power for the composite membrane. This can be attributed to better mass transport and reduced activation loss in the composite membrane. At 0.6 V, the composite membrane gives a current density of 625 mA/cm^2 while PBI bare membrane gives only 400 mA/cm^2 which clearly indicate the lower activation loss in case of composite membrane (Fig. 15(c)).

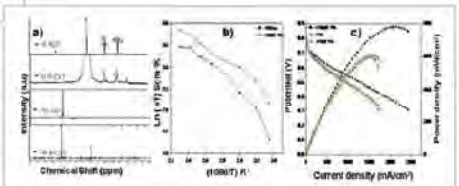


Fig. 15: a) 1H and 31P NMR of AEP and p-CNT measured on 400 MHz bruker instrument. b) Arrhenius plot for the proton conduction of PBI Iso and PBpNT membranes from 25 °C to 160 °C through impedance measurements. c) Polarization plots of PBI Iso, PBpNT and PBNT composite membranes measured at 14° C by passing dry H_2 and O_2 at a flow rate of 0.2 slpm.

Development of micro-patterned electrodes and electrolyte membranes for MEAs: Soft lithography approach

Fig. 16 (a) shows Comparative I-V curves for conventional and patterned MEA at cell temperature 80°C at 100% relative

humidity. In the case of the patterned MEA, the cell performance is maximum, giving power density of 805 mW/cm^2. On the other hand, in the case of the conventional MEA, observed power density is 363 mW/cm^2 under the same operating conditions. A controlled interplay between proton conductivity and water management is essential to ensure improved cell performance. The better performance obtained at higher temperature in the case of the MEA with the micropatterned electrode can be attributed to the better water management due to the micro channels formed on the MEA.

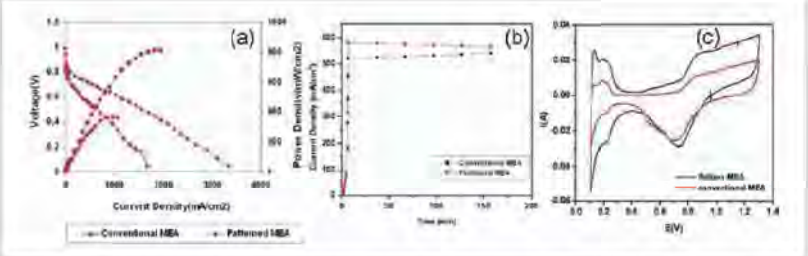


Fig. 16: (a) Comparative single cell polarization curves of Conventional and Patterned MEA having same Pt loading (0.2mg/cm^2) at 80 0C cell temperature. The flow rate of humidified H_2 and O_2 was 0.2 slpm. The area of the MEA tested was 1.68 cm^2, (b) Durability graph of conventional and patterned MEA at 60 °C using H_2/O_2, (c) Comparative cyclic voltammogram of patterned and conventional MEAs, at 200mVs-1scan rate.

Fig. 16 (b) shows the durability study of a single cell, with conventional and patterned MEA, for a period of 3 hr. The single cell performance is studied at constant cell voltage 0.6 V, at 60°C, 100% RH and ambient pressure.

The current density obtained at 30 min intervals at constant voltage. In case of both MEA, the current density is highly stable during the 3 hrs operation, which indicates that resembling the plane MEA, patterned MEA also have higher durability. To understand the realistic perspective of high fuel cell performance of patterned MEA, electrochemical studies has been carried out.

The SSCV is conducted for conventional as well as patterned MEA by passing an H_2 and N_2 at anode and cathode side respectively, at 200 mVs-1 scan rate which is shown in the Fig. 16 (C). The hydrogen adsorption and desorption takes place in the potential range of 0.1 V to 0.3 V and the features in this region resemble very much that of a polycrystalline Pt electrode. The APt has been calculated from the charge required for hydrogen desorption.

Next generation proton exchange membranes: Material development and new strategies for membrane preparation

Phase inversion of ABPBI solution offered power, rather than a continuous film. A continuous, strong film could be obtained if the glass plate after solution casting is immersed directly in water (faster gelation than by the atmospheric moisture). Analysis of these membranes (water and H_3PO_4 content, mechanical properties, etc. are in progress). Also, PBI-BuI membranes were prepared by phase inversion method are mechanically strong, have high H_3PO_4 content (32-41, depending upon the time of exposure to the atmosphere), but are not stable beyond 100 °C (they tend to melt). This indicates that the doping level needs to be lowered or the membrane should be prepared based on an appropriate co-polymer, rather than with just PBI-BuI.

Development and fundamental understanding of the mechanism of proton transport in PEMFCs by quantum chemical investigation using density functional theory

The results of the QM modeling indicate that the optimized geometry in the gas phase always has the proton present on the nitrogen atom of the BI, regardless of whether the input geometry for the structure was made with the proton on the oxygen of the (hydrogen bonding) adjacent H3PO4 molecule, and regardless of the structurally different input structures provided for the geometry optimization.

The full QM, gas phase, optimized structure has the BI nitrogen protonated and hydrogen bonding with the adjacent phosphoric acid. This failure to find minima with the proton present on the oxygen of the phosphoric acid would suggest that the mechanism outlined in Fig. 17 earlier would not be possible in a PBI-H_3PO_4 system, since the proton would only prefer to exist on the PBI. However, if the studied mechanism is correct then this conclusion must be incorrect, because, as is well known, PBI-H_3PO_4 systems do work quite efficiently in transferring the proton from anode to cathode in fuel cells. Overall, the calculations to date indicate that the high dielectric constant of phosphoric acid is an important factor in making it an effective counterpart to PBI in fuel cell systems employing PBI-H_3PO_4 for the purpose of proton transfer from the anode to the cathode.

Conclusions

During 2009-10, 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. R&D activities on Hydrogen storage using carbon nanotubes (CNTs), metal incapsulated mesoporous materials and Metal Organic Frame works (MOFs) have enabled promising candidates with enhanced gravimetric storage. For hydrogen utilization using polymer electrolyte membrane fuel cells, many new materials for components such as electrocatalysts, catalyst supports, bipolar plates and polymer electrolyte membrane for membrane electrode assembly (MEA) have been developed. Hybrid membranes of Nafion/PBI and functionalized multi walled carbon nanotubes show enhanced proton conduction as well better thermal stability.

Similarly for maximum platinum utilization, modification in the catalyst support (Vulcan Carbon) by polypyrrole shows enhanced catalytic activity and many unique materials have been developed to reduce platinum loading in the electrode including core shell type materials like Fe@Pt, and Cu@Pt. Despite all these promising results, investigations of some of these materials will require another two years of concerted efforts to establish their full benefits and limitations for hydrogen energy with respect to durability and performance criteria.

Center of EXCELLENCE

Scientific Computing

The Center of Excellence in Scientific Computing is presently an active Center at NCL promoting scientific computing in different domain areas. Scientific computing is used not just to analyze the experimental results, but also to predict phenomena. Formally, the Center is in existence from 1st April, 2008. This report presents detailed activities of the Center in its second year i.e. 1st April 2009 - 31st March, 2010.the work has resulted in thirteen publications.

Sourav Pal (Physical and Materials Chemistry)
Members: Subrata Banik, R. Lalitha, Mudit Dixit, Tuhina Kelkar, Sapana Shedge, Himadri De

Development and coding of many-body coupled-cluster methods for properties

The Fock space multi-reference coupled-cluster (FSMRCC) response approach has been implemented in singles and doubles approximation to calculate the first hyper-polarizabilities of molecules. This required coding of the first derivatives of Lagrange multipliers. The code was completed and test results were obtained for proto-typical small molecules. Earlier, the codes for polarizabilities and magnetic susceptibilities using FSMRCC response theory were extensively tested. Subsequently, triples corrections to the dipole moment using FSMRCC at low order have also been included and pilot results have been produced for test molecules. The results show improvement of dipole results with the low order triples.

Vibrational coupled-cluster method has been used to calculate the vibrational transition matrix elements and expectation values of dipole moment of different states. The method is implemented on water molecule and its isotropic variants. The quartic potential energy surface and cubic dipole moment surface are used in the calculation. The results at different level of truncation of cluster operator are compared with the converged full configuration interaction results and a good agreement is observed.

Improving hydrogen storage of metal-organic framework (MOF-5) by metal doping

MOFs are used as hydrogen storage materials. Hydrogen adsorption process is a physisorption process in MOF and hence dehydrogenation kinetics is quite good. However, the main challenge is to bind the hydrogen to MOF more strongly. First-principle computations were carried out to improve the energies of adsorption by decorating MOF-5 by use of Li_2, Be_2, Mg_2, Li_2 using density functional theory. Our results show only Al_2 and Li_2 can improve the binding of hydrogen to MOF-5.

Non-iterative coupled-perturbed Kohn-Sham theory

We have performed a detailed theoretical study of the polarizabilities of free and disubstituted azoarenes employing auxiliary density perturbation theory (ADPT) and the noniterative approximation to the coupled perturbed Kohn-Sham (NIA-CPKS) method developed at NCL. Both methods are noniterative but use different approaches to obtain the perturbed density matrix.

NIA-CPKS is different from the conventional CPKS approach in that the perturbed Kohn-Sham matrix is obtained numerically, thereby yielding a single-step solution to CPKS. ADPT is an alternative approach to the analytical CPKS method in the framework of the auxiliary density functional theory. It is shown that the polarizabilities obtained using these two methods are in good agreement with each other.

Comparisons have been made for disubstituted azoarenes, which give support to the push-pull mechanism. Both methods reproduce the same trend for polarizabilities because of the substitution pattern of the azoarene moiety. Our results are consistent with the standard organic chemistry "activating/deactivating" sequence. We present the polarizabilities of the above molecules calculated with three different exchange-correlation functionals and two different auxiliary function sets. The computational advantages of both methods are also discussed.

Understanding the reactivity properties of Aun($6 \leq n \leq 13$) clusters using density functional theory based reactivity

Relativistic Density Functional Theory (DFT) based calculations have been performed on gold clusters with six to thirteen atoms (Aun; n=6-13). The ground state geometries of these clusters as obtained from our calculations are presented and discussed.

This work proposes that atoms in a ground state conformation can be classified into distinct types of reactive sites in a given geometry. Based on symmetry, susceptibility of various types of reactive sites in the ground state geometry towards an impending electrophilic and/or a nucleophilic attack has also been studied using DFT based reactivity descriptors. The studies were also extended to high energy isomers in these cluster sizes. The reactivity of various sites as a function of cluster size and shape was thus analyzed.

The study shows that as a general rule the size and shape of the cluster influences the number and position of available sites for an electrophilic and/or nucleophilic attack. This makes the reactivity patterns of these clusters highly complex. The study also highlights as to how for a cluster with seven atoms (Au7) various conformations are likely to co-exist indicating that the reactivity patterns of various high energy conformations are also important while dealing with small sized Au clusters.

V. Ravi Kumar (Chemical Engineering and Process Development)
Members: Rahul Doiphode, Ketan Sarode

Studies of complex networks in chemical and biological systems

Studies with chemical systems

The focus of the work here is to study, develop and use multiscale methodologies for identification and characterization of flow structures from complex data monitored from reactors. In this connection, our earlier work developed a general formalism for studying monitored process space-time velocity data from different types of reactors (viz., annular centrifugal contactor, jet loop, ultrasound, channel flow, stirred tank and bubble column reactors) to study and identify the formation of structural networks, i.e., micro- and macro structures in turbulent flow fields **[2008, Chem. Engg. Sci., 63, 5330-5346]**.

For this background, in the current year 2009-2010, we studied the effects of micro and macro structures and their flow effects on heat transfer in single and multiphase jet reactors. Jet reactors have important applications as a cost effective way to achieve high degree of mixing in systems and was therefore chosen for a detailed study.

High frequency measurements by hot film anemometry (HFA) of liquid velocities and temperature in the region of vapor-liquid (VL) and solid-liquid (SL) interfaces for two types, namely, condensation jet and jet loop reactors, were planned and the experiments carried out at ICT, Mumbai.

The data obtained formed the basis for identifying flow structures and studying the heat transfer properties. An algorithm for flow structure identification has been devised from velocity data based on (i) zero crossings and (ii) continuous wavelet transform to study the heat transfer behavior in the VL and SL interfaces employing a multi-scale framework.

The wavelet transform algorithm is especially found to be useful in accurately estimating both the age and size distributions of eddies near interfaces. Using these distributions, it is shown that the calculated values of heat transfer coefficients (HTC) at the SL and VL interfaces show remarkable correspondence with the HTC values obtained experimentally from instantaneous temperature measurements. For this purpose, a modified capacitance model has been proposed that takes into account the information about both the age and size distributions. The results obtained by the present methodology show the improvements possible for calculating the HTC at interfaces when compared with the earlier surface renewal models. It may therefore be used to study the interaction between flow dynamics and heat transfer behavior in chemical process equipment. The results of the above study have been published in **[(2009) Ind. Eng. Chem., 48, 9428-9440]**.

In the coming year (2010-2011), we plan to study further the characteristics of the flow structures and study their energy properties especially with respect to their break-up distribution and the associated local turbulence phenomena. Another objective will be to study 1D and 2D energy spectra using these multiscale formalisms as envisaged here and bring out its advantages on comparison with known classical ones such as FFT, proper orthogonal decomposition (POD) and eddy identification methodologies (EIM).

Studies with 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 was earlier carried out for various patterns of locomotion and the parameters tuned by genetic algorithms.

During the year 2009-2010, studies with respect to the stability of the system for perturbations and changes in network topology have been carried out. A student working on the problem has been awarded an M.Tech. degree by Pune University. The work also won a best poster award in the Engineering Sciences category during the Science Day Celebrations held at NCL on Feb 27 2010.

Center of Excellence

Scientific Computing

Nayana Vaval (Physical and Materials chemistry)
Member: Sayali Joshi

Relativistic coupled cluster method for molecular properties

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 at the Indian Institute of Astrophysics, Bangalore. The Coupled cluster code for the calculation of the energies of the heavy atom with the relativistic effects has been developed. The calculation of properties with the proper spin orbit factors is under development and the expressions have been derived.

We have also done work on magnetic properties of closed shell molecules using coupled cluster method. In particular we have calculated magnetic shielding constant of some closed shell molecules.

C. G. Suresh (Biochemical Sciences)
B. M. Khan (Plant Tissue Culture)
Members: Manas Sule, Priyabrata Panigrahi, Ranu Sharma

In-silico study of the recognition process involving proteins possessing wide binding specificity for small biomolecules and thus to design proteins for specific applications.

Out of the seven genes involved in the lignin biosynthetic pathway of the plant *Leucaena leucocephala* we have modeled the structure of two proteins. The plant has two genes for Cinnamoyl-CoA reductase (CCR) which catalyses the conversion of cinnamoyl-CoAs into their corresponding cinnamaldehydes.

This is also the first step of the phenylpropanoid pathway specifically dedicated to the monolignol biosynthetic branch. A second protein modeled in the pathway is that of the coniferaldehyde-5-hydroxylase (Cal5D) sequenced in our lab.

The modeling of the three-dimensional structures of CCR1 and CCR2 has already been accomplished. The models have been further energy minimized using molecular dynamics. The putative active sites of the enzymes identified. The differences in the amino acid residues at the active site of the two enzymes could be responsible for their difference in activity. However, the present docking programs available to us could not correctly place the substrate at the active site.

Coniferaldehyde-5-hydroxylase could be modeled using six structures that showed around 25% sequence identity. A phylogenetic tree generated narrowed down the final template to human microsomal cytochrome P450 1A2 (2HI4), which was used as the reference structure for modeling coniferaldehyde-5-hydroxylase sequence. The overall PROCHECK G-factor was -0.11 which confirms the acceptability of the model.

The structural comparison helped to identify heme-binding domain. The residues Phe, Gly, Arg, Cys, Gly in 2nd, 5th, 7th, 9th, and 11th position of heme-binding domain are conserved in Cal5D also. It is possible that the residues namely Arg108, Trp129, Arg133, His379 and Arg 446 interacting with the heme group also might be important for the binding the substrate.

Glycosyl transferase is an enzyme which carries out post-translational modification to stabilize and solubilize metabolic products. We have modeled the three-dimensional structure of the sequence of a glycosyl transferace determined in our laboratory. It belongs to the family GT-B. The structure has two domains made up of Rossman fold. Enzyme contains the conserved C-terminal domain that is believed to bind activated sugars. Further investigations on the substrate specificity etc. are in progress.

In the case of Ntn-hydrolases we have been trying to find out the features that provide information on the variation of substrate specificity. We have identified several conserved residues through alignment of more than 500 sequences. Even though we could correlate the conserved residues to enzyme mechanism we are yet to find a method to annotate sequence to substrate specificity.

Sudip Roy (Physical and Materials chemistry)

Molecular dynamics simulation of polyleucine in hexane, water and hexane water interface

We have performed atomistic molecular dynamics simulation on polyleucine for sufficiently long simulation time in water, hexane and in water hexane interface. Polyleucine has propensity to be in α-helix form. Hydrophobic nature of side chains helps it to interact well with non-polar environment and hence making it a good candidate to be a trans-membrane peptide. Folding and unfolding times of polyleucine in water membrane interface is quite large.

So it is good to start with model but similar system such as water-hexane interface, which retains the most important property of the water membrane interface. Thus carefully interpreted results from water-hexane interface can be helpful to understand the story of water membrane interface.

Structure prediction of a multi-domain protein pleckstrin and PcrA using molecular dynamics simulation

The objective of our study was to predict the structure of the multi-domain protein pleckstrin, which is a major phosphoprotein in the blood platelets. We have used molecular dynamic simulations and spin-labeling techniques to predict the structure of pleckstrin. The cysteine residues in the protein have been labeled with EPR spin label (SSS) to get distances as constraints in predicting the pleckstrin structure. Quantum chemical calculations were used for parameterization and to obtain the force fields of these attached spin labels.

The simulations carried out in water as a solvent and different water models like the SPC, TIP3P and TIP4P were also used. Optimized Potentials for Liquid Simulations (OPLS) force field was used to define a set of parameters for each atom present in the protein.

Molecular Dynamics trajectories were used to obtain the distance histograms and these were compared to the experimental histograms and it was found that the conformation of the protein changed with the change in water models used.

Our study shows the effect of solvent on the conformation of the protein and also the use of spin labeling technique to predict the structure of proteins, which cannot be crystallized.

PcrA, standing for Plasmid copy reduced, is a helicase that catalyses the unwinding from a free 3' end of double stranded plasmid DNA using ATP. PcrA contains all of the signature helicase motifs and, consequently, is also related to the vast number of RNA helicases that have been identified in eukaryotes.

We are exploiting the site directed spin labelling (SDSL) technique in GROMACS for determining the structural features of PcrA's (3PJR, 2PJR, 1QHH, 1PJR). By incorporating, atleast, two spin labeled side chains, distance between elements of secondary structure can be determined. The range of distances measured will provide a useful ruler for determining the spatial arrangement of known elements of secondary structure in a protein. These distances are characterized by PELDOR (Pulsed electron spin resonance spectroscopy) experimentally.

In our study, MTSSL [3-(methanesulfonylthiomethyl)-2,2,5,5-tetramethylpyrrolidin-1-yloxy)], the spin label, was used to modify the cysteine residues. Rationalization of the distances and their distributions, with the experimental datas, will be subsequently carried out by molecular dynamics simulations.

Molecular dynamics simulation of benzimidazole and phosphoric acid mixture: A potential polymer for fuel cell polymer membrane

Fuel cells are, in terms of economic and environmental concerns, an interesting alternatives to existing power conversion systems because they combine high efficiency with the usage of fuel that have the potential to be renewable. Polymer exchange membrane fuel cell (PEMFC) are becoming of great interest because of their low operating temperatures and their applications in transportation and portable electronics.

There are high demands to optimize the efficiency of PEMFC such as high conductivity at a wide temperature range. Especially to design a membrane that are stable at temperature above 100°C.

Benzimidazole (BI) and phosphoric acid (PPA) shows interesting properties in this respect. For different concentrations of phosphoric acid shows high proton conductivity well above T=100°C. While Nafion based fuel cells exhibit high conductivity only when hydrated, (Poly) BI/PPA systems operate even at low humidity. These membranes will be able to operate at high temperature (above 80°C).

We have done molecular dynamics simulation of BI, which is a monomer of Polybenzimidazole and phosphoric acid mixture to understand the underlying mechanism of proton conductivity in such system. Different proportion (1:2, 1:4, 1:6, 1:8, 1:14 and 1:16) of BI and PPA has been simulated at temperatures 380K and 450K. BI and PPA mixtures are analyzed hence proton conduction mechanism.

Adsorption of hydrogen gas on fluorinated metal organic framework by ab-initio quantum chemical method

We have computed the binding energy (adsorption energy) of the hydrogen molecule in Cu metal -centred fluorinated Metal Organic Framework (F-MOF-4) which was synthesized by P. Pachfule. We also carried out calculations on the non-fluorinated counterparts (exchanged fluorine atom by hydrogen atom)of the F-MOF-4 to get the difference in binding energy due to the change of organic ligand chemistry.

These quantum chemical calculations were performed using geometries obtained from x-ray crystal structure of F-MOF-4. We have performed cluster-based HF and MP2 calculation to get the binding energy of hydrogen molecule and probable binding sites by scanning different positions of F-MOF-4. We have performed calculations on F-MOF-4 clusters using the Gaussian 03 software suite.

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Kumar Vanka (Physical and Materials chemistry)

Members: Manoj Mane, Shantanu Kadam, Nishamool Kuriakose

Ziegler-Natta heterogeneous catalysis

In the previous year, the focus had been on understanding how internal and external donors stabilized the magnesium chloride support, before the binding of the octahedral titanium catalyst to the $MgCl_2$ surface. This year, computational investigations have been done on the nature of the enantiomorphic site control made possible by the proximity of adjacent donor groups. Results indicate that the zip coordination of donors provides an environment which can facilitate the experimentally observed heightened isotacticity in the presence of internal donors such di-iso-butyl phthalates.

Study of the structures of metal organic frameworks (MOFs)

As potential candidates for (i) the storage of gases that may be the fuel of the future, such as hydrogen, or (ii) the sequestration of Greenhouse gases such as carbon dioxide, MOFs have become the subject of intense research activity over the past decade. Computational investigations have been done to determine the structure in solution of new MOF structures that have been prepared experimentally at NCL and to rationalize the experimental observations with regard to the nature of the structures in different solvents.

Nickel-based oligomerization catalysis

Nickel-oxime systems have recently been found to be effective in dimerizing and trimerizing ethylene - leading to the formation of butene and hexene respectively. Last year, computational investigations were done to investigate the means of monomer insertion and termination. This year, the focus has been on understanding the means by which catalyst degradation can take place.

Development of an alternate accelerated stochastic simulations method to model chemical reactions

The Gillespie Algorithm is a well established means of using Kinetic Monte Carlo to determine the change in reactant, intermediate and species amounts during the course of a chemical reaction.

However, its principal weakness is that it is inhibitingly slow to track changes in species amounts, especially when the reactant amounts are large. To solve this problem, Gillespie has proposed an accelerated method, which expedites the process of determining the change in species amounts with change in time, but which is more complicated than the simple and elegant Exact Gillespie Algorithm.

We have attempted to develop an improved accelerated stochastic algorithm method that will combine the speed of Gillespie's accelerated algorithm with the simplicity of the Exact algorithm.

Study of the mechanism of oligomerization of ammonia borane

Ammonia borane is being considered a serious candidate for the efficient chemical storage of hydrogen, which makes it one of the most important molecules in chemistry today. Catalysts have been found that can dehydrogenate ammonia borane efficiently to produce hydrogen at room temperature, but the key problem that persists in such dehydrogenation processes is the failure to subsequently regenerate ammonia borane - which is turned into an oligomer during the process.

We have attempted to understand the means by which the oligmerization might be taking place, with special emphasis on the role of the catalyst in the process.

Neelanjana Sengupta (Physical and Materials chemistry)

Protein conformational disorders: Probing the mechanisms and pathways for protein misfolding and aggregation under ambient conditions.

The Amyloid β peptide

We have attempted to develop an understanding of the early events that give rise to amyloidogenesis, by studying the structural and dynamical changes taking place in the helical form of the Amyloid β(Aβ) peptide. Recent experiments suggesting the role of the helical form in membrane poration.

Further, the Aβ peptide is itself created from a larger, membrane spanning precursor protein, and there exist experimental evidence pointing to a helical form of the 42-residue segment within the membrane. Thus, the pathway from the helical to the amyloidogenic, extended β-sheet form may provide insight into ways of trapping the peptide into non-amyloidogenic conformations.

Molecular dynamics (MD) simulations of the helical form of the Aβ 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. 120 nanosecond MD trajectories were generated by solvating the peptide with more than 2000 water molecules, using the TIP3P water model, at 1 atmosephere pressure and at the room temperature. The CHARMM22 force field and the NAMD simulation package were used.

The radius of gyration (R_g) shows distinct conformational changes in the peptide over the 120 ns simulation run. Specifically, there

is sudden loss of compactness between 25 and 80 ns (approximately), when the R_g value increases by 40%. This is followed by refolding, marked by decrease in the R_g. A more compact structure is noticed at about 100 ns. To narrow down on the location of the conformational change, we have calculated the root mean squared deviation (RMSD) of the peptide backbone, separately of three segments, residues 1-14, 15-28 and 29-42.

The results show that the 3rd (hydrophobic) segment has the greatest structural fluctuation, and that the 2nd segment, with the least amount of solvent penetration, is the most stable. 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 time correlation function.

Based on a geometric criterion, we have looked at hydrogen bonding between the peptide and the surrounding solvent, and have calculated hydrogen bonding time correlation functions and the mean decay times.

The α Synuclein peptide

The aggregation of the α-synuclein protein is the prime reason behind Parkinson's disease. It has been reported in the literature that certain amino acid mutations with the protein polymer increase the likelihood of the disease. We have begun MD simulation work to compare the structural fluctuations of the native and the mutated state, to probe solvent effect on conformational changes, and to understand how the mutations affect the stability and the rates of formation of the aggregated (diseased) state.

M. Karthikeyan (Digital Information Resource Center)

ChemScreener : Distributed In silico library design under drug-likeness constraints

In this project we are highlighting the progress made in developing a chemoinformatics application for distributed in silico library generation from known biologically active molecules under the additional constraint of drug-likeness and lead likeliness.

In this work we attempted to expand the scope of distributed computing environment using the server/client communication infrastructure Java RMI technology to design focused virtual library of molecules from molecules known to have biological active properties published in scientific literature.

This virtual library of molecules could be effectively used for further in-silico modeling and simulation studies related to drug design or material science in a virtually unlimited size of "chemical space", which can't even be sampled exhaustively for typical small molecules containing up to about 30 heavy atoms.

The server/client communication infrastructure employed is based on Java RMI and distributed as open source. Earlier we already described the application of the Java RMI architecture to distributed "harvesting" of chemical information from the Internet in combination with the Google API16, an application termed ChemXtreme[1], as well as the distributed computation of molecular properties via ChemStar[2]. While in both cases computational tasks are carried out in a distributed fashion, the kind of analysis performed is very different.

It is adoptable to virtually every computing task that can be parallelized, as earlier applications on such diverse tasks as distributed computing and distributed data mining of chemical information from the Internet demonstrated.

Early high-throughput screening and combinatorial library design both suffered from unfavorable physicochemical properties of the molecules they contained, giving for example too large or poorly permeable compounds unsuitable as leads. To circumvent this problem, in the application presented here the generation of structures in silico is combined with a drug-likeness filter which currently obeys the 'rule of five' but can be set to any user-definable filter and other advanced QSAR/QSPR/QSTR components.

This enables the generation of libraries of compounds which are tailored to specific targets or target classes, given that both the fragments employed for virtual synthesis as well as the drug-likeness filter can incorporate knowledge about the drug class considered.

In addition to calculating, as it is performed in the current implementation, drug-likeness for each structure in a distributed manner, further evaluations such as docking can also be implemented in this fashion.

Center of Excellence

Scientific Computing

Dr. Sanjeev Tambe (Chemical Engineering and Process Development)

Design, development and application of Artificial Neural Networks, and a Machine Learning

Design, development and application of Artificial Neural Networks (ANNs), and a Machine Learning (ML) for a variety of classification/pattern recognition/clustering/dimensionality reduction applications such as fault detection and diagnosis in chemical and biochemical processes.

Design, development and application of ANNs, fuzzy logic (FL), support vector regression (SVR), and genetic programming (GP) for a variety of chemical process engineering tasks such as steady-state and dynamic modeling, identification, monitoring, control and soft-sensor development.

Design, development and application of artificial intelligence based optimization formalisms such as genetic algorithms, Ant colony methods, Taboo search, simulated annealing, particle swarm, for optimization and scheduling of chemical and biochemical processes.

Application of artificial intelligence based modeling, optimization, data reconciliation, data validation formalisms for the power station of National Thermal Power Corporation (NTPC) (Sponsored project by NTPC).

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 40,000 lines of Java code.
- 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.

The software generates advisory for the power plant operators to control and optimize the power plant efficiency.

K. Selvaraj (Catalysis and Organic Chemistry)

Members: Sivaraj, Devendra Dixit

Catalysis / computational materials science

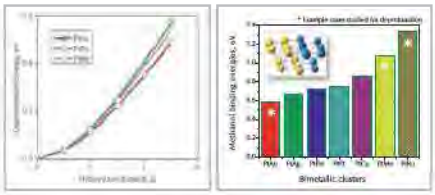
Background / objectives

The efficiency of noble and non-noble metal based the catalytic materials for direct methanol fuel cell (DMFC) applications are known to be sensitive for their chemical composition and also their size.

The small nano-clusters of the metallic catalysts are of great interest interms of their synthesis and structure property correlations for utilizing in solving specific application related problems such as methanol crossover. However, a basic understanding about their dependencies between the molecular level structure and the catalytic properties are known little. The present project attempts to understand this area using first principle methods specifically with the use of relativistic quantum mechanics.

Work done and discussion

Various subnono-bimetallic clusters of different noble and non-noble metals were modeled with different combinations of promising catalytic metallic elements. Their structure and stability aspects were studied using density functional theory based on both relatisitic and non-relativisitc quantum mechanics.



Several geometries were optimized and the most stable clusters have been identified. More over the methanol adsorption on them were studied in detail with calculated energetic related to adsorption and de-protonation of methanol etc.

were studied in detail with calculated energetic related to adsorption and de-protonation of methanol etc.

The results showed the a selective combinations of Pt based bi-metallic subnano clusters exhibit the best adsorption possibilities and also effective to deprotonate the methanol to start the methanol oxidation process at anode.

Microreaction Technology

With NCL's strengths in synthesis, catalysis, analysis, engineering and direct relevance with the industrial research, a Centre of Excellence on Microreaction Technology (CoE) was established in 2008. The CoE is a long term program 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. Currently, the CoE is an internal network of activities between 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. New proposals are considered for inclusion in the CoE annually and Director, NCL takes the decision on the basis of the recommendations of the monitoring committee. In the second year, the following four projects were considered under the CoE:

1. Understanding hydrodynamics and scale-out strategies using microreactors
2. Microreactor based organic process development
3. Continuous process for functionalized nanoparticles and nanogels
4. Microreaction technology for development of hydrogel based prototype diagnostic disposable devices

Amol A. Kulkarni (Chemical Engineering and Process Development)

Members : Chaitanya M. Karale, Akshay Singan (IIT-Madras), Sujoy Debnath, P. R. Naren
Collaborators : Prof. Niket Kaisare (IIT-Madras), Prof. Achim Kienle (MPI-Magdeburg)

Understanding scale-out strategies using microreactors

In the present report, we have focused our attention on the following specific components that fall in the large class of issues under the 'development of scale-out strategies' for microreactor systems: (i) External scale-out strategy: flow distribution and residence time distribution, (ii) Understanding the flow in spiralmicroreactor, (iii) Modelling and simulation of a complex network of reactions for flow synthesis of 5-nitro salicylic acid and (iv) Flow and heat transfer in small channels

Flow distribution in a fractal based network of mini channels

Micro-channel devices are increasingly being used in the industry because their small dimensions provide precise control of residence time, fast heat and mass transfer rates, and practically isothermal conditions even for highly exothermic reactions. Industrial scale production of fine chemicals requires "numbering up" or "scale-out".

Typical methods of scale-out can be classified as internal and external scale-out. An important consideration in scale-out is to ensure identical flow conditions in every channel of the scaled-out network. The performance of such networks has a significant effect of the design and the relative orientation of channels.

In view of this, here we demonstrate an external scale-out approach and bring out the associated hydrodynamics in a fractal based mini channel network for single and two-phase flow. The focus will be on the effect of the channel geometry, orientation of the network, flow rate and the flow ratio of the two fluids on flow distribution in individual channels of the network.

Fig. 1 shows a network of mini-channels constructed from 10 cm long stainless steel tubes and diameters varying from 1/2" to 1/16". The inset figure shows single in-house designed and fabricated flow splitter which divides the flow from a parent channel (1/2", 1/4", 1/8") to four daughter channels (1/4", 1/8", 1/16", respectively). The diameter of a daughter channel is half its parent channel to ensure that the total volume of the reaction channels is the same at every level of splitting.

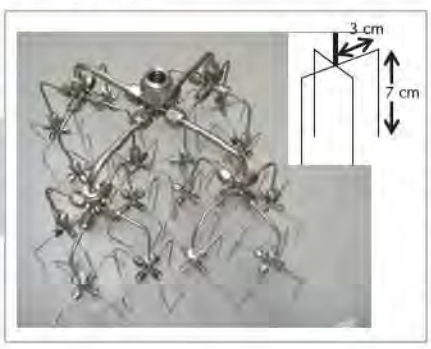


Fig. 1: The 64 channel network in vertically downward orientation. Inset: schematic of a single split

The network in Fig. 1 is in vertically downward orientation. The flow distribution was obtained by measuring the volume of fluid collected from each channel in a fixed time span. Measurements were made for water (single phase flow), and kerosene-water mixtures (two-phase flow).

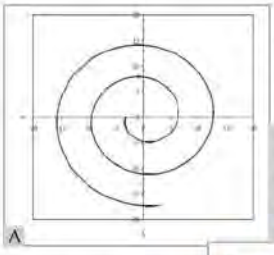
The flow rates were varied to achieve the inlet Re in the range 40-400. The effect of variation in the Water : Kerosene flow ratio at the inlet on % deviation as well as the residence

Microreaction Technology

time distribution studies were performed. The detailed observations are skipped for brevity. Further experiments to elucidate the effect of wetting behavior with different fluids are ongoing.

Flow modeling in spiral minichannel reactor

Earlier we had done the continuous flow synthesis of Ag nanoparticles in a spiral mini channel reactor. It was seen that the spiral geometry helps develop secondary flows that lead to better local mixing and reduced back mixing. Further this was concept was extended for in-line separation of nanoparticles. It was observed that in order to realize a reliable design, it would be necessary to know the flow in the device. And hence, to quantify the effect of spiral geometry and inlet flow rates further, it was thought desirable to do a detailed CFD simulation of the geometry.



The 3D geometry was developed using Gambit and the flow was simulated using Fluent 6.3.26. The fluid was considered as water and all simulations were at steady state with laminar viscosity model. On simulating the flow when fluid enters from the actual outlet of the spiral (i.e. inlet at the end of the outer most curve), it was seen that the Deans flow becomes strong towards the centre of the spiral. The simulation results are shown below as the contour plots of different flow parameters.

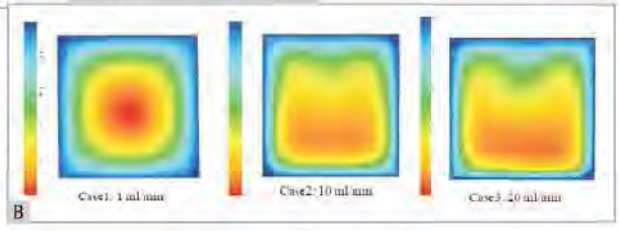


Fig.: 2(A): Spiral geometry, (B): Velocity contours at the exit of spiral at 1 ml/min, 10 ml/min and 20 ml/min inlet flow rates.

Reaction engineering model for continuous flow nitration of salicylic acid

The nitration of Salicylic acid (SA) forms an important intermediate, 5-Nitrosalicylic acid (5NSA), which is used in the synthesis of Mesalazine, a drug for the treatment of ulcerative colitis. Recently, Kulkarni et al. have shown that the reaction is feasible when done in continuous flow using microreactor at higher temperature and in very small time ~ 60 s with the complete homogeneity in the solution by using excess of acetic acid.

Here we aim to identify the optimal design of such a tubular reactor and the operating conditions that yield the best performance from this reaction, avoid the formation of dangerous hotspots that may lead to runaway situation and also establish guidelines towards its scale-out. An attempt is made using a phenomenological model that uses the reaction scheme.

A tubular reactor (1mm i.d. and 1 m long) is considered for developing the model. The model is 2d axisymmetric in r and the z coordinates for framing the governing equations. 10 grids in radial and 100 grids in the axial direction are used. Typical species transport equation is shown here (for 5NSA). The mass fraction of the species at each grid point is calculated by solving the above equation. Constant temperature wall boundary condition or gradient temperature condition was used. The equations were discretized using control volume method and Thomas algorithm. The time step is calculated using CFL criterion.

The simulations were carried out for understanding the effect of inlet composition, temperature of the medium surrounding the tube, tube diameter (heat transfer area) and the residence time/inlet velocity (v). The simulations help to identify the design guidelines, operational effects and the situations to yield the best performance. Further, the developed model will be validated with experimental data.

$$\frac{\partial(\rho C_{5NS})}{\partial t}+\frac{\partial}{\partial z}(u\rho C_{5NS})+\frac{1}{r}\frac{\partial}{\partial r}(rpVC_{5NS})=\frac{\partial}{\partial z}\left(\mu\frac{\partial C_{5NS}}{\partial z}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial C_{5NS}}{\partial r}\right)+S_{C5NS}$$

$$where\ S_{C5NS}=k_1C_{AS}C_{HNO3}-k_4C_{5NS}C_{HNO3}-k_5C_{5NS}C_{HNO3}$$

Single phase flow and heat transfer in parallel channels

The present research work is focused on developing models, methodology and quantitative understanding of flow, mixing and heat transfer in small channels. The size of the channels under the study ranges from few micrometers (700 µm) to millimeters (2 mm). Single phase flow and heat transfer in small channels was studied.

The study involved experimental as well as numerical investigations. Flow and heat transfer experiments were carried out with a micro-channel plate comprising of 20 parallel channels. Pressure drop and heat transfer coefficients were experimentally measured.

Flow and heat transfer in the experimental set-up were simulated using CFD models to provide useful and quantitative information on developing flow regions, axial heat conduction, conjugate heat transfer, effect of the design inlet and outlet manifolds. It was found that including the entrance effects, the experimental Poiseuille number was in agreement with that of conventional theory of laminar flow in macro channels.

In case of heat transfer, the Nusselt number calculated from the experimental data was well predicted by the CFD analysis. The conjugate heat transfer methodology was therefore found to be useful for detailed understanding of wall heat conduction. The methodology and the results presented here will be useful for further work on flow and heat transfer in micro-channels.

Microreaction Technology

Dr. R. A. Joshi (Organic Chemistry),
Dr. R. R. Joshi (Organic Chemistry),
Dr. A. A. Kulkarni (Chemical Engineering and Process Development)
Members : M. Munshi, N. T. Nivangune

Microreactor based process development

Continuous flow homogeneous nitration of benzaldehyde

Recently, the nitration of benzaldehyde using a nitrating mixture has been reported in a microreactor (Kulkarni et al. 2009). While it is known that benzaldehyde is not a very active molecule, its nitration with nitrating agent can be expedited in the presence of acetic anhydride. It is known that the presence of acetic anhydride along with the nitrating mixture helps to rapidly generate nitronium ions thereby expediting the nitration.

In the absence of any quantitative information on this system, here we report our observations from the nitration of benzaldehyde using the nitrating agent (HNO_3 + H_2SO_4) in the microchannel reactor. For the continuous flow experiments, the experimental set-up consisted of two syringe pumps (Boading Longer, China) loaded with 20 ml glass syringes connected to SS316 tubes (1/16" o.d.) through an in-house developed and fabricated glass to metal connector made in PTFE.

Experiments in continuous flow showed different features. Even after repetitive experiments at different temperatures and the necessary residence time (observed from batch experiments), no fluid came out of the reaction tube and it was completely blocked. The experiments were repeated several times and the observation was consistent. This was an effect of the presence of acetic anhydride in the reaction media, which makes the solution homogeneous.

Thus, all the products and impurities that are formed during the reactions remain in the reaction mixture. However, the solubility of the product (nitro derivatives of benzaldehyde as well as the benzoic acid formed due to over-oxidation) in the reaction mixture is relatively less.

This results in precipitation of the products and subsequent blocking of the channel path. In the case of two phase reaction (Kulkarni et al. 2009), the slug formation takes place and reaction occurs at the liquid-liquid interface and byproducts remain in the aqueous layer and products in organic layer which are further separated by ether extraction.

The homogeneous system (with acetic anhydride), relatively higher yield of ortho isomer can be obtained by having smaller residence time yet, at the cost of lower conversion.

Two step continuous flow syntheses of Azodyes using T-micromixers

Diazotization and diazocoupling reactions are important class of organic reactions, which are currently performed with mineral acids and alkalies as catalysts. In the present work we have demonstrated the diazotization of aromatic amines between the temperature range 0-30°C and its azocoupling with 2-naphthol at room temperature (25-28 °C) for the synthses of azodyes.

Continuous flow process for the preparation of sulphoxide compounds

A continuous process for the preparation of sulphoxide compounds is developed and demonstrated. Particularly the invention relates to an efficient micro reactor based continuous flow process for the synthesis of sulphoxide compounds such as modafinil compounds and proton pump inhibitors.

Programs in progress

Reactions generating solid particles ($MgCl_2$ precipitation reaction), continuous flow synthesis of Schiff bases (l-hydroxy cetronellal + methyl antranilate, benzaldehyde + methyl antranilate, carvone + cyclohexyl amine), b-chrotonate esters.

Microreaction Technology

B. L. V. Prasad (Physical and Materials Chemistry)
V. Ravi Kumar (Chemical Engineering and Process Development)
A. A. Kulkarni (Chemical Engineering and Process Development)

Continuous process for functionalized nanoparticles and their scale-up

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. In order to develop a synthsis protocol and methodology for the nanoparticles, initially, the studies were done for the model systems viz. synthesis of Ag and Au nanoparticles.

The silver nanoparticles were synthesized in a microreactor which has a spiral geometry at different flow rates in continuous flow method.

The process parameters to synthesize silver nanoparticles using a biosurfactant called as sophorolipid were optimized and the particles were synthesized in continuous flow by using a helical coil of i.d 1.38 mm.

Since the velocity profiles in helical coil are parabolic, there was a time deviation of the particles spent at different location and this leads to the broader size distributions. To eliminate this limitation silver nanoparticles were synthesized in a microreactor which has spiral geometry.

This microreactor has channel dimensions of 70 cm length and 0.5 mm depth and width, made up of PMMA material using micro machining technique. The silver nanoparticles synthesized in both the microreactors (helical coil and spiral) for same residence time were compared.

The particles which were synthesized in helical coil are of size 8-10 nm with some irregularity in shapes, but the particles which were synthesized in spiral reactor were monodisperse with 3-4 nm in size.

In continuation to this work the segmented flow synthesis of silver nanoparticles were studied in spiral microreactor.

Here silver nanoparticles were synthesized in segmented flow using air and kerosene as gas and liquid phases respectively. Silver nanoparticles were synthesized using stearic acid sophorolipid as reducing and capping agent in basic medium and the experimental set up was as follows.

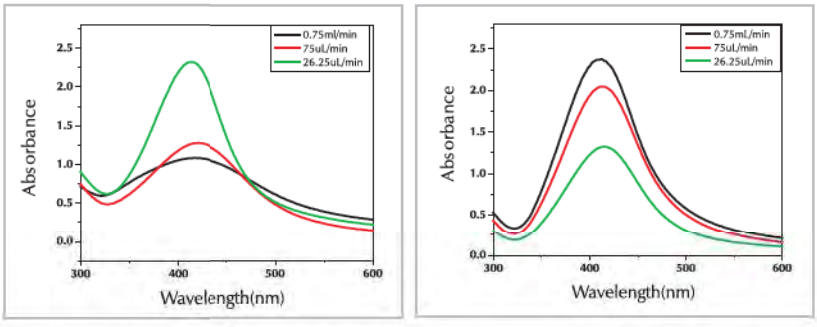
The UV-Visible and DLS studies of the silver nanoparticles synthesized in segmented flow using air as inert phase shows that the particles are smaller and mono disperse at lower flow rates. This is the general trend which was observed in continuous flow synthesis also.

The particle size decreased and became mono disperse from 180 to 10nm when the flow rate had decreased from 1mL/min to 35μL/min. The TEM results are also comparable with the DLS results and both TEM and DLS results are from uncentrifuged samples. In case of kerosene and liquid two phase flow the results were not clear.

The UV-Visible results shows that the particle sizes are comparable in all the cases and the intensity of the particles synthesized at lower flow rates were less and this can be conformed with DLS particle size distributions.

The TEM image of the Ag NPs synthesized at 35 μL/min were well shaped and with a size of 4-5 nm which is less than the particles synthesized in Gas-liquid segmented flow (10nm).

Here also all the results are from uncentrifuged samples. Further work and analysis of these results are under progress.



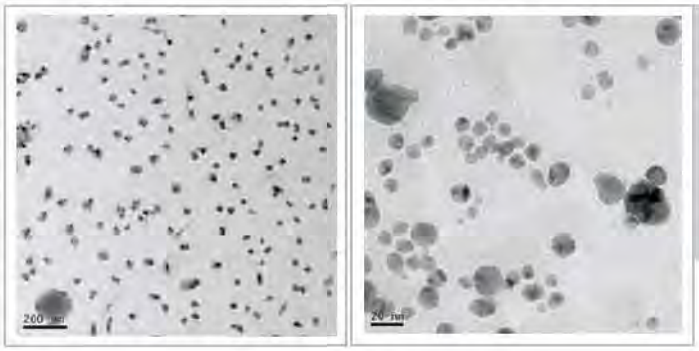


Fig. 3: (Top Row) UV-Visible spectra of Ag NPs synthesized in spiral microreactor which was operated in segmented flow and (Bottom Row) TEM images obtained for (Left) air as inert phase, (Right) kerosene as inert phase. Legends indicate the total flow rate

Resource Centers

Catalyst PILOT PLANT

Catalyst Pilot Plant (CPP) is well equipped with all the facilities required for the synthesis of catalytic materials and environmentally benign batch processes at different scale of operations. Facilities include mixing vessels; stirred reactors with capacity ranging from 100 mL to 1000 L, filtration equipments, dryers, calciners, mixtruder, laboratory hand operated extruder, and fixed bed micro-reactors.

CPP is also well supported by an array of physico-chemical characterization facilities required for various products. 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, development of the scalable and cost-effective synthesis route, improvement in catalytic processes, scale up and supply the client-specific materials. Some of the activities are described below:

R & D Activities

- Oxyanion-induced hydrothermal crystallization of Sn-BEA molecular sieve in fluoride medium
- Recycling of mother liquor produced during the hydrothermal crystallization of K-LTL zeolite
- Esterification of carboxylic acid with alcohol
- Transesterification of sunflower oil with alcohol
- Development and supply of catalyst for tert-butyl amine from isobutylene and ammonia

Services Offered

Supply of D.M.Water, raw materials, finished catalysts, chemical analyses by AAS to research community

Center for MATERIALS CHARACTERIZATION

Center for Materials Characterization (CMC) houses some of the most sophisticated equipments utilized for R & D projects of the Laboratory. The 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, inorganic, bioorganic, organometallic and natural product novel 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 AXS 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 with EDAX)
- **Environmental scanning electron microscopy** (FEI Quanta 200 3D with EDAX)
- **High resolution transmission electron microscopy** (Tecnai F 30 with 300 kV FEG; FEI make)
- **Transmission electron microscopy** (Tecnai T20 with 200 kV LaB6; FEI make)
- **Electron spectroscopy** (ESCA 3000 system)
- **Mass spectrometry** (LC-MS/MS-TOF, HR-MS, and MALDI-TOF-MS)
- **Magnetic measurements** (EG & G PAR 4500 vibrating sample magnetometer)

	In-house	Outside
Samples analysed	44647	228
Total number of samples	44875	
Total earning from outside samples	₹ 26,32,504/-	

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 activates 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 the expertise in the following areas

- Solid and solution state NMR methodology development.
- Structural elucidation of organic and bio-organic molecules
- Impurity profiling of pharmaceuticals
- Micro structural analysis of polymers
- NMR of molecular self assemblies
- NMR of gels
- Protein- ligand binding studies
- NMR in Bio transformations
- Protein-nucleic acid interactions
- Diffusion by pulse field gradient NMR
- Application of solid-state NMR in Materials Science (polymers, molecular sieves, layered oxides, biomaterials, 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)
- 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}P, ^{13}C, ^{15}N and ^{1}H), a 5mm inverse broad band probe (^{95}Mo-^{31}P) with gradients, a 10 mm high temperature ^{13}C probe for polymer characterization, a 5mm triple resonance TXI probe with gradients (^{13}C,^{15}N,^{1}H) and a 5mm broad band BBFO probe with gradients (^{109}Ag-^{31}P and ^{1}H,^{19}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}Mo-^{31}P) observe (BBO) probe with gradients, ^{1}H-^{13}C inverse (SEI) probe with gradients, high temperature (SEX) ^{13}C probe and a broad band observe probe (BBFO) with gradients (^{109}Ag-^{31}P and ^{1}H,^{19}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}P-^{15}N, ^{1}H), a 2.5mm MAS probe with STMAS attachment, a 4mm double resonance probe with low gamma nuclei capability, a wide line probe (^{109}Ag to ^{31}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 carousal auto-sampler. This has a QNP (^{1}H,^{13}C,^{31}P and ^{19}F) probe and a dedicated 1H probe.

	In-house	Outside	
		Industry	R&D and academic institutes
Samples analysed	25,539	754	57
Total number of samples	26,350		
Total earning from outside samples	₹ 50,83,969/-		

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.

Network Administration Unit

The Unit enhanced its existing Internet Bandwidth from 34 Mbps standard leased line to 100 Mbps dedicated leased line on fail safe OFC link with Ethernet connectivity to fulfill all the Internet requirements of the lab, 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. 24x7 these services provide 100% throughput with 100 Mbps dedicated BW and network uptime >99%. This has helped to overcome all our limitations in dealing with various BW critical applications.

Additionally, Unit enhanced the existing Internet Bandwidth of NCL Innovation Park from 2 Mbps shared leased line to 6 Mbps standard one. Both the links are regularly monitored using web-based tool that enables to gain a real-time, end-to-end view with respect to various applications, system and network performance.

During this year, Unit procured state-of-the-art server/storage hardware consisting of latest technology blade servers, SAN (storage access network) and NAS (Network array storage). The hardware was mainly utilized for the deployment Microsoft Dynamics platform based EMIS (ERP) software and Microsoft Exchange 2007 server based mailing system in the laboratory. The Unit also procured Gigabit switches in the form of Chases to be deployed in various divisions to upgrade their network to Gigabit.

The Unit newly deployed Microsoft Exchange 2007 server based E-mailing system, for the benefit of all the E-mail ID users in the lab. The activity also included deployment of 'Root Domain Controller' and 'Additional Domain Controller' along with the configuration of DNS and DHCP servers and creation of User Objects, User Groups and their mailboxes. Mails of all the E-mail ID users were migrated from their old mail clients such as Thunderbird, Mozilla, Eudora to 'Outlook Express' or 'Outlook Web Access'. All the desktop PCs in the lab were migrated from work group to a newly created domain (ncl.res.in), common for all, maintaining uniformity in the names of these assets. An SSL certification was procured from Entrust (USA) in order to make the MS Exchange a secure product, so that we can use mailing securely and in the recipient's desired encryption format. A backup solution was procured and installed for generating periodic backups.

Unit has procured license for deploying server grade antivirus software, which provides virus-free network environment at NCL. Also its older version was upgraded to the higher version. This antivirus software helps in web based monitoring and management of about 60 servers and 1000 network PCs in the lab, securing them from viruses, malware, grayware, Web threats and spyware. It also helps to minimize the risk of spyware-related slowdowns, crashes, and support calls.

1500 E-mail ID users in the lab daily send or receive average 8000 mails. Even though all our mail servers are well equipped with adequate anti-virus solution, there are daily additions of many more attacks which need to be constantly prevented from receiving unsolicited mails getting delivered to the mail recipients. For this purpose Unit has deployed an anti-spamming solution called IMSS (Inter Scan Messaging Security Suite) to guard emails against hazards like spam, viruses, Trojans. This deployment has brought down SPAM control rate from 50 to 55 % to 4 to 5 %.

The deployment also helps storing all spam mails received by the domain, on spam quarantine server for a period of six days. Its spam-notify feature provides daily spam digest on mail to every user so as to release any clean mail using the username / password, without involving the administrator. The deployment also facilitates every individual to consider certain mails to be non spam so that they can be released from his / her quarantine area and delivered as clean mails.

Unit provided Internet connectivity to the new P&AM building by activating over 350 LAN ports into its premises. Also all the newly created hub centers which were previously provided copper uplink from the nearby hubs, are provided Fiber uplink to boost the network speed. All these backbone links are created using OFC and the associated structured-cabling components. As on today 2500 LAN ports are active, all across the laboratory. Additionally, Unit has installed wireless network devices (Access points) to provide wireless connectivity in the conference halls / lecture halls of various divisions in the lab. To avoid any inconvenience to the users, no security is deployed at this moment and a plane unsecured network is made available to all.

Unit connected all the offices and labs of NCL Innovation Park by LAN. In addition to the activation of more than 200 data points, Unit also deployed state-of-the-art VoIP Technology using hard IP phones and soft phones with cameras and receptionist (IP) console in these premises. Almost all the area including open air lounge and canteen in this campus is converted into a secured Wi-Fi zone, using high power access points.

As an essential requirement of NKN, all the CSIR labs are suggested to ensure that in near future they will be equipped with Gigabit LAN Ethernet connectivity. In this regard, from this year Unit has taken up the mission of step-by-step migration of NCL network from Megabit to Gigabit LAN. Accordingly LAN network in the CMC, CEPD, PSE and part of P&AM

buildings is migrated from Megabit to Gigabit connectivity, by providing 10G backbone uplink and using advanced high performance Gigabit Ethernet switches, which provide high scalability, reliability and security needed to deliver the critical service levels of various Internet / intranet / data sharing applications.

While deploying WI-FI Technology to connect all the area of NCL colony and establishing a secured wireless network across the colony, the Unit also provided secured VPN Connectivity to allow many scientists to connect to their NCL office computers from home.

Unit initiates an Annual Maintenance Contract (AMC) for all the desktop, laptop PCs as well as other Computer Peripherals in the lab. This involves managing a help desk on campus that helps users logging all hardware, software issues including installations, reinstallations, repairs, reformatting, updating software, virus issues, etc. A web based 'Network Operations Center (NOC)' tool is made available to the users, from which control is exercised over the lab IT assets so as to provide an automated monitoring and management of services and service support.

Unit also avails 'Network and server Infrastructure Facility Management Services' to be provided for the Data Center. The scope of work involves monitoring & managing WAN / LAN network assets installed in the data center as well as NCL campus and various servers including blade servers, used for various applications in the data center.
Unit is also responsible for maintaining Web based 'Time attendance and Access control' Management system in NCL, NCL-Innovation Park, Medical center, GJ Hostel as well as new P&AM building. The responsibilities include 1) Time & Attendance Management 2) Access Control Management 3) Visitor Management and 4) Printing and activation of smart cards. A central database of all the online readers is collected on a high end server and its web based access is provided to all the responsible officials for viewing the attendance and access control related reports. Web based Visitor Management System (VMS), deployed by the Unit helps scientists to pre-book their appointments of future dates and alerts the VMS operator at the reception. The system saves operator's time and repeated work of data entry for the regular visitors.

Unit also manages to issue biometric printed ID cards to all the newly joined staff, students, library members, etc and provide access privileges to them. While managing this activity, Unit takes care of 65 LAN based readers. Till date, more than 2500 staff members and library visitors are provided printed RF cards.

Ever since we have switched over to Microsoft based (Exchange 2007) mailing system, E-mail system has become a powerful and speedy means of communication and every Scientist, Staff, Research Student, Project Assistant as well as any authorized person who is provided E-mail access uses this facility for research / (official) business. Considering this fact, as a 'System Admin' the Unit considers this as its prime duty to ensure that E-mail ID users of the lab are utilizing this tool in a responsible, effective and lawful manner. Therefore, to make users adhere to certain guidelines, while writing, replying and maintaining E-mails, Unit has published an 'E-mail password Policy' as well as an 'E-mail Retention Policy'. The purpose of these policies is to ensure proper use of NCL's email system and make users aware of what everyone should treat as an acceptable or an unacceptable usage of our E-mail system and minimize the legal risks involved in the use of e-mail and also make them alert of the penalty clause in case of misuse / violation of rules, mentioned therein.

During this block year the Unit also helped CSIR HQ in conducting on line CASE (combined administrative services examination 2009) exams for the recruitment of Section Officers and Executive Assistants in CSIR. All the IT facilities were provided to conduct this examination. About 450 candidates appeared for the exam, as per the scheduled program.

Unit has also developed its own intranet website, made available from ncl@home page that provides all the related information, guidelines, and announcements. The site is maintained by regularly updating its contents.

Knowledge Resource Centre

Print collection: NCL KRC as on March, 2010, has a total collection of 1.39 lakhs, which includes books and bound volumes of journals. During 2009-10, 553 Books were purchased and 148 Indian and Foreign print journals were subscribed. KRC subscribed 56 Electronic journals. Research students submitted 55 theses and link has been provided on intranet to the awarded theses.

Electronic Resources: This year KRC subscribed to American Chemical Society & Elsevier journals only in electronic form. This has been initiated keeping in view the future changes in the publication policies, inflation in subscription costs & users preference to Electronic version.

During 2009-10, KRC subscribed to Springer & RSC E books.. Access to, Annual Reviews, Methods in Enzymology series, Chemical Abstracts on CD, India Patents, Chemical Business News Base was continued.

NCL KRC, being the part of CSIR consortium project, provided access to more than 3300 journals of 10 publishers. Access to databases like Web of Science, Delphion, DII was also available under consortium project

KRC Homepage provides links to all the subscribed E-resources and also information about the services offered.

KRC Services: During 2009-10, nineteen new pharmaceutical companies availed information related services like document delivery of journal articles, patents, searching of specialized online databases and translation of scientific documents. Membership to the KRC is also open to research students of various colleges, universities and to the industries from all over India. This year 355 outside members referred the library. A reading lounge with conducive atmosphere encourages readers to browse the latest arrivals of journal issues and books.

RFID Library System: KRC's RFID system is working up to the mark for last two years. Radio Frequency Identification (RFID) system for KRC helps for self check-outs by members, stock verification, misplaced documents search and documents security. This year sample physical verification of books & bound volumes was done with the help of RFID system.

Annual Events: Book Exhibitions was arranged in Aug. 09, which provided an opportunity to readers to browse latest books and select books of their choice for purchase. This year KRC organized two exhibitions to broaden the scope of book selection published by various publishers.

National Collection of INDUSTRIAL MICROORGANISMS

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 about ₹ 77 lakhs during the year by providing cultures to industries and research organizations 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.

	Number of cultures		Total
	Government organization	Private organization	
Nos	1940	6526	8466
Amount(₹)	5,35,522	71,98,645	77,34,167

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, e.g., 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.

The patent has been licensed to one of the pharmaceutical industries, Hygeia Laboratories, Jejuri, Pune. Presently, 5 kg of the final product is produced per year using this technology as one of the steps (U.S. patent No. 6,448,051 B1).

NCL INNOVATIONS

NCL Innovations was founded to champion the cause of technology innovations within the organization. Its mission is to find means and ways to help the birth of new technology ideas and assist and support their translation into products and successful exploitation.

NCL Innovations 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.

A schematic illustration of the various aspects of technology commercialization and various groups that play a role

NCL Innovation Park

The year 2009-2010 saw efforts from the NCL Innovations team in forging longer-term public-private partnerships for NCL. Operational models were conceptualized and presented to potential partners.

NCL Innovations is expecting to take at least one of these initiatives to fruition during the year 2010-2011.viz. CSIR Innovation Complex, Pramod Chaudhari Innovation Centre and setting-up of CII- Biotechnology Resource Centre.

NCL Technology and Entrepreneurship Club

NCL Students at TLEP, Hyderabad

CSIR conducts a yearly program on Technology Led Entrepreneurship for research students in CSIR labs. NCL Innovations facilitated the participation of twelve NCL students this programme.

A talk by Mr. Rajmohan and Mr. Anish (both PhD students from National Institute of Immunology) on the topic "PLA based Artificial Skin Substitute: Concept to Market", on 21st May 2009. Mr. Anish and Mr. Rajmohan won the Intel-U of Berkeley business plan competition.

Lectures on "How to Write a Good Resume (Academic and Industrial/Business Resume)" by Dr. K. Guruswamy, NCL, "Writing resumes for industry/business jobs" by Dr. V. Premnath, "Careers in academic and research organizations" by Dr. Ashish Lele, "Taking up entrepreneurship as a career" by Mr. Kaushik Gala and "Careers in industry" by Dr. Chetan Gadgil were organized.

Mr. M.V. Shankar Principal Scientist, Dow Chemical International Pvt. Ltd., Pune and Dr. Gopakumar G. Nair, Founder and CEO, Gopakumar Nair Associates, Mumbai delivered lectures under NCL Innovations Seminar Series.

Outreach, networking and talks

Given NCL Innovations goal to promote a supportive environment for technology innovation/ innovators and a spirit of celebration of technology innovation, outreach activities by NCL Innovations staff is an important aspect of the group's activities. Networking with potential partners and other stakeholders is also important to NCL Innovation. This year, NCL Innovations staff made small beginnings in this direction: Dr. Premnath delivered the talks on Technology Commercialization : Perspectives and insights from NCL at Indian Institute of Technology Mumbai and Inventing, Patenting and Technology Commercialization in Practice: Some Insights for the "Indian Bayh Dole Act" Review of Indian bay Dole Bill at NUJS Kolkata

Institutional mechanisms

The NCL Innovations contributed in significant ways in shaping the new schemes of the CSIR. With the intention of promoting technology entrepreneurship and better technology commercialization results, the Government of India on 25 May 2009 announced the "Knowledge-to-Equity" scheme whereby that CSIR institutions shall be allowed to transfer knowhow and provide related support services to an entity in lieu of equity.

CSIR Innovation Complex @ NCL Campus is intended as a world-class innovation eco-system build by using a PPP model that will leverage CSIR strengths to develop and efficiently take technologies to the market. NCL Innovations initiated this project and made significant contribution in planning, coordinating with Director, NCL, DG-CSIR, and relevant officials from CSIR-HQ and other govt. agencies, creating various documents and strategizing as to how to take it forward.

CSIR Tech

CSIR is working on creating a new company (CSIR Tech)which is intended to work closely with CSIR laboratories to commercialize CSIR technologies and intellectual property primarily (but not exclusively) through technology start-ups.

NCL Innovations scientists were involved in planning, coordinating and executing various initiatives aimed at creation of CSIR Tech. Starting from exploring various models (from India and around the world) that could be adopted, working out the structuring of the company (should it be private or public limited etc.), financial details, potential investment patterns, technology transfer issues, interacting closely with potential partners, sorting out financial, legal, structuring questions, and creating necessary documents, and supporting materials and coordinating with DG-CSIR and Director, NCL and high-level committees empowered to create CSIR Tech.

Technology Marketing

NCLInnovations.org is the technology platform for NCL. The site was created to showcase NCL technologies, achievements, and to market and publicize

NCL INNOVATIONS

current technology/knowhow available at NCL to potential collaborators and industry partners. This website details the various tech transfer policies and how NCL would engage with potential partners.

NCL Innovations scientists screened NCL's technology/patent portfolio and identified technologies with high-potential for commercialization and highlighted them in the "Available Knowhow" section in the website. Also, they created attractive write-ups for each technology portfolio listing their value, market feasibility and technology status, etc. These write-ups provide a glimpse into NCL's capabilities into those technologies in a nutshell. This website also contains various topics highlighting

NCL's track record in technology transfer and commercialization, list of patents, history of technology at NCL, etc

IP Valuation/Support for Licensing Deals/Negotiations

NCL Innovations scientists provided support and financial/market analysis to negotiate deals for licensing out NCL technology/IP. This involved conducting detailed market analysis of the technology products, collecting market data, using financial models to estimate the value of the IP/technology being sought, and recommending to the negotiating team/leadership about how much NCL's technology is worth for the company.

Valuation analysis for two licensing deals (NAVE-10 - Celanese and ATBS - Vinati) was performed by NCL Innovations scientists. These analyses helped the negotiation team to make informed decisions.

NCL Technology Fund

NCL Innovations scientists proposed the creation of a dedicated "Technology Fund" at NCL to fund early stage technology ideas. This fund was created by Director, NCL in Jan 2010. Proposals for technology development were called for, and two such proposals were received.

NCLI scientists evaluated these technology proposals from NCL scientists and provided feedback as to how to position the projects to create maximum value. Evaluation of one such proposal ("Depolymerization of Lignin Using Catalyst") led to a patent landscape analysis being conducted. Even though no proposals were funded through this fund, other technology ideas from NCL scientists are being scouted for.

Program planning, proposals and fund raising

During the year, NCL Innovations along with Venture Center wrote several proposals to build facilities, resources, programs and activities focused around various aspects of technology innovation. It is expected that several of these will reach fruition during 2010-2011.

IP Group at NCL

NCL has entered into an agreement with M/s Gnanlex Hermeneutics, Mumbai last year and continued their services for the financial year 2009-10, to provide necessary support to IPG for identifying inventions through discussions with scientists, carry out patentability assessments and drafting of patent specifications.

Other services offered by M/s Gnanlex Hermeneutics, Mumbai include

- Prior art search report for Dr. Satyanarayana titled "Catalysis for conversion of pentenenitrile to pyridine"
- Prior art search report for "Catalyst for toluene alkylation"
- Patent landscape report for Dr. Paresh Dhepe titled "Depolymerization of lignin using catalysts"

Number of invention disclosure (Calendar year)	39
Number of patents filed in India (Calendar year)	19
Number of patents filed outside India (Calendar year)	4
Number of patents licensed/ assigned	1
Number of Indian patents granted (calendar year)	83
Number of foreign patents granted (Calendar year)	21

Licenses and patents for the calendar year 2009

Licensing

One portfolio was licensed to Sud-Chemie India Pvt. Ltd. In Feb. 2009 for a process for the preparation of crystalline microporous titanium silicate. The process is covered by two US and two Indian patents.

S & T Support Services

Business DEVELOPMENT

Business Development Division (BDD) takes care of various aspects of business planning, contracts management, strategy consulting, and event management. Significant portion of NCL's budget is generated through contract R&D services, consultancy and technology licensing.

The division is staffed with management graduates who work as technology facilitators interfacing with scientists, industries, government, financial institutions, other statutory agencies, etc.

Business facilitation

NCL is constantly exploring opportunities to work with industrial customers on challenging research problems which have an impact on their performance. 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 plays a technology facilitation role through discussions related to project proposals, pricing issues and contracts management. NCL believes in the credo that NCL wins only if its customer wins. Consequently, NCL constantly aims at building a win-win relationship with all its customers. During the year NCL worked with 38 Indian and 13 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. NCL also actively participates in the exhibitions related to scientific achievements organized by other agencies.

The Division organized CSIR Programme on Youth for leadership in Science (CPYLS) for standard X meritorious students during 28-29 January 2010. The division coordinated the visits of Shri. Prithiviraj Chavan, Vice president of CSIR to NCL and Dr. Manmohan Singh, President of CSIR on the occasion of NCL Diamond Jubilee Celebrations.

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 challan 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 systems 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 NCL performance, 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.

PMIS is a centralized document management system holding all project records at one place. The project records are available to the concerned scientists through MIS website (24 x 7 hours). MIS group creates all the project records internally and same is made available on the MIS website to the scientists. The scientists are provided with a login and password to access their project records directly from their desktops. All project documents like agreement, project proposal, project initiation, challans, and funds received and due are available on

the fly as and when the records are created by MIS group. In addition, there is an upload facility for 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 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. PMIS sends alert mails, whenever a payment is due. This helps MIS group to raise invoice and collect the funds in time.

The alert mail is also sent to the scientists, whenever a report to the client is due and scales up the alerts to HOD and 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.

MIS is responsible for the budgeting exercise of the laboratory. MIS along with 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, 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 equipments for the laboratory, divisional office requirements for office equipments, consumables and small scientific equipments required in the divisions. The requirements are compiled into appropriate formats and studied. The allocations are made based on the 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. MIS along with Director monitors 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

- Alkyl Amines Chemicals Ltd.
- Aquapharm Chemicals P. Ltd.
- Aquatech Systems (Asia) P. Ltd.
- Asian Paints (India) Ltd.
- Biopore Implant
- Biopore Surgicals
- Chemspec Chemicals Pvt. Ltd.
- Chemtall-Rai india Ltd.
- Emcure Pharmaceutic als Ltd.
- Engenious Engineering Pvt. Ltd.
- FMC India Pvt. Ltd.
- Galaxy Surfactants Ltd.
- GE India Technology Centre Pvt. Ltd.
- Gharda Chemicals Ltd.
- GMM Pfaundler Ltd.
- Godavari Sugar Mills Ltd.
- Godrej Sara Lee Ltd.
- Gujarat Fluorochemic als Ltd.
- Hughes & Hughes Chem Ltd.
- Hygeia Laboratories
- I S Industries Pvt Ltd
- Indian Centre for Plastics in the Environment
- Kamud Drugs Pvt. Ltd.
- Kirloskar Oil Engines Limited
- Lupin Research Park
- MITSU Pvt. Ltd.
- Racold Thermo Ltd.
- Reliance Industries Ltd.
- Ross Lifesciecne Pvt Ltd.
- S C Johnson Products Pvt. Ltd.
- SANDOZ Private Ltd.
- Shree Baidyanath Ayurved Bhawan Pvt Ltd
- SRF Ltd.
- Sudarshan Chemical Industries Limited
- Sud-Chemie India Pvt. Ltd. (SCIL)
- Tata Chemicals Limited
- Torrent Pharmaceutic als Ltd.
- Wanbury Ltd.

Foreign customers

- BASF Catalysts LLC
- Celanese Ltd.
- Colgate Palmolive Company
- Dow Corning Ltd
- Eastman Chemical Company
- GE Plastics
- Honam Petrochemica l Corporation
- Johnson & Johnson Vision Care, Inc.
- New Century Lubricants Inc./Benefuel Inc.
- Solvay Solexis
- The Max Planck Society
- The Procter & Gamble Company
- Wellcome Trust

Human Resource MANAGEMENT

The Human Resource Management (HRM) Unit helps in promoting the competencies of the employees of NCL, student's community and guest workers to enable the laboratory to achieve its mission as well as strengthening scientific fraternity. The activities of Unit are listed below.

Training programmes arranged for NCL staff

Name of Programme	For	Date	No of Participants
Outbound training program on "Self-development"	Gr DNT Gr I & II	Aug 28, 2009	25
Multi-skill Training Program	Gr DNT	Sept 09 & 10, 2009	26
Multi-skill Training Program	Gr DNT	Sept 16 & 17, 2010	22
Noting & Drafting and Record Management	Administration Staff	Mar 10 & 11, 2009	25
Noting & Drafting and Record Management	Administration Staff	Mar 12 & 13, 2010	22

Short Term Summer/Winter Project

More than 310 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; as well as two students from abroad were trained at NCL.

The students for the short term projects worked normally for the period of two months to one year.

Guest workers

Fifty-four Guest-workers worked at NCL during the year including twelve fellows of various Indian sciences and engineering academies and two fellows from abroad.

Institutional visits

NCL receives many requests throughout the year from various academic and research institutes including PG colleges fifteen 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.
to visit NCL facilities. The Unit coordinated fifteen 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.

Joint CSIR-UGC Test for JRF/LS - NET Examination

The above tests were successfully conducted at Pune Centre on June 21, 2009 and Dec 20, 2009 for 7154 and 9571 registered candidates respectively.

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 lab's mission, 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 and www.ncl.org.in / www.ncl.res.in), prints annual reports and brochures, communicates impact making work from the laboratory in the form of R&D features, prepares video for general information to its stakeholders from scientific community, industry, public etc.

During the year, the brochures for the newly built Polymers and Advanced Materials Laboratory, NCL: Sixty years and beyond, NCL Research Foundation were brought out. Designing, production and printing of the revised and enlarged edition of book on NCL Flora and Fauna by Dr. Mukund Deshpande and Dr. Vandana Ghormade was co-ordinated, whereas Recording and Communicating Research Results A primer by Dr. Dinesh Agrawal was formatted and edited and was made available on the intranet portal for the students. The brochure on Fuel cell was revised. NCL input for CSIR brochure on Healthcare was provided.

Four R&D features namely, A new strategy for developing thin fuel cell electrodes, Artificial (Synthetic) Protein Structures, Predicting localization of subnuclear protein, and Dressing-up nanoparticles with antibiotics and their concurrent bimodal growth at infancy were prepared covering impact making work from NCL. These reports are further published by various newspapers.

The Unit provides one-point contact for press/ media and releases, issued press releases, attended press queries, provided customised reports on request to the stakeholders and co-ordinated interviews with NCL scientists on request from various science magazines/ newspapers / electronic media. Press releases were also issued on receiving fellowships, awards, medals, recognitions to the staff etc.

Reports covering various events such as National Science Day, National Technology Day, NCL Foundation Day, CSIR Foundation Day, Memorial and Endowment Lectures, symposia / conferences were prepared and released to the press, CSIR News, CSIR Samachar, besides uploading at NCL website.

About forty press notes were prepared covering these achievements / events and released to the press besides regular announcements such as announcement of programmes, outreach lectures, CSIR - UGC exam etc.

Interviews with the Director and the scientists were arranged during the year for the science magazine NanoDigest and the newspapers Sakaal Times, Loksatta, Agrowon etc.

Business and academic websites were continuously updated and modified and new scientists were encouraged to prepare their profiles for uploading at the websites.

Conference management

The organisers of the conferences were provided various type of support such as launching the website for the particular conference, printing of conference material, logistics etc.

During the year organizers of Symposium on Advances in Chemical Engineering and Process Technology, Workshop on Nanotechnology and Advanced Functional Materials, Symposium on Leveraging Digital Information for Research Productivity, Discussion Meeting on Chemical Reactions in Unusual Media, NCL - University of Gottingen, Germany Workshop on Catalysis, INSA Platinum Jubilee Symposium on Research in Molecular Medicine Based on Natural Resources and Traditional Knowledge, RSC-CSIR Chemical Sciences Innovation Symposium, Workshop on Accelerating Innovation Strategies for Collaboration and Commercialization by University of Toronto and NCL, 50th Annual Conference of Association of Microbiologists of India were given various types of support.

Internal communication

All the internal communications are announced through ncl@home portal. Development of new applications is done continuously and the admin rights were given to the users for managing pages wherever necessary. Memos / OMs from CSIR Hq., DG-CSIR, Other Govt. agencies, and from within NCL are announced using intranet portal ncl@home, besides announcement of major events and lectures.

The unit also announced internal and external job vacancies through ncl@home portal. Search facility application was prepared to facilitate the search of content at ncl@home.

Archive

Reports published in print media and appeared in electronic media such as NCL in news, CSIR general science articles, photos of major events, audio and video of major events science day posters, press notes were archived.

Publications database

R&D work at NCL results in about 400 research papers annually. To manage publication database, 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 customized NCL publication database to the Director, NCL, NISCAIR for CSIR Research Output database and also to CSIR HRDG.

Multimedia facilities

The Unit provided support for multimedia facilities including video conferencing in Board Room and CE Building, public address system, projectors, video and still photography.

Events

Logistic support was provided to the events organized during the year such as Prof. B.D. Tilak Memorial Lecture, Prof. L.K. Doraiswamy Lecture in Chemical Engineering, Prof. J. W. McBain Memorial Lecture, NCL Diamond Jubilee Lectures, Prof. K. Venkataraman Memorial Lecture, CSIR Foundation Day Lecture, NCL Foundation Day Lecture, National Science Day Lecture, besides assisting organization of the visit of the honourable MoS for S&T and the Prime Minister. Guidelines and checklist for event organizers were prepared.

The Unit maintains the online database of the mailing list to organize the dispatch of NCL Annual Reports, NCL RF Brochures etc. The Unit provided project training to two M.Sc. (Tech.) students in web development. A one-week internship was hosted to the editor of Cactus Communications Pvt. Ltd.

The Unit co-ordinated the publication of the Book on NCL History written by Dr. L.K. Doraiswamy, former Director of NCL and satisfied all the queries raised by the editorial team of Taylor and Francis Books (I) Pvt. Ltd.

Posters of Noble Prize winning work for last three years requested from the Nobel Foundation were displayed in the snap frames in New Polymers and Advanced Materials Laboratory.

Research planning and AUDIT

Research Planning and Audit Unit (RPA) has been involved in areas of project planning, project monitoring, budget, liaison with CSIR, etc. Technical and scientific audit of all on-going projects is a key activity. Highlights of the major activities during the year 2009-10 are:

In-House projects

All internal research programmes are funded through a system of In-house projects. Research proposals are invited twice a year. Similarly, the progress for all on-going projects is reviewed twice a year.

During the year, a total of thirty-one new proposals were received that were reviewed during two meetings held in May 2009 and October 2009. Of these fifteen proposals were approved for inclusion in the In-house projects.

In addition, funding was also continued to projects under the theme Centre of Excellence for a) Scientific computing (seven projects) and b) Micro reaction technology (four projects).

Periodic reviews are conducted to monitor the progress in the projects. During the past one-year, two such reviews were conducted. During the reviews on 19th May 2009, twenty-two projects were reviewed, while during the review conducted on 10th Nov. 2009, thirty ongoing projects were put under the scanner. Eleven start-up grant projects were continued, while five were concluded.

Four projects that were a part of the NCL-IGIB joint research initiative and were funded through internal resources were also concluded as the CSIR funding under the XI FYP network projects was received.

Research funded through the In-house projects produced eighteen publications, while ten are under the process of publication. Besides, these leads also led to the initiation of four public funded (DST/DBT) projects and the sponsorship of an industrial project and four technical services projects. It also helped train several M.Sc. and M.Tech. students.

During the year 2009-10, four newly joined scientists were given a start-up grant of ₹ 12 lakh for two years. In addition, the start-up grants for eleven scientists (who joined in the previous years) were continued into the second/third year.

The total funding to all fifty-three In-house projects (including start up grant) during 2009-10 amounted to ₹ 90 lakh.

Projects under 11th Five-year plan

NCL has a total of 16 network projects under the XI Five Year Plan. The unit has an overall responsibility for the governance and coordination of all these projects, both within NCL and also with other participating labs and CSIR.

The highlight of the activity involves keeping a track of expenditure, purchase of equipments, fresh / additional demand of funds and monitoring of all the project reports etc.

NCL is the Nodal Laboratory for two Network Projects (NCL-IGIB joint research initiative and Hydrogen energy initiatives).

In addition two new Centers of Excellence in Micro-reaction engineering for fine and specialty chemicals and Computational chemistry: A tool for multi-scale simulation for design of materials and processes" have been created.

Annual plan

During the current year a report entitled Annual Plan 2010-11 was prepared for

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Annual plan

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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 XI FYP projects, Non-network projects of the lab with a consolidated accomplishment and performance of the lab for the year 2009-10 and projections for the next year.

Interface with auditors

The unit interacted and provided detailed supporting information for submission to the external audit of CSIR. It also interfaced with the audit parties from the Principal Director of Audit, Scientific Department (Mumbai) on matters relating to projects at NCL, which resulted in dropping of many audit objections.

Research Council meetings

During the last one year, two RC meetings were conducted and actions taken to follow-up and implement the recommendations. The Unit also made available the information on several items that reported to RC and made a presentation on "status reports of In-house projects 2009-10"

Liaison with CSIR

The Unit liaises with CSIR in providing timely information on many aspects of the laboratory, which may be required from time to time. Moreover, the consolidated performance reports on two major network projects and Research utilization data of NCL are sent to CSIR on a monthly basis.

This involves providing current status on the 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 RTI has also been provided to CSIR. Response to questions from Parliament is also attended to on priority.

Communication GROUP

Critical job of rerouting of telephone connections for main building was taken up by Communication group. NCL main building telephone connections were routed through main building basement through ducts up to laboratories and rooms. From safety, security and maintenance point of view it was necessary to reroute all these connections on respective floors logically and remove the connectivity from basement MDFs.

Accordingly about 370 telephone connections were logically rerouted through casing up to rooms and were energised from main MDF main building exchange hardware. Old telephone cables were then totally removed from the basement.

A telephone node to take care of 400 telephones was made functional to take care of telephone connections in new Polymer and Advanced Material building. Out of these, 200 telephone connections were made functional to take care of PAM building telephone connections. A provision is made at node for extra 200 telephone connections in future for first floor of PAM laboratory.

New armoured underground telephone cable was laid for biochemistry building and further saddling of cables were done up to all floors. Provision is made for 100 telephone connections for biochemistry building from main building exchange hardware. All telephones were then reenergised from new cable.

Telephone connections for Glass blowing building, Civil engineering godown, refrigeration laboratory, physical laboratory near catalysis pilot plant were made functional by hanging connections. These hanging connections were removed by laying underground telephone cables for respective buildings. Critical work was completed to shift field cables directly onto the main MDF of main building exchange.

Due to this work, about 800 jumpers were totally removed between main MDF and field MDF in main exchange. Due to this, day-to-day maintenance has become easy for field personnel. Presently about 1300 telephones are now functional in NCL laboratory and NCL area.

Safety MANAGEMENT

Authorization from MPCB

This year, Maharashtra State Pollution Control Board (MPCB) granted consent to the NCL to operate under sec 26 of the water act (prevention and control of pollution) Act 1974, under sec 21 of the Air (prevention and control of pollution) Act 1981 and Authorization /renewal of authorization under Rule 5 of the Hazardous wastes (Management, *Handling and transport) movement* Rules 2008.

Disposal of hazardous waste and solvents

Further, this consent to operate under the Hazardous wastes (Management, Handling and transport) movement Rules 2008 cleared the path to disposal of waste solvents by incineration to a government appointed agency. Accordingly, all the waste solvents have henceforth been sent outside for disposal. With the addition of new facility, solvents that had been lying in NCL for last several years have been successfully disposed off. Currently, almost 2000 L of waste solvents are disposed off every month. With this, the toxic and hazardous waste disposal systems have now been standardized. Earlier waste disposal was being carried out in an incinerator within NCL.

Facilities up-gradation

In tune with the mission of the safe labs, the facility up-gradation has been a continuous activity. Several labs have been renovated with the installation of state of the art steel lab furniture; fume hoods, safety showers and eye wash fountains.

During the year 2009-10, the solvent storage facility in labs was upgraded with the procurement and distribution of fire proof solvent storage cabinets and solvent storage cans at a cost of ₹120 lakh. The purpose was to do away with solvent storage in HDPE cans, which are not fire resistant and have other problems as well.

The new metal solvent storage systems have many inbuilt safety features (double brass, wire mesh flame arrestor and a self-closing spout for automatic pressure relief. Such safe solvent storage cans do not normally explode even in the event of a fire). Similarly the storage cabinets for solvents also provide sufficient safety against fire.

To protect the staff from different types of exposures (extremely high and ultra low temperature, toxic vapours, corrosives etc) several pairs of suitable grades of gloves and masks were procured and distributed.

Orientation and Training

The newly joined staff and students were given hands on practical training for tackling small fires and the use of portable fire extinguishers during the orientation programme on the safety practices.

Two research students were deputed to a one-day practical workshop organized in Pune on fire safety, first aid and emergency preparedness with emphasis on Life saving skills (procedures for treating casualties during any emergency).

In the context of the IUPAC mandate to undertake safety awareness programmes to improve safety, health and environment in India, several public lectures and workshops were conducted. An oral paper was also presented in an international conference in Glasgow on aspects of safety awareness programme, limitations and path forward.

Accidents in NCL

A minor fire incident was reported in one of the catalysis labs. The incident was investigated to find the underlying cause of the fire. The recommendations of the committee are being implemented. The laboratory room did not house any expensive equipment or instrument. The book value of the loss of the equipment, furniture, etc. is approximately ₹ 27.00 lakhs based on purchase value.

Management of infrastructure

All the fume hoods, safety showers, eye wash fountains portable fire extinguishers, the fire alarm and detection systems etc were periodically checked for their working and efficiency The divisional safety coordinators conducted an inspection of all the labs and all deficiencies and safety non-compliance were brought to the attention and rectified.

Engineering SERVICES

The Engineering Services Unit comprises Mechanical, Electrical and Civil Engineering departments. The Glass Blowing Section is also attached with this unit. The unit provides support to the research activities alongside maintaining various lab facilities.

The Electrical Section has added a power back up of 210 KVA by installing generators for strategic work areas. With this, the total back up power available is increased to 940 KVA.

The work of construction Polymer & Advance Material laboratory building was completed during this financial year. The building is spread over an area of 8 acres and is connected to the main approach road near NCL Cafeteria. This building was dedicated to the nation by Hon. Prime Minister of India Dr Manmohan Singh.

The highlights of the building are as follows

- Areas of Engineering involved: Civil, Electrical, Mechanical, Communication, Networking & Laboratory Furniture.
- Total Built-up Area : 80000 sq ft
- Total Laboratory Area : 65000 Sq ft
- State of the art laboratory furniture
- Sitting area separated from working area for better human safety
- Fire Detection and Fire Fighting System
- Gas Piping provided on each working table with ample points
- Ventilation System to evacuate the harmful produce of reactions
- The analytical laboratory rooms are air conditioned
- Air-conditioned Auditorium of 100 seat capacity
- Admin Block and Laboratory area is separated by Access Control System to prevent entry of aliens in the lab area.
- Conference room, exhibition hall, meeting rooms are housed in the Block.
- Total Cost : ₹16 Crores

The design of the building is such that all the services such that electrical control panels, telephone panels, network hub, cold storages are housed separately, away from the lab areas. For access to these installations a separate service corridor in kept to minimize disturbance to the lab working areas.

The structural design of the building is made so as to take the load of an additional floor. All the services are laid considering the construction of one more floor in the future.

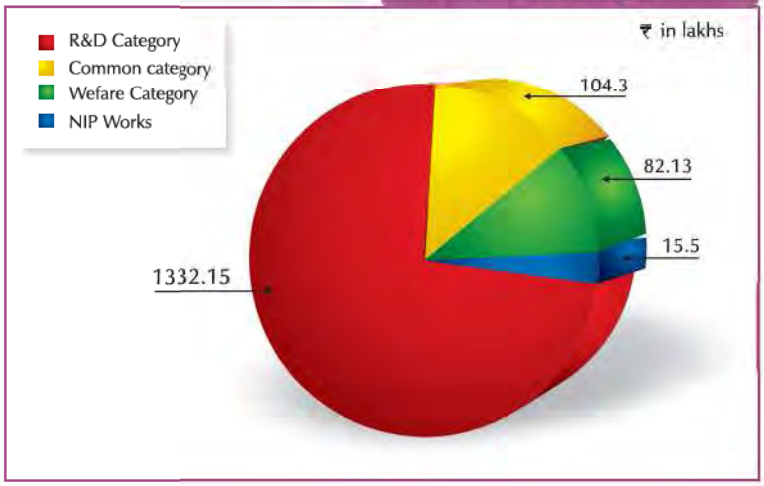
The Unit continued the work of renovation of laboratories and maintenance of the infrastructure facilities. The financial break-up of the works carried out under various categories is as follows:

1) R&D Category : ₹ 1332.15 lakhs
2) Common category : ₹ 104.30 lakhs
   Welfare Category : ₹ 82.13 lakhs
4) NIP Works : ₹ 15.5 lakhs

The Glass Blowing Section caters to the need of glass-wares for the laboratory work. The section fabricates various set-ups and modifications as per the need of scientific community. The section has carried out about 1200 such fabrications and modifications during this financial year.

The in-house Liquid Nitrogen Plant produced 10,000 l of liquid nitrogen and distributed additional 44000 l brought from an identified source.

Expenditure During 2009-10



वित्त एवं लेखा

यह विभाग प्रयोगशाला के नियमित स्टाफ, कनिष्ठ शोधछात्र/वरिष्ठ शोधछात्र, अनुसंधान सहयोगी, परियोजना सहायक, ऐमरिटस 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 रजिस्टरों 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 वैट भी लागू किया गया ।

1. निधि की उपयोगिता

सीएसआईआर अनुदान राशि (31.3.2010 तक)

परियोजनाएँ	(रु.लाख में)
नेटवर्क (एचसीपी परियोजना सहित)	1947.650
गैर-नेटवर्क	7303.202
नमिटली परियोजनाएँ	145.989
ईएमआर एवं वैज्ञानिक पूल	553.633
प्रयोगशाला आरक्षित निधि	600.217
बाहरी वित्तपोषित परियोजनाएँ	1570.907
विविध/फुटकर जमा राशि	74.494
बाहरी संगठनों द्वारा किया गया भुगतान	110.990
प्रायोजित सम्मेलनों/संगोष्ठियों हेतु जमा राशि	23.872
कुल (1)	**12330.954**

2. प्रयोगशाला आरक्षित निधि का अर्जन	(रु. लाख में)
वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर से भिन्न) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	299.948
अन्य लेखाशीर्षों से	454.372
कुल (2)	**754.320**

3. 31.3.2009 को अतिरिक्त निधि का निवेश (रु. लाख में)	1880.000

4. आपत्ति पुस्तिका मदों का निपटारा

वर्ष के दौरान किए गए समायोजन	(रु. लाख में)
सरकारी	
निजी	1760.957
यात्रा भत्ता/छुट्टी यात्रा रियायत	16.641
स्थानीय	25.368
कुल	**1802.966**
मदों की संख्या	

5. निम्न प्रकार के वाउचर तैयार किए गए

भुगतान	16570
प्राप्त राशि	4105
टी.ई.	279
कुल	**20954**

भण्डार एवं क्रय

भण्डार एवं क्रय अनुभाग एनसीएल के लिए वैज्ञानिक/विश्लेषणात्मक, अत्याधुनिक उपकरणों के अलावा रसायनों, विलायकों, उपभोज्य 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 क्लिअरिंग 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 (₹ करोड़ में)	
	2008-09	2009-10	2008-09	2009-10
कुल प्राप्त एवं निष्पादित माँगपत्र	1817	1507	57.11	36.57
कुल दिए गए ऑर्डर (आयातित)	849	945	28.63	21.40
कुल दिए गए ऑर्डर (स्वदेशी)	729	487	12.24	4.66
कुल प्राप्त सामग्री (आयातित)	1009	973	19.11	17.68
कुल प्राप्त सामग्री (स्वदेशी)	1575	1189	9.78	7.99
ऑनलाइन माँगपत्र	1517	1665	0.90(*)	1.06(*)
स्थानीय खरीद (ऑनलाइन आर सी सहित)	14046	7278	4.09	5.47
भण्डार से जारी की गई कुल सामग्री	35340	18138	0.64	0.52
वित्त वर्ष 2009-10 में समायोजित बकाया शेष			15.43	11.44
सीमा शुल्क छूट से प्राप्त राशि का उपयोग			19.22	14.68
उत्पाद शुल्क छूट से प्राप्त राशि का उपयोग			6.49	0.67

*_ऑनलाइन माँगपत्र

खरीदे गए प्रमुख उपकरण /अन्य वस्तुएँ

क्र. सं.	मदें	मूल्य (₹ लाख में)
1.	लिक्विड क्रोमैटोग्राफ-मास स्पेक्ट्रोफोटोमीटर	95.18
2.	जीपीसी प्रणाली	20.00
3.	एचपी एम 5314 बी एफसी ड्राइव	58.00
4.	एचपी प्रोलिएंट बीआई 460	50.00
5.	नेटवर्क संचार घटक	41.42
6.	नेटवर्क घटक	55.85
7.	एनसीएल वेबसाइट की डिज़ाइन पुनः बनाना	28.10
8.	ब्लेड सर्वर एवं सम्बद्ध घटक	41.35
9.	जस्टराइट सॉल्वेन्ट कैन्स एवं कैबिनेट्स	54.80
10.	एचपीएलसी प्रणाली	20.90
11.	पोर्टेबल ईंधन सेल परीक्षण केन्द्र	37.00
12.	लेज़र माइक्रोडिसेक्शन प्रणाली	94.76
13.	एचपीएलसी प्रणाली	26.50
14.	क्लस्टर	21.50
15.	फ्लौ क्रोमैटोग्राफी प्रणाली	22.25
16.	टेम	350.00
17.	एचपीसी क्लस्टर	28.15
18.	मैग्नेटोमीटर	280.00
19.	प्रिपरेटिव एचपीएलसी प्रणाली	36.00
20.	हाइ स्पीड रेफ्रिजरेटेड सेन्ट्रीफ्यूज	20.70
21.	यूवी/वीआईएस/एनआईआर	30.00
	कुल	**1412.46**

वर्ष के दौरान किए गए अन्य कार्य

- 4 प्रेस निविदाएँ जारी की गईं ।
- 2 बोली-पूर्व बैठकें आयोजित की गईं ।
- 16 मर्यादित निविदाएँ वेबसाइट पर अपलोड की गईं ।

अनुपयुक्त वस्तुओं का निपटान

- मास अक्तूबर, 2009 में किए गए अनुपयुक्त वस्तुओं के निपटान से रु. 3,28,03,433/- की राशि प्राप्त हुई ।
- अतिरिक्त रसायनों का निपटान दिसम्बर, 2009 में किया गया जिससे रु. 54,600/- की राशि प्राप्त हुई ।

Finance & ACCOUNTS

1. Funds Utilization

a) CSIR Grant (by 31.3.2010)

Projects	Amount (₹ in lakh)
I) Network (including HCP Project)	1947.650
ii) Non -network	7303.202
iii)NMITLI Projects	145.989
b) EMR & Scientist Pool	553.633
c) Laboratory Reserve	600.217
d) Externally Funded Projects	1570.907
e) Misc. Deposits	74.494
f) Payment on behalf of outside bodies	110.990
g) Deposits for Sponsored conf./ seminars	23.872
Grand Total (1)	**12330.954**

2. Generation of Lab Reserve (a) through earning of interest on investment of surplus funds (other than CSIR) during the year.	299.948
(b) From other heads	454.372
Total (2)	**754.320**

3. Investment of surplus funds as on 31.3.2009 — **1880.000**

4. Clearance of OB items

Adj. made during the year	(₹ in lakh)
Govt.	-
Private	1760.957
TA/LTC	16.641
Local	25.368
Total Amount	**₹ 1802.966**

5. Generated the following types of vouchers

Payment	16570
Receipt	4105
TE	279
Total	**20954**

Stores & 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 like 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 (₹ in Crores)	
	2008-09	2009-10	2008-09	2009-10
Total Indents received and Processed	1817	1507	57.11	36.57
Total orders placed(imported)	849	945	28.63	21.40
Total order placed (indigenous)	729	487	12.24	4.66
Total consignments received (Imported)	1009	973	19.11	17.68
Total consignments received (indigenous)	1575	1189	9.78	7.99
On-line indents	1517	1665	0.90(*)	1.06(*)
Local Purchases (Including on-line RC)	14046	7278	4.09	5.47
Total Stores Issues	35340	18138	0.64	0.52
Outstanding balance adjusted during the financial year 2009-10			15.43	11.44
Utilization of Custom Duty Exemption during Financial year 2009-10			19.22	14.68
Utilization of Excise Duty Exemption during financial year 2009-10			6.49	0.67

(*) On-line indents

Major Equipment/other items procured/processed

S. No.	Item	Value ₹ in lakh
1	Liquid chromatograph-mass spectrophotometer	95.18
2	GPC system	20.00
3	HP M5314 B FC drive	58.00
4	HP Proliant Bl 460	50.00
5	Network communication components	41.42
6	Network components	55.85
7	Redesign of NCL website	28.10
8	Blade server & related components	41.35
9	Justrite solvent cans & cabinets	54.80
10	HPLC system	20.90
11	Portable fuel cell test station	37.00
12	Laser microdessection system	94.76
13	HPLC system	26.50
14	Cluster	21.50
15	Flash chromatography system	22.25
16	Tem	350.00
17	HPC cluster	28.15
18	Magnetometer	280.00
19	Preparative HPLC system	36.00
20	High speed refrigerated centrifuge	20.70
21	UV/VIS/NIR spectro-photometer	30.00
	Total	**1412.46**

Press/Web Tenders

during the period two press tenders issued, two pre-bid meeting were conducted, and sixteen limited tenders uploaded on website.

Disposal of Unserviceable items

a) Disposal activity of un-serviceable items was taken up in the month of October, 2009 and a sum of ₹ 3,28,03,433/- was realized from this disposal.

b) Disposal of surplus chemicals was taken up in the month of December, 2009 and a sum of ₹54,600/- has been realized from this disposal.

Student Academic PROGRAMME

In NCL, around 400 students are pursuing for their doctoral degree in Chemical and allied sciences. PhD students are admitted through a centralized interview held twice a year. Candidates, who are holding M.Sc. degree or equivalent in all branches of science and have qualified in CSIR/UGC-NET under CSIR/UGC fellowship scheme or DBT/ICMR JRF examination scheme or BioInformatics National Certification (BINC) examination, are eligible for admission to the Ph.D. programme.

The advertisements are sent twice in a year, following the announcement of CSIR/UGC NET examination results. Selection for admission to the Ph.D. programme is done on the basis of an interview held at NCL in broad disciplines of Organic Chemistry, Catalysis, Life Sciences, Physical & Theoretical Chemistry, Chemistry & Physics of Materials, Polymer Science and Chemical Engineering.

Candidates are selected depending on the vacancy and requirements of research guides under the above broad disciplines. Admission to the Ph.D. programme through direct Senior Research Fellowship (SRF) program of CSIR is also continued as per usual procedures.

Overall academic activities of students working at NCL are monitored by the Student Academic Committee (SAC) headed by a chairman who is a senior scientist and scientists from different disciplines as members.

The committee meets at least once every three months to discuss various issues related to the academic and other activities of the students. All the activities related to the PhD students, including their accommodation are handled by the student academic office (SAO). The student academic office works directly under the chairman of the SAC.

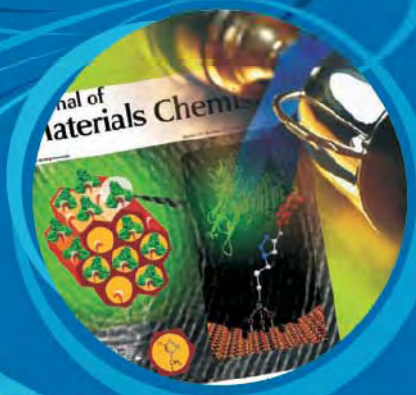
Every batch of students joining the Ph.D. program at NCL undergoes a two-day orientation programme, which provides an introduction to the laboratory, its systems, procedures and functioning, safety, security, scientific ethics, scientific record keeping and access to scientific information. Participation in the orientation programme is compulsory.

Additionally, students (JRFs as well as selected through direct SRF scheme) are required to complete the credit courses that is offered by NCL, appropriate to his/her research area. The courses are selected and offered with a view to bridge the gap between Masters Education and what is required for Ph D research. This is waived in the case of students registered with IIT Mumbai or ICT Mumbai.

The resource persons are drawn from the staff of NCL, and neighboring Institutions. This course work was made compulsory for all students, joined after 1 July 2004.

Students are required to present two seminars, one general seminar related to their topic of research (overview) to be preferably completed before registration and second one on the research theme to be completed before synopsis submission.

An academic committee comprising the research guide, a subject expert from NCL and an external expert evaluate the seminars and periodically assess the progress of the student. Similarly, all the students are required to make poster presentations on National Science Day, at least twice during their stay in NCL. Partial financial support is provided to selected students, who excel in the course work and research activities, to attend international conferences outside India.



Annexures

Research PAPERS PUBLISHED

Biological Sciences

- **Katre U.V., Suresh C.G.**

  Features of homotetrameric molecular association in protein crystals
  Acta Crystallographica Section D: Biological Crystallography
  65(1),1-10

- **Bogdanovic X., Singh R.K., Hentschke J., Gudmundsdottira B.K., Hinrichs W.**

  Crystallization and preliminary X-ray diffraction studies of AsaP1-E294A and AsaP1-E294Q, two inactive mutants of the toxic zinc metallopeptidase AsaP1 from Aeromonas salmonicida subsp. achromogenes
  Acta Crystallographica Section F: Structural Biology and Crystallization Communications
  65(7),695-697

- **Sridevi N., Prabhune A. A.**

  Brevibacillus sp: A novel thermophilic source for the production of bile salt hydrolase
  Applied Biochemistry and Biotechnology
  157(2),254-262

- **Kumar A., Singh S., Poddar P., Prabhune A., Pundle A.**

  Effect of cultural conditions and media constituents on production of penicillin v acylase and CTAB treatment to enhance whole-cell enzyme activity of rhodotorula aurantiaca (NCIM 3425)
  Applied Biochemistry and Biotechnology
  157(3),463-472

- **Khan F., Gaikwad S.M., Khan M.I.**

  Entropy driven binding of O-glycan and glycoproteins to Artocarpus hirsuta lectin: An SPR study
  Asian Journal of Biochemistry
  4(4),106-116

- **Sreejith R. K., Yadav V. N., Varshney N. K., Berwal S. K., Suresh C. G., Gaikwad S. M., Pal J. K.**

  Conformational characterization of human eukaryotic initiation factor 2 : A single tryptophan protein
  Biochemical and Biophysical Research Communications
  390(2),273-279

- **Adikane H. V., Dixit J. N.**

  Effect of different operational conditions on the decolorization of molasses spent wash using once developed soil inoculum
  Biodegradation
  20(6),867-874

- **Chaudhary P.M., Chavan S.R., Shirazi F., Razdan M., Nimkar P., Maybhate S.P., Likhite A.P., Gonnade R., Hazara B.G., Deshpande M.V., Deshpande S.R.**

  Exploration of click reaction for the synthesis of modified nucleosides as chitin synthase inhibitors
  Bioorganic and Medicinal Chemistry
  17(6),2433-2440

- **Mohapatra D.K., Maity P.K., Shabab M., Khan M.I.**

  Click chemistry based rapid one-pot synthesis and evaluation for protease inhibition of new tetracyclic triazole fused benzodiazepine derivatives
  Bioorganic and Medicinal Chemistry Letters
  19(17),5241-5245

- **Sunil Kumar, Mehta U.J., Hazra S.**

  In Vitro Studies on Chromium and Copper Accumulation Potential of Pongamia glabra Prierre Seedlings
  Bioremediation, Biodiversity and Bioavailability
  3(1),43-48

- **Khan A., Bhide A., Gadre R.**

  Mannitol production from glycerol by resting cells of Candida magnoliae
  Bioresource Technology
  100(20),4911-4913

- **Adsul M.G., Bastawde K.B., Gokhale D.V.**

  Biochemical characterization of two xylanases from yeast Pseudozyma hubeiensis producing only xylooligosaccharides
  Bioresource Technology
  100(24),6488-6495

- **Singh R., Varma A.J., Seeta Laxman R., Rao M.**

  Hydrolysis of cellulose derived from steam exploded bagasse by Penicillium cellulases: Comparison with commercial cellulase
  Bioresource Technology
  100(24),6679-6681

- **Mhetras N.C., Bastawde K.B., Gokhale D.V.**

  Purification and characterization of acidic lipase from Aspergillus niger NCIM 1207
  Bioresource Technology
  100(3),1486-1490

- **Adsul M.G., Terwadkar A.P., Varma A.J., Gokhale D.V.**

  Cellulases from Penicillium janthinellum mutants:Solid state production and their stability in ionic liquids
  Bioresources
  4(4),1670-1681

- **Kotwal S.M., Shankar V.**

  Immobilized invertase
  Biotechnology Advances
  27(4),311-322

- **Poopal A.C., Laxman R.S.**

  Chromate reduction by PVA-alginate immobilized Streptomyces griseus in a bioreactor
  Biotechnology Letters
  31(1),71-76

- **Jaitak V., Kaul V.K., Bandna, Kumar N., Singh B., Savergave L.S., Jogdand V.V., Nene S.**

  Simple and efficient enzymatic transglycosylation of stevioside by -cyclodextrin glucanotransferase from Bacillus firmus
  Biotechnology Letters
  31(9),1415-1420

- **Gurulingappa H., Tare V., Pawar P., Tungikar V., Jorapur Y.R., Madhavi S., Bhat S.V.**

  Susceptibility of Aedes aegypti and Culex quinquefasciatus larvae to gedunin-related limonoids
  Chemistry and Biodiversity
  6(6),897-902

- **Sridevi N., Srivastava S., Khan B.M., Prabhune A.A.**

  Characterization of the smallest dimeric bile salt hydrolase from a thermophile Brevibacillus sp.
  Extremophiles
  13(2),363-370

- **Pandit S.S., Chidley H.G., Kulkarni R.S., Pujari K.H., Giri A.P., Gupta V.S.**

  Cultivar relationships in mango based on fruit volatile profiles
  Food Chemistry
  114(1),363-372

- **Chavan P., Mane S., Kulkarni G., Shaikh S., Ghormade V., Nerkar D.P., Shouche Y., Deshpande M.V.**

  Natural yeast flora of different varieties of grapes used for wine making in India
  Food Microbiology
  26(8),801-808

- **Sridevi N., Vishwe P., Prabhune A.**

  Hypocholesteremic effect of bile salt hydrolase from Lactobacillus buchneri ATCC 4005
  Food Research International
  42(4),516-520

- **Telang M.A., Giri A.P., Pyati P.S., Gupta V.S., Tegeder M., Franceschi V.R.**

  Winged bean chymotrypsin inhibitors retard growth of Helicoverpa armigera
  Gene
  431(40180),80-85

- **Tamhane V.A., Giri A.P., Kumar P., Gupta V.S.**

  Spatial and temporal expression patterns of diverse Pin-II proteinase inhibitor genes in Capsicum annuum Linn
  Gene
  442(40180),88-98

- **Telang M.A., Pyati P., Sainani M., Gupta V.S., Giri A.P.**

  Momordica charantia trypsin inhibitor II inhibits growth and development of Helicoverpa armigera
  Insect Science
  16(5),371-379

- **Varma R.J., Gaikwad B.G.**

  Biodegradation and phenol tolerance by recycled cells of Candida tropicalis NCIM 3556
  International Biodeterioration and Biodegradation
  63(4),539-542

- **Shashidhara K.S., Gaikwad S.M.**

  Class II -mannosidase from Aspergillus fischeri: Energetics of catalysis and inhibition
  International Journal of Biological Macromolecules
  44(1),112-115

- **Dhaneshwar S.R., Mahadik M.V., Kulkarni M.J.**

  Column liquid chromatography-ultraviolet and column liquid chromatography mass spectrometry evaluation of stress degradation behavior of escitalopram oxalate
  Journal of AOAC International
  92(1),138-147

- **Dharker P.N., Gaikwad S.M., Suresh C.G., Dhuna V., Khan M.I., Singh J., Kamboj S.S.**

  Comparative studies of two araceous lectins by steady state and time-resolved fluorescence and CD spectroscopy
  Journal of Fluorescence
  19(2),239-248

- **Jagtap S., Rao M.**

  Fluorescence study on interactions of -crystallin with the molten globule state of 1, 4-D-glucan Glucanohydrolase from Thermomonospora sp. induced by guanidine hydrochloride
  Journal of Fluorescence
  19(6),967-973

- **Shah P., Bhavsar K., Soni S.K., Khire J.M.**

  Strain improvement and up scaling of phytase production by Aspergillus niger NCIM 563 under submerged fermentation conditions
  Journal of Industrial Microbiology and Biotechnology
  36(3),373-380

- **Kotkar H.M., Sarate P.J., Tamhane V.A., Gupta V.S., Giri A.P.**

  Responses of midgut amylases of Helicoverpa armigera to feeding on various host plants
  Journal of Insect Physiology
  55(8),663-670

- **Sreekanth D., Syed A., Sarkar S., Sarkar D., Santhakumari B., Ahmad A., Khan M.I.**

  Production, purification, and characterization of taxol and 10-DABIII from a new endophytic fungus Gliocladium sp. isolated from the Indian yew tree, Taxus baccata
  Journal of Microbiology and Biotechnology
  19(11),1342-1347

- **Kumar A., Pundle A.**

  Effect of organic solvents on cell-bound penicillin V acylase activity of Erwinia aroideae (DSMZ 30186): A permeabilization effect
  Journal of Molecular Catalysis B: Enzymatic
  57(40182),67-71

- **Sekhar Pagadala N., Arha M., Reddy P.S., Kumar R., Sirisha V.L., Prashant S., Janardhan Reddy K., Khan B., Rawal S.K., Kavi Kishor P.B.**

  Phylogenetic analysis, homology modelling, molecular dynamics and docking studies of caffeoyl-CoA-O-methyl transferase (CCoAOMT 1 and 2) isoforms isolated from subabul (Leucaena leucocephala)
  Journal of Molecular Modeling
  15(2),203-221

- **Kumar A., Gowda N.M., Gaikwad S., Pundle A.**

  Rhodotorula aurantiaca penicillin V acylase: Active site characterization and fluorometric studies
  Journal of Photochemistry and Photobiology B: Biology
  97(2),109-116

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- **Pandit S.S., Kulkarni R.S., Chidley H.G., Giri A.P., Pujari K.H., Kollner T.G., Degenhardt J., Gershenzon J., Gupta V.S.**

  Changes in volatile composition during fruit development and ripening of 'Alphonso' mango
  Journal of the Science of Food and Agriculture
  89(12),2071-2081

- **Bhosale S.H., Pant A., Khan M.I.**

  Purification and characterization of putative alkaline [Ni-Fe] hydrogenase from unicellular marine green alga, Tetraselmis kochinensis NCIM 1605
  Microbiological Research
  164(2),131-137

- **Gowda S.J.M., Radhika P., Kadoo N.Y., Mhase L.B., Gupta V.S.**

  Molecular mapping of wilt resistance genes in chickpea
  Molecular Breeding
  24(2),177-183

- **Gurjar G., Barve M., Giri A., Gupta V.**

  Identification of Indian pathogenic races of Fusarium oxysporum f. sp. ciceris with gene specific, ITS and random markers
  Mycologia
  101(4),484-495

- **Kulkarni A., Rao M.**

  Differential elicitation of an aspartic protease inhibitor: Regulation of endogenous protease and initial events in germination in seeds of Vigna radiata
  Peptides
  30(12),2118-2126

- **Shaik N.M., Arha M., Nookaraju A., Gupta S.K., Srivastava S., Yadav A.K., Kulkarni P.S., Abhilash O.U., Vishwakarma R.K., Singh S., Rawal S.K., Khan B.M.**

  Improved method of in vitro regeneration in Leucaena leucocephala - a leguminous pulpwood tree species Physiology and Molecular Biology of *Plants*
  15(4),311-318

- **Singh S., Hazra S.**

  Somatic embryogenesis from the axillary meristems of peanut (Arachis hypogaea L.)
  Plant Biotechnology Reports
  3(4),333-340

- **Pawar K.D., Thengane S.R.**

  Influence of hormones and medium components on expression of dipyranocoumarins in cell suspension cultures of Calophyllum inophyllum L.
  Process Biochemistry
  44(8),916-922

- **Panda B.V., Hazra S.**

  Seedling culture of Semicarpus anacardium L.
  Seed Science Biotechnology
  3(2),54-59

- **Kautharapu K., Pujari N.S., Golegaonkar S.B., Ponrathnam S., Nene S.N., Bhatnagar D.**

  Vinyl-2-pyrrolidone derivatized guar gum based aqueous two-phase system
  Separation and Purification Technology
  65(1),9-13

- **Banu S., Lagu M.D., Gupta V.S.**

  Phylogeographical studies in disjunct populations of Symplocos laurina Wall. using cytoplasmic PCR-RFLP approach
  Tree Genetics and Genomes
  6(1),13-23

Catalysis and Surface Science

- **Choudhary V.R., Jana P.**

  Direct H2 -to-H2 O2 oxidation over highly active selective Br-F-Pd Al2O3 catalyst in aqueous acidic medium: Influence of process conditions on the H2O2 formation
  Applied Catalysis A: General
  352(40180),35-42

- **Lucas N., Bordoloi A., Amrute A.P., Kasinathan P., Vinu A., Bohringer W., Fletcher J.C.Q., Halligudi S.B.**

  A comparative study on liquid phase alkylation of 2-methylnaphthalene with long chain olefins using different solid acid catalysts
  Applied Catalysis A: General
  352(40180),74-80

- **Sahoo S., Kumar P., Lefebvre F., Halligudi S.B.**

  Oxidative kinetic resolution of alcohols using chiral Mn-salen complex immobilized onto ionic liquid modified silica
  Applied Catalysis A: General
  354(40180),17-25

- **Garade A.C., Kshirsagar V.S., Rode C.V.**

  Selective hydroxyalkylation of phenol to bisphenol F over dodecatungstophosphoric acid (DTP) impregnated on fumed silica
  Applied Catalysis A: General
  354(40180),176-182

- **Joshi M.M., Labhsetwar N.K., Mangrulkar P.A., Tijare S.N., Kamble S.P., Rayalu S.S.**

  Visible light induced photoreduction of methyl orange by N-doped mesoporous titania
  Applied Catalysis A: General
  357(1),26-33

- **Taralkar U.S., Kalita P., Kumar R., Joshi P.N.**

  Synthesis, characterization and catalytic performance of Sn-MCM-48 in solvent-free Mukaiyama-type aldol condensation reactions
  Applied Catalysis A: General
  358(1),88-94

- **Kshirsagar V.S., Garade A.C., Mane R.B., Patil K.R., Yamaguchi A., Shirai M., Rode C.V.**

  Characterization of clay intercalated cobalt-salen catalysts for the oxidation of p-cresol
  Applied Catalysis A: General
  370(40180),16-23

- **Jagtap N., Umbarkar S.B., Miquel P., Granger P., Dongare M.K.**

  Support modification to improve the sulphur tolerance of Ag Al2O 3 for SCR of NOx with propene under lean-burn conditions
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Process for the preparation of hydrocarbon fuel	Srinivas; Darbha, Srivastava; Rajendra, Ratnasamy; Paul	US	7482480
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Thermoprecipitating polymer containing enzyme specific ligands, process for the preparation thereof, and use thereof for the separation of enzymes	Vaidya; Alankar Arun; Lele; Bhalchandra Shripad; Kulkarni; Mohan Gopalkrishna; Mashelkar; Raghunath Anant	US	7501478
Water soluble polymers containing vinyl unsaturation, their crosslinking and process for preparation thereof	Prerana Maruti Patil, Mohan Gopalkirshna Kulkarni	RU	2361884

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Title	Inventors	Patent No.
A method for the improvement of gas-solid contacting in a bubbling fluidized bed reactor	Choudhary VR, Choudhary TV	227056
A method for the manufacture of a hybrid organic - inorganic composite film	Gole AM, Kumar A, Phadtare S, Sastry M	227520
A novel 2, 3-diaryl-4-(ter-butyldimethylsilyloxy) cyclopent-2-en-1-one	Gurjar MK, Wakharkar RD, Borate HB, Shinde PD, Mahajan VA, Dadhav VH, And Wagh AM	232568
A polymer composition for the selective removal of cobalt, a process for the preparation thereof and the process for removal of cobalt	Mohan Gopalkrishna Kulkarni, Rohini Nitin Karmalkar	235750
A process for electrocatalytic oxidation of alkenes	Radhakrishnan S, Adhikari A	231010
A process for preparation of 2-acrylamido - 2-methyl-1- propane sulfonic acid	Purushottam BP, Shankar J, William SR, Yashwant GM, Narayan JC, Madhukar GS, Venkatrao NR, Anantrao KR, Narayan BA	233606
A process for preparation of 2-phenyl ethanol	Chandrashekhar Vasant Rode, Vikas Shripat Kshirsagar, Vilas Hari Rane, Raghunath Vitthal Chaudhari	232572
A process for preparation of highly pure 2-methyl-2- propene -1- sulfonic acid, sodium salt	Purushottam BP, Shankar JS, Madhukar GS, Williams SR, Yashwant GM, Narayan JC, Venkatrao NR	227498
A process for preparing mono and bimetallic nanoparticles	Murali Sastry, Absar Ahmad, Sangaru Shiv Shankar	237381
A process for the acylation of aromatic compound using solid catalyst comprising metal oxide(s)	Chourhary VR, Jana SK	231559
A process for the derivatisation of macroporous beaded crosslinked copolymers	Ghadge VB, Rajan CK, Ponrathnam S	231059
A process for the oxidation of paraffins to primary alcohols	Ratnasamy P, Raja R	232260
A process for the preparation of (20r)-20-hydroxy -3b- tosyloxypregna -5- en-22-aldehyde	Hazra BG, Basu S, Pore VS	232482
A process for the preparation of 2(2-chloro ethoxy) - acetic acid	Ravindranathan, T., Deshpande, V.H., Patil, V.B., Mehendale, A.R., Lahoti, R.J., Joshi, R.A., Joshi, R.R., Kalkote, U.R., Shivakumar, I.	232403

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A process for the preparation of 2, 3-diaryl-4-(tert -butyldimethylsilyloxy) cyclopent -2-en-1-one	Gurjar MK, Wakharkar RD, Borate HB, Shinde PD, Mahajan VA, Jadhav VH, Wagh AM	232567
A process for the preparation of 2-hydroxy carboxylic acids	Raghunath Vitthal Chaudhari, Sunil Sopana Tonde	234310
A process for the preparation of a lactone from a cyclic ketone,	Mandal D, Ahmad A, Khan MI, Kumar R	230892
A process for the preparation of a mixture of methanol and formaldehyde through the oxidation of methane	Puthusseril Varkey, Chandra Ratnasamy, Sarada Gopinathan	231586
A process for the preparation of carboxylic acid	Anant KA, Sopana T, Vitthal CR	232933
A process for the preparation of conducting co-polymer having enhanced thermal stability	Subramaniam Radhakrishnan, Shripad Dagdopant Deshpande	232901
A process for the preparation of conducting polyketone polymers	Jog JP, Kulkarni SM, Priya L, Chaudhari	RV 233329
A process for the preparation of cyclodextrin bound polymer bound support	Debaprasad Nayak, Arika Koyha, Sima Atmaram Mule, Anant Patkar, Surendra Ponrathnam, Chelanattu Khizhakke Madath Raman Rajan	232355
A process for the preparation of enantiometrically pure cyclohexylphenyl glycolic acid	Pradeep Kumar, Rodney Agustinho Fernandes, Prii Gupta	231243
A process for the preparation of encapsulated oxo-bridged organometallic cluster catalysts	Srinivas D, Chavan SA, Ratnasamy P	230861
A process for the preparation of impregnated thin film hydrocarbon sensor materials using spray pyrolysis technique	Ramgir NS, Chaudhary VA, Pillai VK, Mulla IS	233595
A process for the preparation of ion conducting polymer blend useful for separation of proteins using an isoelectric focussing unit	Chinnathambi S, Lachke AH, Radhakrishnan SR	232836
A process for the preparation of macroporous bis(picolyl) amine polymers	Sunny Skaria, Varsha Bhikoba Ghadge, Surendra Ponrathnam, Chelanattu Khizhakke Madath Raman Ranjan	232371
A process for the preparation of novel bidentate ligands	Raghunath Vitthal Chaudhari, Avinash Narendra Mahajan, Vinod Sankaran Nair	232398
A process for the preparation of novel polyimides	Jinu Suju Mathew, Subhash Pundlik Vernekar, Reges Mercier, Rachid Kerboua	231770
A process for the preparation of novel water soluble palladium complexes and supported aqueous phase catalysts thereof	Seayad J, Seayad AM, Sarkar BS, Chaudhari RV	231614
A process for the preparation of polymeric absorbents useful for gelling organic liquids	Lele, Ashish Kishor (Pune, In), Varghese, Shyni (Pune, In), Badiger, Manohar Virupax (Pune, In), Mashelkar, Raghunath Anant (Pune, In)	233536

Title	Inventors	Patent No.
A process for the preparation of soluble polyanilines by micro emulsion technique	Madathil Rethi, Chelunattu Khizhakke Madath Raman Ranjan, Surendra Ponrathnam	232775
A process for the preparation of water soluble poly anilines	Madathil Rethi, Chelunattu Khizhakke Madath Raman Ranjan, Surendra Ponrathnam	232759
A process for the purification of penicillin g acylase from crude enzyme extract	Ghadge VB, Rajan CK, Ponrathnam S, Mujawar SK, Nanda RK	231061
A process for the selective artification of tertiary alcohol by an acid anhydride using a reusable solid catalyst	Vasant Ramchandra Choudhary, Kshudiram Mantri, Suman Kumar Jana	232085
A thermoprecipitating polymer containing enzyme specific ligands and a process for the preparation thereof and a process for the separation of enzyme	Vaidya, Alankar Arun (Pune, In), Lele, Bhalchandra Shripad (Pune, In), Kulkarni, Mohan Gopalkrishna (Pune, In), Mashelkar, Raghunath Anant (Pune, In)	233331
A tissue culture medium formulation for induction and proliferation of multiple shoots in excined embryo axes of cotton	Dinesh Chandra Agarwal, Anjan Kumar Banerjee, Satish Manohar Nalawade, Sulekha Hazra, Venkata Krishnamurhty	232855
An improved composition for treatment of effluents from paper and pulp industry and the process thereof	Panchanadikar Vv, Suresh Babu S	232573
An improved hydrocarbon reforming process	Tapan Kumar Das, Asha Jeevan Chandwadkar, Subramanian Sivasanker	233544
An improved process for preparation of polypropylene moulding compound having high tensile strength and toughness value	Subramaniam Radhakrushna, Comandur Saujanya,	230368
An improved process for the preparation of 2-(aryl-1- hydroxy methylene) cycloalkanones	Satya Varahala Nadimpalliraju, Suresh Subramaniam, Kumar Venkataraman Srinivasan, Chelanattu Khizhakke Madhath Raman Ranjan, Surendra Ponrathnam, Claudine Noel	232938
An improved process for the preparation of 2-aryl propionic acids	Raghunath Vitthal Chaudhari, Seayad. A. Jayasree Seayad	231089
An improved process for the preparation of acetic acid or methyl acetate,	Kelkar AA, Tonde SS, Devekar SS, Chaudhari RV	230372
An improved process for the preparation of adipic acid	Srinivas D, Chavan SA, Ratnasamy P	227368
An improved process for the preparation of aldehydes	Chaudhari, R.V., Deshpande, R.M., Bhanage, B.M., Mahajan, A.N.	232932
An improved process for the preparation of aromatic polymers	Idage BB, Mahajan SS, Sivaram S	232152
An improved process for the preparation of bis (picolyl) amines	Sunny Skaria, Varsha Bhikoba Ghadge, Raman Ravishankar, Surendra Ponrathnam, Chelanattu Khizhakke Madath Raman Ranjan	232365
An improved process for the preparation of immobilized nano sized metal particles	Mukherjee P, Ahmad A, Mandal D, Senapati S, Khan MI, Sastry M, Kumar R	231058

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Title	Inventors	Patent No.
An improved process for the preparation of microcellulose beads	Harshavardhan Vishvanath Adikane, Sanjay Narayan Nene	230975
An improved process for the preparation of poly alkyl(meth) acrylates	Durairaj Baskaran	232765
An improved process for the preparation of saturated carboxylic acid esters using supported aqueous phase palladium complex catalysts	Seayad J, Seayad AM, Sarkar BS, Chaudhari RV	231571
An improved process for the preparation of styrene	Parthasarathy Ganguli, Shivaram Dattatraya Sathaye, Shirish Dattatray Pradhan, Imtiaz Sirajuddin Mulla, Suguna Dayanand Adyanthaya	232093
An improved process for the preparation of supported metallocene catalyst	Swaminathan Sivaram, Soumen Sensarma	232750
An improved process for the preparation of surface modified thin film sensor material	Alok Kalra, Sushil Kumar, Neetu Katiyar, Janak Raj Bahl, Ravi Prakash Bansal, Harmesh Singh Chauhan, Arun Prasad, Rakesh Pandey, Om Parkash Dhawan, Alok Krishna, Ramesh Srivastava	227551
An improved process for the production of glutaryl -7- amino cepherlosporanic acid	Shewale JG, Mujawar SK, Kotha A, Rajan CK, Ponrathnam S	232542
An improved process for the production of immobilization milk clotting protease	Shewale JPG, Channe PS, Ghadge VB, Rajan CK, Ponrathnam S	232820
An improved process for the removal of colour and sugar from black liquor	Adikane HV, Thakar DM, Nene SN	227896
An improved process for the single step isolation of albumin	Hashavardhan Vishvanath Adikane, Dnyaneshwar Maruti Thakar, Sanjay Narayan Nene	230985
An improved process for the single step isolation of alkaline protease from fermentation broth	Adikane HV, Thakar DM, Nene SN	232755
An improved process for the treatment of spent wash using marine sponge to produce potable water	Promod Prabhakar Moghe, Vinita Vinay Panchanadikar, Arvind Gajanan Untawale, Vinod Kashinath Dhargalkar, Baban Shravan Ingole	232096
An improved process for treatment of agro-industry waste water to produce colourless waste water	Ashok Nagesh Gokarn, Narendra Vasant Sankpal, Mohan Keraba Dongare	232487
An improved process for treatment of cane sugar industry waste water along with spent wash & black liquor	Moghe VV, Panchanadikar VV, Pol AV, Bahirat PK	231017
An improved process for treatment of viscose effluent from rayon pulp industry	Moghe PP, Panchnadikar VV, Pol AV, Bahirat PK	232342
An imroved process for the fabrication of ultracapacitor electrodes using activated lamp black carbon	Mukta Shripad Dandekar, Girish Vilas Arabale, Vijayamohanan Kunjukrishna Pillai, Subhash Pundalic Vernekar	234759

Title	Inventors	Patent No.
Antiozonant based on functionalized benzotriazole uv absorbers and the process for the preparation thereof	Shailendra Singh Solanky, Shrojal Mohitkumar Desai, Raj Pal Singh	234568
Copolymers and preparation thereof	Mohan Gopalkrishna Kulkarni, Jayant Jaganath Khandare	233328
Hybrid organic - inorganic composite film	Gole AM, Kumar A, Phadtare S, Sastry M	231082
Improved process for the preparation of polyesters from aromatic diodide and alkyl or aryl diol and carbon monoxide	Kelkar AA, Kulkarni SM, Chaudhari RV	231053
Novel antiozonant cum antioxidant and the process for the preparation thereof	Desai S M, Solanky S S, Singh R P	233563
Oligomers and containing n-acetyl glucosamine	Kulkarni Mohan Gopalkrishna, Khandare Jayant Jagannath	236017
Polymerizable macromer and preparation thereof	Mohan Gopalkrishna Kulkarni, Jayant Jagannath Khandare	233301
Polymerizable monomers and preparation thereof	Kulkarni MG, Khandare JJ	233479
Process for recovery of sulphur from sour/natural gas using biodegradable carboxylic acid metal chelates	Aniruddha Subhash Deshpande, Narendra Vasant Sankpal, Bhaskar Dattatraya Kulkarni	233617
Process for the activation of a catalyst comprising metallic palladium, useful for the direct oxidation of hydrogen to hydrogen peroxide	Choudhary VR, Gaikwad AG, Sansare SD	232145
Process for the continuous production of carbon monoxide free hydrogen from methane or methane rich hydrocarbons	Choudhary VR, Rajput AM	228341
Process for the epoxidation of liquid olefinic organic compound using a supported nano-gold catalyst	Vasant Ramchandra Choudhary, Nilesh Sudhir Patil, Balu Shivaji Uphade, Prabhas Jana	236024
Process for the preparation of a mixture of alkyl phenols	Dongare MK, Patil PT, Malshe KM	227865
Process for the preparation of a novel catalyst composite material suitable for hydrocarbon transformations	Tapan Kumar Das, Asha Jeevan Chandwadkar, Subramanian Sivasanker	232391
Process for the preparation of arylamines	Ashutosh Anant Kelkar, Nandkumar Manikrao Patil, Raghunath Vitthal Chaudhari	233826
Process for the production of aromatic carboxylic acids	Srinivas D, Chavan SA, Ratnasamy P	230567
Selective hydrogenation of nitrogen containing aromatics	Avinash Narendra Mahajan, Prakash Shivanand Ozarde, Raj Madhukar Deshpande, Raghunath Vitthal Chaudhari	235913
Tinuvin p-hindred amine light stabilizer and derivatives thereof, and a process for the preparation thereof	Mohitkumar Shrojilal Desai, Raj Pal Singh	233398
Vapor phase nitration of benzene using nitric acid over molybdenum silica catalyst	Dongare MK, Patil PT, Malshe KM	234033

Ph.D. THESES

Devi Ahilya University, Indore

Author	Title	Guide
Kautharapu, K. B.	Aqueous two phase systems for down stream processing of proteins	Ponrathnam, S.

IIT Mumbai

Author	Title	Guide
Dasmahapatra, A.K.	Studies of phase transition in polymeric system in the presence of hetero species by dynamic monte carlo simulation	Kumaraswamy, G.
Gorasia, A.K.	Multiphase flow and mixing in microreactors	Ranade, V. V.
Iyer, V.S.B.	Dynamics of Ring Polymers in an Obstacle Environment	Lele, A. K.

University of Kalyani

Author	Title	Guide
Bhattasali, D.	Synthesis Studies Towards New Alfa - Glucosidase Inhibitors Penarolide Sulfate A1, Schulzeines B and C	Gurjar, M. K.

University of Mumbai

Author	Title	Guide
Naren, P. R.	Modeling of High Solid Flux Circulating Fluidized Bed Reactors	Lali, A. M. and Dr. V. V. Ranade
Salunke, G.B.	Enantioselective Synthesis of Bioactive Molecules	Gurjar, M. K.

University of Pune

Author	Title	Guide
Abhilash, O. U.	Studies on Peroxidases and their Potential Role in Lignin Metabolism of Leucaena Leucocephala	Khan, B. M.
Aher, N. G.	Design and Synthesis of Bile Acid Based Conjugates, Dimers, Oligomers and their Pharmacological and Supramolecular Applications	Pore, V. S.
Bag, A.	Linear Response Approach to Fock Space Multi Reference Coupled Cluster	Pal, S.
Bavikar, S. N.	Design and synthesis of Sterol-Polymides, Sterol-Polymines and bile acid bistriazoles: a new class of antimicrobials	Hazra, B. G.
Chandran, S. P.	New Methods Towards Synthesis and Controlled Functionalisation of Inorganic Nanoparticles	Prasad, B. L. V.
Chavan, S. B.	Biocontrol of Insect Pests in a Agriculture Using Chitinolytic Enzyme Complex of Myrothecium Verrucaria	Deshpande, M. V.
Chincholkar, P. M.	Studies on the Synthesis of Azetidin-2-Ones and their Application in the Synthesis of Biologically Important Compounds	Deshmukh, A. R. A. S.
Chopade, A.U.	Total Synthesis of Thia- Calanolide A and Analogues, Asymmetric Aziridination of Alkenes and Development of Environmentally Benign Green Methodologies	Chanda, B. M.
Dakarapu, R.	Towards the Total Synthesis of 15 Hydroxygeldanamycin, KOSN 1655 and Herbimycin A	Gurjar, M. K.
Delori, A.	Molecular recognition study of some amino derivatives of pyrimidines and triazines	Pedireddi, V. R.
Deshpande, A. S.	In-Situ Chemo-Bioremediation for Gas Clean-up	Kulkarni, B. D.
Devi, G.(Ms)	Synthesis and Biophysical Studies of PNA Analogues Derived from 4 Substituted Proline and 1,2,3 Triazole in the Backbone	Ganesh, K. N.
Dharkar, P.	Investigation into the structures of a lectin from Trichosanthes dioica and one from Erythrina indica & biophysical characterization of Araceae lectins from Sauromatum guttatum and Arisaema tortuosum	Suresh, C.G.
Didgikar, M. R.	Studies in catalytic carbonylation of amines for the synthesis of disubstituted ureas and carbamates	Gupte, S.P.
Durugkar, K.A.	Cross Metathesis Approaches for Broussonetine C, G & 12-C-Glycosyl-Dodecanoic Acids and Exploration of Click Reaction in Crystal Engineering	Ramana, C.V.
George, S.	Enantioselective Synthesis of Bioactive Molecules and Asymmetric Oxyfunctionalization of Alkenes	Sudalai, A.
Gupta, D.F.	Modeling of Coal Fired Boiler	Ranade, V.V.
Ingavle, G.C.	High Internal Phase Emulsion: Synthesis of Novel, Highly Porous, Functional Polymers, Characterisation and Applications	Ponrathnam, S.

Author	Title	Guide
Jagannathan, R.	Surface Functionalisation of Nanoparticles and Their Biological Applications	Prabhune, A.(Ms)
Jagtap, N.(Ms)	Selective Catalytic Reduction of NOx Under Lean Burn Conditions Using Supported Metal Oxide Catalysts	Dongare, M.K.
Joshi, V.P.	Studies on Synthesis & Characterization of Thermoplastic Polyurethane Urea Copolymers	Lele, A.K.
Kar, R.	Study of a rational model of gas phase molecules in external electric field and in solvents using local reactivity descriptors	Pal, S.
Kelkar, T.	Computational Study of Hydrogen Storage Materials for Fuel Cells	Pal, S.
Kondekar, N.B.	Synthesis of biologically active compounds employing proline catalysed reactions, asymmetric dihydroxylation, aminohydroxylation and Jacobsen's hydrolytic kinetic resolution	Kumar, P.
Kothawade, S.S.	Synthesis and Characterization of Polyimides: Membrane Material for Gas Permeation and Polymer Electrolyte for Fuel Cell	Kharul, U.K.
Kshirsagar, V.S.	Heterogenized transition metals/complexes into the clay matrix for liquid phase oxidation of phenol derivatives	Rode, C.V.
Kulakarni, P.(Ms)	Isolation and Characterization of Cinnamyl Alcohol Dehydrogenase Gene from Leucaena Leucocephala	Khan, B.M.
Kulkarni, M.P.	Synthesis and Characterization of Heterocyclic Polymers as Polymer Electrolytes for Fuel Cells and other Applications	Vernekar, S.P., and Vijayamohanan, K.
Mallik, R.	Studies Towards the Total Synthesis of Cyclodidemniserinol Trisulfate by Employing Pd Mediated Alkynol Cycloisomerizations and A [2+2+2] Alkyne Trimerization Approach for Synthesis of some Carbapenems	Gurjar, M.K.
Mallikarjuna, S.R.	Synthesis and Properties of Polymer Layered Silicate Clay	Sivaram, S.
Manje, G.S.J.	Molecular Analysis of Fusarium Wilt Resistance and Yield Related Traits in Chickpea(Cicer Arietinum L.)	Gupta, V.S.(Ms)
Mapa, Maitri	Synthesis, characterization and catalytic studies of heteroatoms incorporated ZnO	Gopinath, C.S.
Meera, P.	Nafion Based Hybrid Polymer Electrolytes and Nanocomposites: Design and Electrochemical Investigations	Vijayamohanan, K.
More, A.S.	Synthesis of new monomers starting from renewable resource materials and polymers derivd therefrom	Wadgaonkar, P.P.
Panchgalle, S.P.	Organocatalytic Asymmetric Synthesis of Bioactive Molecules and Oxidation Studies in Ionic Liquids	Kalkote, U.R.
Panda, B.M.	Studied on Semecarpus Anacardium L. for in Vitro Regeneration and Identification of Biologically Active Compounds	Hazra, S.
Pandey, A.K.	Synthesis and Characterization of Biodegradable Polymers	Garnaik, B.
Patil, P.M.(Ms)	Synthesis and Characterization of Novel Copolymers	Kulkarni, M.G.

Author	Title	Guide
Patwa, A.N.	DNA Ferrocene Covalent Adducts for Studying DNA Conductance and Engineering Molecular Recognition Switch of DNA Base Pairing	Ganesh, K.N. and Vaijayanti, Anilkumar
Potrekar, R.A.	Novel Polybenzimidazoles as Polymer Electrolytes for Fuel Cell	Vernekar, S.P.
Prabhakaran, R.(Ms)	Intra Specific Map Development and Molecular Analysis for Agronomically Important Traits in Chickpea (Cicer arientinum L.)	Gupta, V.S.(Ms)
Shabab, M.	Study on Cysteine Protease and their Inhibitors	Khan, M.I.
Shaik, N.M.	Molecular Cloning and Characterization of Leucaena Leucocephala Beta Glucosidase, a Family 1 Glycosyl Hydrolase	Khan, B.M.
Shaikh, T.M.	Enantioselective Synthesis of Bioactive Molecules via Asymmetric Hydroxylations, Aminoallylation and Synthetic Methodologies Involving Activation of C-H Bonds	Sudalai, A.
Shashidhara, K.S.	Studies of structure function relationship of Alpha mannosidase from Aspergillus Fischeri NCIM 508	Gaikwad, S.M.
Sidhaye, D.S.(Ms)	Studies on Synthesis and Assembley of Metal Nanoparticles	Prasad, B.L.V.
Singh, J.	Studies on low molecular mass cysteine protease inhibitor from Actinomycetes	Gaikwad, S.M.
Singh, N,	In vitro conservation, ecological mapping with chemical and molecular characterization of garcinia species occurring in Maharashtra	Thengane, S.R.(Ms)
Soni, S.K.	Phytase from Aspergillus niger NCIM 563: isolation, purification, characterizaion and its applications	Khire, J.M.
Srivastava, S.	Molecular Characterization of Cinnamoyl CO a Reductase (CCR) Gene in Leucaena Leucocephala	Khan, B.M.
Sulake, R.S.	Synthesis of Two Bromotyrosine Derived Natural Alkaloids and Analogues, Total Synthesis of Mutisianthol and Enzyme-catalysed Resolution of Fine Chemical and Intermediates in the Presence Phosphorus Ionic Liquids	Chanda, B.M.
Suryawanshi, S.B.	Studies towards Total Synthesis of Pachastrissamine, Cephalosporolide E/F and their Analogs and some Metal Mediated Reactions on Sugar Templates	Ramana, C.V.
Thakar, D.M.	Studies of Penicillin Acylase Immobilization Using Membranes for the Production of 6-Aminopenicillanic Acid (6-APA)	Adikane, H.V.
Tiwari, S.S.	How do Ionic Liquids and Aqueous Media Promote Organic Reactions?	Anilkumar
Upadhyay, P.K.	Development of New Methodology Using Phosphorus Ylides and Enantioselective Synthesis of Pyrrolidine and Piperidine Alkaloids	Kumar, P.
Vaidya, B.K.	Chiral Separation of Drugs and Drug Intermediates by Immobilized Biocatalyst	Kulkarni, B.D.
Vatmurge, N.	Design synthesis and bioevaluation of bile acid B-lactam conjugates, studies directed towards the synthesis of squalamine and enantioselective reduction of prochiral ketones using chiral amino alcohols	Hazra, B.G.
Yadav, A.K.	Molecular Studies of Lignin Metabolism in Leucaena Leucocephala	Khan, B.M.

Academic COLLABORATIONS

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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
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 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. Vijayamohanan
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
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)
Towards improvement of flax for agronomic and disease resistance traits	Dr. Vidya Gupta	Dr. Raju Datla, NRC-PBI, University of Saskachewan, Saskatoon, Canada Dr. Sylvie Cloutier, Agriculture and Agri- Food Canada, Winipeg, Canada
Towards an understanding of Nox 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.
Magnetic nanoparticles for applications in biomedicine and spintronics	Dr. B.L.V. Prasad	Prof. Mathias Brust Department of Chemistry, University of Liverpool, UK
Preparation of Metamaterials through self-assembling nanostructures	Dr. B.L.V. Prasad	Prof. Olivier Mondain-Monval Centre de Recherche Paul Pascal (CRPP CNRS) University of Bordeaux, France
Conformational Investigation of Synthetic Oligomers	Dr. G. J. Sanjayan	Prof. H. J. Hoffman, University of Leipzig, Germany
New PiP3-K antagonists	Dr. C. V. Ramana	Prof. Alexei Degtrev Sackler School of Graduate Biomedical Sciences, Boston, USA

Academic COLLABORATIONS

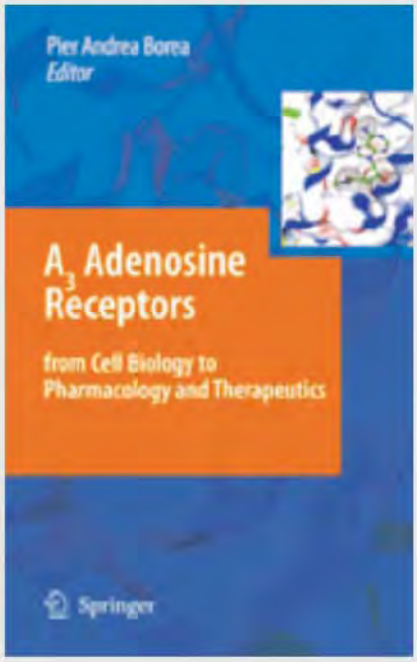
Project Title	NCL Partner(s)	External Partner(s)
Potential antidiabetic agents: Synthesis and enzymatic evaluation of sugar-derived inhibitors of glycogen phosphorylases	Dr.Vincent Paul Dr. Hotha Srinivas Dr. Thomas Daniel	Prof. Somsák Lazlo Dr. Gergely Pal Dr. Czifrák Katalin Tibor Docsa Department of Organic Chemistry University of Debrecen, Debrecen, Hungary
Novel method for the synthesis of enantiomerically pure ?-amino acids and its application towards antispastic drug Baclofen and epileptic drug Pregabalin	Dr.Vincent Paul Dr. Hotha Srinivas	Prof. José Mario Ordóñez Palacios Prof. Mario Fernández Zertuche Centro de Investigaciones Químicas-Universidad Autónoma del Estado de Morelos. Av. Universidad Cuernavaca, or. Mexico
Dimorphism in a marine isolate Yarrowia lipolytica: Significance of ornithine decarboxylase in oxygen dependent yeast-hypha transition and its correlation with alkane degradation	Dr. M.V. Deshpande	Professor J.Ruiz-Herrera, Centro de Investigacion y de Estudios, Avanzados del IPN, Unidad Irapuato, Apartado Guanajuato, Mexico

Books / CHAPTERS in BOOKS

- Doiphode N., Joshi C., Ghormade V. and Deshpande M.V., The biotechnological applications of dimorphic yeasts. In: Yeast biotechnology - Diversity and applications (Ed.: Satyanarayana and Kunze), Springer, 2009, pp. 635-650.

- Khire J. M., Bacterial Biosurfactants and their role in Microbial Enhanced Oil Recovert (MEOR) In: Biosurfactants (Ed.: Dr. Ramakrishana Sen), Landes Biosciences / Eureka Publications, 2010, pp. 146-157.

- Jacobson, K.A., Gao, Z.G. Tosh, D.K., Sanjayan, G.J., de Castro, S., A3 Adenosine receptor agonists: History and future perspectives, In A3 Adenosine Receptors from Cell Biology to Pharmacology and Therapeutics. (Ed.: P.A. Borea), Springer, 2010, pp. 93-120.



Deputation ABROAD

Business Development activity

- **Srinivas D,**
  USA,
  12-26 August 2009
  21 Nov - 01 Dec 2009
- **Raja T,**
  USA,
  12-26 August 2009
  21 Nov - 01 Dec 2009

Bilateral/ Collaborative/ Exchange programme

- **Kelkar A A,**
  France,
  7-28 April 2009
- **Hotha S,**
  USA,
  14-25 June 2009
- **Ogale S B,**
  Singapore,
  19 June -03 July 2009
- **Shukla P G,**
  UK,
  15-24 June 2009
- **Gopinath C S,**
  UK,
  7-28 June 2009
- **Guruswamy K,**
  UK & France,
  26 June-08 July 2009
- **Rode C V,**
  Japan,
  08-13 July 2009
- **Vidya S Gupta,**
  Canada,
  7-8 Oct 2009
- **Dongare M K,**
  Germany,
  14 Sep - 13 Oct 2009
- **Ogale S B,**
  France,
  07-20 Oct 2009
- **Singh A P,**
  Germany,
  18 Nov-09 Dec 2009
- **Satyanarayana C V,**
  S Africa,
  21 Jan 2010-05 Feb 2010
- **Giri A P,**
  Germany,
  01 Aug-31 Oct 2009
- **Thomas Daniel,**
  Russia,
  30 Oct-08 Nov 2009
- **Vincent Paul Swamy,**
  Russia,
  30 Oct - 08 Nov 2009
- **Umbarkar S B,**
  France,
  09-19 Dec 2009
- **Shukla P G,**
  UK & The Netherlands,
  09-19 Feb 2010
- **Giri A P,**
  USA,
  18 Jan - 04 Mar 2010

- **Vincent Paul Swamy,**
  Ukraine,
  04-12 Mar 2010
- **Premnath V,**
  Canada,
  08-12 Mar 2010
- **Nene S,**
  Germany,
  07-21 Mar 2010

EOL/ Fellowship/ Sabbatical Leave/ Visiting Professor

- **Patil K R,**
  Spain,
  02-31 July 2009
- **Amol A Kulkarni,**
  Germany,
  30 Aug-12 Sep 2009
- **Chaudhary S K,**
  Spain,
  18 Jan-16 Apr 2010
- **Pradeep Kumar,**
  Germany,
  01 Mar-31 May 2010
- **Amol A Kulkarni,**
  USA,
  31 Dec 2009-11 June 2010
- **Deshpande S D,**
  S Korea,
  13 July 2009-12 July 2010

Meeting

- **Krishnan S,**
  Denmark,
  05-08 June 2009
- **Sivaram, S.,**
  South Africa,
  June 7-13, 2009
- **Sivaram, S,**
  Russia,
  15 September 2009
- **Sivaram, S,**
  Brazil,
  September 21, 2009
- **Ogale S B,**
  USA,
  30 Nov - 10 Dec 2009
- **Guruswamy K,**
  USA,
  15-19 Mar 2010
- **Kendurkar S V,**
  China,
  22-25 Mar 2010

Training

- **Panchnadikar V V,**
  Japan,
  16 Nov - 04 Dec 2009

Conferences/ Seminars/ Symposia/ Workshops

- **Varma A J,**
  Italy,
  21-23 April 2009
- **Sivaram, S,**
  The Netherlands,
  April 22-23, 2009
- **Bhattacharya A K,**
  Thailand,
  4-6 May 2009
- **Wadgaonkar P P,**
  Korea,
  17-21 May 2009
- **Rode C V,**
  Italy,
  14-17 June 2009
- **Ajith Kumar T G,**
  USA,
  19-23 July 2009
- **Gadgil C J,**
  Canada & USA,
  26-31 July 2009
- **Grover G S,**
  UK, 01-04
  August 2009
- **Srinivas D,**
  Japan,
  03-07 August 2009
- **Pal Sourav,**
  Germany,
  6-12 August 2009
- **Prasad B L V,**
  UK,
  02-16 August 2009
- **Anil Kumar,**
  Spain,
  09-11 Sept 2009
- **Sivaram, S,**
  Russia,
  September 13-14 and 17, 2009
- **Sivaram, S,**
  Brazil,
  September 19-20, 2009
- **Vijayamohanan K, S**
  Korea,
  03-06 Nov 2009
- **V A Kumar,**
  USA,
  16-26 August 2009
- **Srinivas D,**
  Russia,
  12-15 Sep 2009
- **Dhepe P L,**
  Russia,
  12-15 Sep 2009
- **Ogale S B,**
  Brazil,
  17-22 Sep 2009
- **Shukla P G,**
  The Netherlands &
  Germany,
  23-30 Sept 2009
- **Vaval Nayana,**
  Greece,
  29 Sep - 04 Oct 2009
- **Pal Sourav,**
  Greece and Germany,
  29 Sep -11 Oct 2009
- **Lele Ashish K,**
  USA & UK,
  18-24 Oct 2009
- **Pedireddi V R,**
  China,
  22-25 Oct 2009
- **Pal Sourav,**
  China,
  16-18 Nov 2009
- **Kulkarni M G,**
  Singapore,
  15-18 Dec 2009
- **Ogale S B,**
  Egypt,
  22-28 March 2010
- **Wadgaonkar P P,**
  Brazil,
  01-21 Feb 2010
- **Pal Sourav,**
  Japan,
  23-24 Feb 2010

Deputation ABROAD

Fellows and Students participation in conferences/ research projects

- **N Khuspe, SRF,**
  Australia,
  29 May-04 June 2009
- **Yogesh Manjare, SRF,**
  Canada,
  24-30 July 2009
- **Ramya Jagannathan, SRF,**
  Germany,
  26-29 July 2009
- **Hamid Shaikh, SRF,**
  Italy,
  14-18 Sept 2009
- **T Kotbagi, SRF,**
  Germany,
  21-30 Sept 2009
- **B S Kulkarni, SRF,**
  Germany,
  04-07 Oct. 2009
- **Himadri Dey, SRF,**
  Germany,
  04-07 Oct 2009
- **S Pandhare, JRF,**
  Germany,
  04 Nov 2009-29 Jan 2010
- **Urvashi, SRF,**
  France,
  07-15 Dec 2009
- **Deepak Jadhav, SRF,**
  Germany,
  08 Jan-31 Aug 2010
- **V Sreeja, SRF,**
  Australia,
  22-26 Feb 2010

Lecture / Seminar delivered at NCL by VISITORS

Date	Topic	Speaker
16/04/2009	Synthesis, Characterization, and Application of New Mesoporous Materials	Dr. Rani Jha, Cook Physical Science, Burlington, USA
17/04/2009	Soft Chemistry Route for Materials	Prof. P. Pramanik, Department of Chemistry, Indian Institute of Technology, Kharagpur
22/04/2009	Modeling room temperature ionic liquids	Prof. S. Balasubramanian, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore
24/04/2009	Microrheology of a sticking transition	Prof. Shankar Ghosh, TIFR, Mumbai
14/05/2009	Electrospinning and extensional rheology of polymer solutions	Dr. Pradipto Bhattacharjee, Post-doctoral Fellow, MIT, USA, Massachusetts, USA
18/05/2009	Electro-chemical Characterization of PS-PEO Block Copolymer Electrolytes	Ashoutosh Panday, UC Berkeley, California, USA
25/05/2009	Enlightening Chemical Genetics with Libraries of Fluorescently Tagged Small Molecules	Dr. Suvadeep Nath, Research Associate, Chemistry & Biochemistry, University of Colorado, Boulder, USA
26/05/2009	Nucleoside and Nucleotide Chemistry at the Surface of Chemistry and Biology	Dr. Shantanu Pal, Karmanos Cancer Research Institute, Detroit, USA
17/06/2009	Resolution enhancing strategies in solid-state NMR	Dr. Rajendra Singh Thakur, Postdoctoral Fellow, Tata Institute of Fundamental Research, Mumbai
18/06/2009	Dyspepsia	Dr. Harshal Gadhikar, Gastro-enterologist, Pune
30/06/2009	Decoding Mechanisms involved in Generating Metabolic Diversity	Dr. Rajesh S. Gokhale, Institute of Genomics and Integrative Biology, New Delhi
10/07/2009	Recent developments in the synthesis of nitrogenated heterocycles	Prof. Yannick Landais, Universite of Bordex-1, Cedex, France
16/07/2009	Perovskites for NOx removal from mobile and stationary source	Prof. Christophe Dujardine, UCCS, France, Lille, France
24/07/2009	One electron oxidation of DNA: Factors affecting oxidative damage of nucleobases	Dr. Joshy Joseph, Research Scientist II, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA
27/07/2009	Novel Biomedical Applications of Atomic Force Microscopy	Prof. Gunjan Agarwal, Director: Atomic Force Microscopy Lab, Ohio State University, Columbus, USA
30/07/2009	Instability of a Moving Liquid Sheet in the Presence of Acoustic Forcing	Prof. Mahesh Tirumkudulu, IIT-B, Mumbai

Lectures/ Seminars given at NCL by VISITORS

Date	Topic	Speaker
06/08/2009	NMR spectroscopy in solids and mesophases: the golconda of anisotropic interactions	Prof. Olivier Lafon, UCCS, Department of Chemical Engineering, University of Lille, Lille, France
06/08/2009	Theoretical studies of equilibrium structures and their linear stability in block copolymer melts	Dr. Amit Ranjan, Post-Doctoral Research Associate, Harvard Institute, Cambridge, USA
07/08/2009	An intricately networked NF-ÛB system controls immune development and immune responses	Dr. Soumen Basak, University of California, San Diego, USA
10/08/2009	Defects in Ultrathin Cu films on Mo and Ta Studied by Thermal Helium Desorption Spectrometry	Dr. Vinay Venugopal, Institute of Physics, Bhubaneswar
10/08/2009	Subcomponent Self-assembly Approach: An Iron Cage In Water	Dr. Prasenjit Mal, Dept of Chemistry, Cambridge Univ, Cambridge, UK
11/08/2009	Light emitting liquid crystals	N. Somanathan, Scientist, Central Leather Research Institute, Chennai
11/08/2009	Nonlinear Optics: Application to Nanoparticles	Prof. Reji Philip, Raman Research Institute, Bangalore
24/08/2009	Flow of powders into closed cavities	Prof. Csaba Sinka, University of Leicester, UK
26/08/2009	Rheological and Thermal Activity Monitoring Methods for the Characterization of Hydrocolloids	Dr. Abel Gaspar-Rosas, Scientist, TA Instruments, New Castle, USA
27/08/2009	Innovation Flow - the science of flowing Ideas and Inventions into Innovation	Dr. MV Shankar, Principal Scientist, Dow Chemical International Pvt Ltd, Pune
03/09/2009	A Framework for Comprehending the Nature of the Protein Universe	Dr. S. Sri Krishna, Assistant Professor (Research), Joint Center for Structural Genomics, Burnham Institute for Medical Research, La Jolla, USA
07/09/2009	From Reactive Intermediates to Combating Chemical Nerve Agents: Adventures in Physical-Organic Chemistry	Dr. Siva Muthukrishnan, Scientist, Ohio State University, USA
29/09/2009	Selective Reactions of Singlet Oxygen: From Synthesis	Prof. Torsten Linker, Institute of Chemistry, University of Potsdam,Karl-Liebknecht-Straße, Potsdam, Germany
01/10/2009	Conceptualizing Inventions for Commercial Potential	Dr. Gopakumar G. Nair, Founder and CEO, Gopakumar Nair Associates, Mumbai
12/10/2009	MIT Trained Swadeshi: MIT and Indian Nationalism, 1880-1947	Prof. Ross Bassett, Associate Professor of History, North Carolina State University, USA
03/11/2009	Green Polymerization and Protein Conjugation with Phosphorylcholine and poly(ethylene glycol)-based Compounds	Dr. Debasis Samanta, Research Associate, Polymer Science and Engineering Department, University of Massachusetts, Amherst, USA
05/11/2009	Size and Surface effects in Magnetic Nanomaterials	Dr. Balaji Gopalan, Center for Advanced Microstructures and Devices, Louisiana State University, USA

Date	Topic	Speaker
10/11/2009	Present status of Fuel cell Technology	Dr. Subhash Singhal, Director, Pacific North west National Laboratory, USA
11/11/2009	Flavin reductases and oxygen activation: Applications in antibiotic biosynthesis and artificial nuleases	Prof. Marc Fontecave, Director, Academy of Sciences, Cedex, France
16/11/2009	Titanium Based C1 Symmetric Non-metallocene Catalysts from Beta-Amino alcohols for Olefin Polymerization	Dr. Vijayakrishna Kari, CNRS Postdoctoral Fellow, Laboratoire de Chimie des Polymeres Organiques (LCPO), University of Bordeaux 1, Cedex, France
18/11/2009	How do plants coat themselves? Lessons from Arabidopsis and tomato	Dr. Asaph Aharoni, Senior Scientist, Department of Plant Sciences, The Weizmann Institute of Science, Rehovot, Israel
18/11/2009	Molecular Diffusion and Effect due to Confinement	R. Mukhopadhyay, Scientist, BARC, Mumbai
19/11/2009	Selective dehydration of bio-alcohols to olefins and fuels: Novel catalysts and approaches	Dr. Ramesh Kanaparthi, Senior Research Fellow, Institute of Chemical and Engineering Sciences, Singapore, Singapore
25/11/2009	Hypertension	Dr. Nitin Patki, Cardiologist, N.M.Wadia Inst. of Cardiology, Pune
04/12/2009	New Directions in Selectivity with In and Bi Mediated Allylation	Prof. Gregory R. Cook, Professor and Chair, Dept. of Chemistry and Molecular Biology, North Dakota State University, Fargo, USA
08/12/2009	MALDI Imaging	Dr. Ales Svatos, Head, Mass spectrometry, Max Plank Institute, Jena, Germany
08/12/2009	Research in Chem-Bio Center of Kyiv National University, Ukraine	Dr. Dmytro Kovalskyy, Head and Group Leader, Molecular Modelling Department, Kyiv National University, Kyiv, Ukraine
10/12/2009	Single Spins in Diamond-Novel Probes for Nanoscience	Gopalakrishnan Balasubramanian, Research Associate, Physikalisches Institute, Universität Stuttgart, Stuttgart, Germany
11/12/2009	Force generation in the intracellular cytoskeleton	Prof. Tanmay Lele, University of Florida, Gainseville, USA
15/12/2009	Population modeling	Prof. Shripad Tuljapurkar, Morrison Professor of Population Studies, Department of Biology, Stanford University, Stanford, USA
21/12/2009	Marine sponge derived collagen protein and biomaterials	Dr. Arun Ghosh, Scientist (Bio-based Materials), Biocontrol, Biosecurity & Bioprocessing AgResearch Ltd, Crown Research Institute of New Zealand, Lincoln, New Zealand
24/12/2009	Synthetic challenges in Pharmaceutical development	Dr. A. Murugan, AstraZeneca, Bangalore
07/01/2010	Self Detecting Carbon Nanotube Resonators	Mr. Hari Pathangi, Katholieke University, Leuven, Belgium
12/01/2010	Organic Synthesis And Methodology Inspired By Marine Natural Products	Prof. Sivappa Rasapalli, University Of Massachusetts Dartmouth, North Dartmouth, USA

Lectures/ Seminars given at NCL by VISITORS

Date	Topic	Speaker
13/01/2010	Glassy behaviour : Thermodynamics & Kinetics	Prof. Gregory McKenna, Department of Chemical Engineering, Texas Tech University, Texas, USA
13/01/2010	The easy approach to self assembly: Teaching new tricks to old molecules and nanoparticles	Prof. Srinivasa R. Raghavan, Department of Chemical & Biomolecular Engg, University of Maryland, College Park, Maryland, USA
14/01/2010	Biomimetic nanostructured coatings on nano-grained /ultrafined-grained substrate : Microstructure, surface adhesion strength, and biosolubility	Dr. Sachin Mali, Scientist, Department of Biomedical and Chemical Engineering, Syracuse University, New York, USA
14/01/2010	Probing early events in EGFR signaling pathway using nanoparticle and polymer based tools	Dr. Atul Bharde, Humboldt Fellow, Laboratory of Cellular Dynamics, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany
15/01/2010	Integrative Mathematical Modeling of Biological Systems: Opportunities and Challenges	Dr. Frank Tobin, President, Tobin Consulting LLC, USA
19/01/2010	Development of Heterogeneous Polymeric Systems at Macromolecular Institute	Prof. Bluma Guenther Soares, Macromolecular Institute, Federal University of Rio de Janeiro, Brazil
19/01/2010	Molecular Steps in the Fischer-Tropsch Synthesis: A Path Towards Clean Fuel	Dr. Sharan Shetty, Technical University of Eindhoven, Eindhoven, The Netherlands
20/01/2010	BiFeO3: A multifunctional material for new generation devices	Dr. Vilas Shelke, Center for Materials for Information Technology, University of Alabama, Tuscaloosa, USA
21/01/2010	Thermodynamic Studies of Enzyme-Catalyzed Reactions	Prof. Robert N. Goldberg, Department of Chemistry and Biochemistry, University of Maryland, Baltimore, USA
08/02/2010	Aminol Pharm: Asymmetric synthesis and utlilisation of Chiral, non resimic amino alcohol	Prof. Bakhtan Singaram, University of California, California, USA
08/02/2010	From matter to life: chemistry?	Prof. Jean - Marie Lehn, Nobel Laureate, ISIS College, Paris, France
08/02/2010	Gas Hydrates: Opportunities for Innovative Technologies	Dr. Rajnish Kumar, Research scientist, Steacie Institute for Molecular Sciences, Vancouver, Canada
08/02/2010	Sweetness and Light : Continuous Glucose Sensing with Fluorescent Thin-Film Hydrogel	Prof. Bakhtan Singaram, University of California, California, USA
09/02/2010	Progress on the incorporation of cage amino acids into non-natural peptides	Prof. H G Kruger, School of Chemistry, University of KwaZulu-Natal, Durban, South Africa
09/02/2010	Perspectives in Chemistry from Supramolecular Chemistry towards Adaptive Chemistry	Prof. Jean - Marie Lehn, Nobel Laureate, ISIS College, Paris, France
10/02/2010	Nanoengineering Block Copolymer Micelles for Drug Delivery	Prof. T. K. Bronich, University of Nebraska Medical Center, Omaha, USA

Date	Topic	Speaker
10/02/2010	Prevention of heart attack	Dr. Shirish Sathe, Cardiologist, Deenanath Mangeshkar Hospital, Pune
18/02/2010	Electrophoresis of Highly Charged colloids	Prof. Apratim Chatterji, IISER, Pune
22/02/2010	Synthesis of zeolites from mesoporous silica and their catalytic functions ""	Prof. Masaru Ogura, Institute of Industrial Science, University of Tokyo, Tokyo, Japan
24/02/2010	Surface Science and Catalysis	Dr. C. P. Vinod, Post-Doctoral Researcher, Cardiff University, Cardiff, UK
11/03/2010	Buckling and its arrest in drying colloidal droplets	Dr. Debasis Sen, Scientist, BARC, Mumbai
11/03/2010	Small peptides as self-assembling systems	Dr. Aseem Mishra, Wellcome Trust -DBT Alliance Early Career Fellow, International Centre for Genetic Engineering and Biotechnology, New Delhi
19/03/2010	Suicide Inactivation of PLP-dependent Aminoacid Decarboxylases and Analysis of Protein Acetylation Using Semi-Synthesis	Dr. Kannan R. Karukurichi, Post Doctoral Fellow, Johns Hopkins School of Medicine, USA
26/03/2010	Philoshiphy of chemistry	Prof. Sundar Sarukkai, Professor and Director, Manipal University, Manipal

Invited Talks / LECTURES delivered by NCL SCIENTISTS

Dr. Agrawal, D. C.

Transgenic Cotton in India - An Overview, Africa City of Technology, Khartoum, Sudan, 28 Sept. 2009

Dr. Argade, N. P.

Remarkable Chemo-, Regio-and Stereoselective Enzyme Catalysis, Institute of Chemical Technology, Mumbai, 22 Feb. 2010

Deshpande, M. V.

Microbial control of Helicoverpa armigera in pulses
Comparison of Metarhizium isolates to identify strains for commercialization, 5th International Conference on Biopesticides: Stakeholders' Perspectives, New Delhi, 26-30 April 2009

Dr. Sivaram, S.

Catalysis in Polymer Synthesis
Control of Structures and Functionalities, A V Rama Rao Research Foundation Award Lecture, Indian Institute of Chemical Technology, Hyderabad, 2 April 2009

Fostering Innovation in Public Institutions
The NCL-CSIR Experience, M/s. Praj Matrix Innovation Center, Pune, 10 April 2009

Polymers from Renewable Resources
An Indian Perspective, The Netherlands S&T Officers Network, The Hague, The Netherlands, 23 April 2009

The Future of Chemical Sciences R&D in CSIR, CSIR Director's Conference, HRDC, Ghaziabad, 29 Aug. 2009

Ganapathy, S.

CPMG Echo Acquisition and Sensitivity Enhancement in Solid State Hetero and Homonuclear Correlation Experiments, Department of Physics, Central University, Hyderabad, 12 Aug. 2009

Ms. Kendurkar, S. V.

Biotechnology and its application for Propagation and Improvement of Plants, Modern College of Arts, Commerce and Science, Pune, 23 Feb. 2010

Dr. Kulkarni, A. A.

Microreaction Technology
Applications and Engineering Challenges Institute of Chemical Technology, Matunga, Mumbai 30 Sept. 2009

Sinews of Excellence
The Evolution of Scientific Institution, Tata Research, Development and Design Center, Pune, 1 Sept. 2009

Fostering Innovation in Public Institutions
The NCL-CSIR Experience, KPIT-Cummins Infosystems, Pune, 30 Sept. 2009

Reactivity of Some Transition Metal Complexes in the Polymerization of Ethylene, Russia-India Symposium on Catalysis and Environmental Engineering, Novosibirsk, Russia, 13 Oct. 2009

Polymer Nanocomposites
Molecular Approaches to Tailoring Surfaces, Indo-Brazilian Joint Symposium on Advanced Materials, Rio de Janeiro, Brazil, 19 Oct. 2009

Mr Kulkarni, A. D.

IPR and Patent Procedure, Ahmednagar College, Ahmednagar, 20 Nov. 2009

Dr. Ramana, C. V.

From alkynol to nitroalkyne cycloisomerizations
Synthetic Utility and Mechanistic Investigations: International Symposium on organic chemistry - trends in 21st century" IACS, Kolkata, 10-12 Dec. 2009

Dr. Selvaraj, K.

Catalysis - Process and Materials
Insight through Computational Chemistry, Sam Higgin Bottom Institute of Science and Technology (AAIDU), Allahabad 03 Nov. 2009

The Chemical Industry in Transition
The Road Ahead, 11th International Conference Indian Petrochem - 2009, Mumbai, 16 Nov. 2009

Science, Technology and Innovation
Emerging Imperatives for India, National Science Day at ARDE, Pune, 26 Feb. 2010

Awards / RECOGNITIONS

name	Awards / Recognitions
Dr. Amol A. Kulkarni	INSA Medal for Young Scientist 2009
	Young Engineer Award 2009, The Indian National Academy of Engineering
	Indo-US Research Fellowship Awards: 2009
Dr. Rajesh G. Gonnade	INSA Medal for Young Scientist 2009
Dr. L. K. Doraiwsamy	Foreign associate, US National Academy of Engineering
Dr. Anil Kumar	J.C. Bose Fellow
	Homi Bhabha Memorial Award
Dr. Sourav Pal	Prof. R.P. Mitra Memorial Lecture Award
Dr. Ganesh Pandey	Goyal Prize - 2007
	P. C. Ray Memorial Award
Dr. S. Sivaram	Goyal Prize - 2007
	ICC D. M. Trivedi Lifetime Achievement Award for contribution to Indian Chemical Industry (Education & Research)
Dr. Ashish Lele	Fellow of Indian Academy of Sciences, Bangalore
	Young Leader Award by Lakshmipat Singhania - IIM, Lucknow National Leadership Award
Dr. P. P. Wadgaonkar	Tipco-ICT Diamond Jubilee Visiting Fellowship in Thermosets Endowment, Institute of Chemical Technology
Dr. Rahul Banerjee	Young Associate, The Indian Academy of Sciences, Bangalore
Dr. (Ms.) Panchami Prabhakaran	2009 Eli Lilly Asia Outstanding Thesis Award (Second Prize)
Dr. Satyendra Kumar Pandey	2009 Eli Lilly Asia Outstanding Thesis Award (First Prize)
Dr. A. P. Giri	2009 Borlaug Fellow
Dr. Pradeep Kumar	CRSI bronze medal
Dr. B. D. Kulkarni	Festschrift to recognise and honour contributions to Chemical Engineering Science by Industrial & Engineering Chemistry Research, (Issue No. 21, Volume 48 dated November 4, 2009) of American Chemical Society

Members of Board of DIRECTORS of INDUSTRIES

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Dr. V. R. Pedireddi	▪ Co-editor, Acta Crystallographica - Section
Dr. V. V. Ranade	▪ Associate Editor, Asia-pacific Journal of Chemical Engineering, Wiley InterScience
Dr. B. L. V. Prasad	▪ Member of Editorial Advisory Board International Journal of Green Nanotechnology, Taylor and Franscis
Dr. R. P. Singh	▪ Member, Editorial Board, Materials Sciences and Applications
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,
Dr. D. Srinivas	▪ Catalysis Surveys from Asia, Springer, Germanyo ▪ Bulletin of Catalysis Society India, Chennai
Dr. (Mrs) V.S. Tare	▪ Journal of Environmental Biology, Triveni Publishers, Lucknow
Dr. Anjani Varma	▪ Carbohydrate Polymers, Elsevier, The Netherlands ▪ Editorial Board, Trends in Carbohydrate Research, India
Dr. K. Vijayamohanan	▪ 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 Research FOUNDATION

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

Awards and Lectures

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

- Prof. B. D. Tilak Memorial Lecture
- Prof. J. W. McBain Memorial Lecture
- Prof. K. Venkataraman Memorial Lecture
- Dr. R.A. Mashelkar Endowment Lecture
- Dow Endowment Lecture in honour of Dr. Paul Ratnasamy

Award of merit based scholarships to the children of NCL employees

NCL RF awards merit based scholarships for the children, studying in IX to XII Standards, of NCL employees in group D (non-tech) and support staff in group I. The scholarship amount for the students who stood first is Rs.4000/- and for those who stood second is Rs.3500/- from each class. Fourteen students were awarded the scholarship on the occasion of CSIR Foundation Day.

Board of Trustees

Position	Present board	By virtue of
Chairman	Dr. S. Sivaram	Director, NCL
Member	Prof. D. Balasubramanian	Chairman, Research council
Member	Prof. J. B. Joshi	Director, MUICT
Member	Mr. Desh Bandhu Gupta	Representative of donor industry
Member	Dr. B. D. Kulkarni	Deputy Director, NCL
Secretary	Mr. B. B. Kasture	AO, NCL
Treasurer	Mrs. Mariamma John	SFAO, NCL
Jt. Secretary	Mr. G. Prabhakaran	Head, BDD, NCL

Annual Awards

Name of the Award	Award	Award winner	Awarded for
NCL RF Scientist of the Year Award (Sponsored by Maneckji & Shirinbai Neterwala Foundation)	Rs.20,000/- +Citation (Shared Jointly)	Dr. M V Badiger	For significant contributions to the area of superabsorbing polymers, synthesis of 'tailor-made' gels, molecular level studies in stimuli-responsive gels, solid-state NMR and rheo-NMR of gels as well as design and synthesis of hydrophobically associating polymers.
		Dr. C V Ramana	For developing new reactions and/or protocols that are capable of building biologically active small-molecules by integrating the catalyst and substrate designs. Selection of the retrons containing critical stereochemical information and choice of appropriate complex transforms addressing the skeletal and stereochemical complexity of the targeted molecules highlight the accomplished syntheses.
NCL RF Scientist of the Year Award (Sponsored by Dr. R. A. Mashelkar Endowment Fund)	Rs.20,000/- +Citation (Shared Jointly)	Dr. Srinivas Hotha	For developing diversity oriented synthesis (DOS) of small molecules that enables efficient synthesis of complex molecules using carbohydrate scaffolds and for significant contributions in identification and development of alkyl glycosides as glycosyl donors.
		Dr. Pankaj Poddar	For significant contributions to the study of ferroelectricity in nanoparticles and developing a novel microbial biomilling process for reducing larger particles into sub 10 nm particles.
Award for "New Initiative taken by R&D Support System"	Rs.20,000/- + Certificate of Merit (Shared Jointly)	Shri. Atul Mahajan Shri. Jaipal Singh Shri. T S More Shri. D G Naidu Shri. S Y Zope Shri. S R Sayyad Shri. A M Kumbhar Shri. Gopal Prasad Shri. M D Shinde Shri. N R Yadav (Engineering Services Unit)	For planning, designing, installing, operating and efficiently maintaining a wet and dry solid waste handling facility at NCL for composting wet waste. This effort has brought visibility to NCL as a responsible citizen to the city of Pune.

NCL Research FOUNDATION

Name of the Award	Award	Award winner	Awarded for
Director's Commendation Award	Rs. 35,000/- + Certificate of Commendation (Shared Jointly)	Dr. Darbha Srinivas Dr. S A Pardhy Dr. T Raja Dr. K J Waghmare Dr. V V Bokade Dr. S S Deshpande (Catalysis Division)	For developing a robust solid catalyst for transesterification of vegetable oils and having tolerance to high free fatty acids which have been tested and validated in a continuous pilot plant.
	Rs. 5,000/- + Certificate of Commendation	Shri Uttam Thakare (Finance & Accounts)	Having set an example for honesty and probity in public life as a citizen, a quality worthy of emulation by every member of NCL staff.
	Rs. 5,000/- each + Certificate of Commendation (Shared Jointly)	Dr. K. Guruswamy (Polymer Science & Engineering) Dr. V. Premnath (Polymer Science & Engineering)	For championing the cause of taking science to the school children, efficiently putting together an "outreach" programme and motivating young scientists of NCL to give their time to this effort voluntarily.
Individual Merit Award	Rs.5,000/- + Certificate of Merit	Shri. G.S. Krishnan (Finance & Accounts)	For his initiative in ensuring the benefits of "Cenvat Credit Rules 2005" pertaining to service tax payment accruing to NCL, thus realizing significant savings to NCL.
	Rs.5,000/- + Certificate of Merit	Dr. P. K. Ingle (Publication & Science Communication)	For his personal dedication, commitment and diligence in timely completion of Annual Reports, maintaining publication database and coverage of events at NCL for press and the CSIR community, bringing greater visibility to NCL and enhancing its image amongst its stakeholders.
	Rs.5,000/- + Certificate of Merit	Shri. Hasso Raheja (Chemical Engineering & Process Development)	For his conscientious and dedicated services towards providing wide ranging administrative support to scientists irrespective of rank or status and thus being a role model for an efficient Office Assistant.
	Rs.5,000/- + Certificate of Merit	Shri. N. H. Maidargi (Administration)	For efficient organization of the transportation services at NCL and being responsive to the needs of the users.
	Rs.5,000/- + Certificate of Merit	Shri. Agnelo Gabriel Fernandez (Administration)	For his commitment and efficiency in processing cases for approval of foreign travel of NCL scientists and students for attending conferences on deputation, study leave, sabbatical and under various international exchange and collaborative programmes.

Science Day Awards - 2009

Best Research Fellows

Name of the Award	Award	Award winner	Awarded for
Keerthi Sangoram Endowment Awards for "Best Research Scholars" for the year 2009	Rs. 2,500/- each+ Citation	Ms. Manasi B. Kasture Mr. Himadri S. De	Physical / Material Sciences
		Mr. Mukund Adsul Ms. Upasana Singh	Biological Sciences
		Mr. Shailesh P. Nagarkar Mr. Ajit Garade	Engineering Sciences
		Mr. Nagendra B. Kondekar Mr. Tanveer M. Shaikh	Chemical Sciences

Best Research Papers with the highest Impact factor

Name of the Award	Award	Award winner	Awarded to
Dr. Rajappa Award for "Best Publication" in Organic Chemistry with the highest impact factor for the Research Scholars	Rs.1,000/- + Citation	Effect of chirality of L/D- proline & prochiral glycine as the linker amino acid in five-atom linked thymidinyl -(α-amino acid)- thymidine dimers Journal: ChemComm Impact Factor: 5.34 SHARED	Ms. Seema Bagmare
	Rs.1,000/- + Citation	Methyl glycosides are identified as glycosyl donors for the synthesis of glycosides, disaccharides & oligosaccharides Journal : ChemComm Impact Factor: 5.34	Mr. V. Srinivasa Rao
Gupta - Pardeshi - Sainani Award for "Best Research Papers in Biological Sciences"	Rs.2500/- + Citation	Hydrolysis of cellulose derived from steam exploded bagasse by Penicillium cellulases: Comparison with commercial cellulose. Journal : Bioresource Technology Impact Factor: 4.45	Mr. Rajkmar Singh

NCL Research FOUNDATION

Name of the Award	Award	Award winner	Awarded for
	Rs.2,500/- + Citation	SHARED Biochemical characterization of two xylanases from yeast Pseudozyma hybeiensis producing only xylooligo-saccharides Journal : Bioresource Technology Impact Factor: 4.45	Mr. Mukund G. Adsul
Dr. Krishnan Award for "Best publication" for Research Scholars/ Project Assistants Physical / Material Sciences	Rs.5,000/- + Citation	Synthesis of framework Ti -substituted, 3-D hexagonal, mesoporous Ti-SBA-12 for selective catalytic oxidation Journal : ChemComm Impact Factor: 5.34	Mr. Anuj Kumar

Merit Scholarship for the year 2008-09 was awarded to the following students

Master Sushant P. Pawar	Ms. Sayali S. Shukla	Master Prashant P. Pawar
Ms. Tejashree A. Jagtap	Master Akash G. Thombre	Master Sourabh B. Jathar
Ms. Ankita S. Sathe	Master. Vishal R. Bhise	Ms. Deepa Srivastava
Ms. Poonam G. Rathwadkar	Ms. Amrin Punekar	Ms. Jahida Shaikh
Ms. Jyoti D. Chavan	Ms. Apurva R. Jadhav	

Outreach PROGRAMME

This activity has gained momentum and over twenty scientists from NCL, faculty from IISER and IIT-B, staff from the Venture Center, and enthusiastic volunteers are associated with this group, now called the "Exciting Science Group". The activities of this group, apart from the continuing popular science talks, now include outreach lectures at schools for underprivileged students, mentoring for students planning to send in entries to national science fairs and weekly science/ technology video screenings. The group is getting the generous support from NCL, the Venture Center, Battelle India, Forbes Marshall and Praj.

Popular talks for school students

The Popular Talks series of once-a-month talks aims to connect school students to practising scientists. Thus, school students get to hear a first hand account of what it means to do research, and to get a feel for the thrill of discovery. The speakers do not attempt to teach science to the students - rather, the idea is to create a sense of "wow" and to kindle the students' curiosity.

The talks are not meant to be pedantic lectures, but combine live demonstrations, experiments and problem solving exercises to involve the students and engage their attention. The talks are free and open to students and science teachers. The members visited about fifty schools with posters to make them aware of this lecture series.

Talks during the year

Date	Topic	Speaker
26 Apr 2009	How Giant Molecules Wiggle	Ashish Lele
31 May 2009	Bubbles and Drops: Stories from Disney Land, ice cream, laptops and petrol	Amol Kulkarni
28 Jun 2009	Chemical and Biological Analysis: Lets go fishing "molecules"	Venkat Panchagnula
26 Jul 2009	Can we get unlimited energy from sun or wind?	K.Vijayamohanan
25 Oct 2009	Tiny Magnets	Ajith Kumar
15 Nov 2009	Chemistry and Magic	Anil Kumar (IITB)
29 Nov 2009	How cancer begins?	Chitra Manikandan (Dow)
13 Dec 2009	Getting to know solids: How are they built?	Nandini Devi
20 Dec 2009	Ligands: Tools for a nanogoldsmith	BLV Prasad
17 Jan 2010	Excitement in chemistry	Sourav Pal
28 Feb 2010	Why Everyone is talking about Climate Change	K. Guruswamy
28 Mar 2010	Inhaled drug delivery: Science and Technology	Pankaj Doshi

Mentoring school students to do research based projects

An attempt was made to raise the awareness of opportunities such as IRIS (Initiative for Research and Innovation in Science) to spur students from schools in Pune to do research based projects, and NCL scientists, Dr. Chetan Gadgil and Dr. BLV Prasad, have offered to mentor student projects. Chetan and Prasad have already conducted three "mentoring" sessions, following the regular Popular Talks, to help students put together exciting projects.

The idea of our mentoring sessions is to give students with project ideas a forum to discuss their ideas with scientists, and to get further ideas on how to develop their projects.

Students who don't yet have project ideas can learn how to select a topic and how to initiate and plan work on that topic at the mentoring sessions.

Saturday video screenings

The Exciting Science group is now organizing "Saturday Video Screenings" - every Saturday, at 4pm at the Venture Center.

Videos that describe inspiring science or technology are screened.

Outreach PROGRAMME

Communicating with students, teachers, parents

In order to effectively utilize technology to communicate the activities of the Exciting Science group with students, teachers, parents and others who come to our seminars, video screenings, etc., the team at the Venture Center has come up with a redesigned web page.

Registration for our talks can now also be done through a convenient web-based form (or by sending email, as before). Slides from the talks, resources and photographs are uploaded on our site and can be easily shared through our site.

To connect with the students, we also have a presence on Facebook, Orkut and Twitter.

Taking science outreach to schools for underprivileged students

A new programme with the same philosophy as the the NCL Outreach lectures aimed at students at underprivileged schools is developed.

In this programme, we will continue use experiments, demos, etc. to excite children about science - however, we will choose topics for our talks from those that they are taught and will develop modules with appropriate experiments and historical background that will help them make connections with the science.

Six speakers from NCL have been identified who have committed to participating in this exercise. Each speaker will deliver a module to a school (viz. modules will be once a month) starting in the new school year (June 2010).

We are also considering handing out chemistry kits to the students (for example: growing crystals) so that they can get hands-on experience with doing experiments and popular books like "The History of Chemistry", at the end of our lectures. The NCL scientist for this series include: Dr. Sourav Pal, Dr. Ashish Lele, Dr. Sayam Sengupta, Dr. Nandini Devi, Dr. K. Guruswamy, and Dr. Kumar Vanka

Dr. Sayam Sen Gupta (NCL coordinator for this programme) visited Valley View School, Kondhwa on 17th March, after discussions with the Teach for India fellow, Daniel Lobo who is based at this school. The Teach for India team, that had recommended this school to us, and the school principal are very enthusiastic about our initiative, and would also like to encourage their students to submit project entries for the IRIS.

The Valley View school is a private school for the low income community in the area around the school.

A few selected students from this school will also visit NCL in early June since they have very limited exposure to experimental facilities and would like to see cutting-edge laboratories.

Visit to two more schools is planned i.e., Jawahar Navodaya, Shikrapur, and Hutatma Balveer ShirishKumar Vidyalaya, Pune.

Venture CENTER

The Venture Center is a technology business incubator hosted by the NCL that specializes in technology enterprises offering products and services exploiting scientific expertise in the areas of materials, chemicals and biological sciences and engineering.

Venture Center is an initiative of the NCL under CSIR's scheme titled "Scheme for setting up incubation centers in CSIR laboratories". 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).

Venture Center is incorporated as "Entrepreneurship Development Center" under Section 25 of the Companies Act, 1956 (India). During the year, Venture Center added four new members on Board of Directors: Shri H. K. Mittal (Advisor, DST-NSTEDB), Shri A.T.Kusre (Advisor, ICICI Bank), Dr. Rajendra Lagu (Ex-Director, SINE) and Dr. K N Ganesh (Director, IISER-Pune). Venture Center also created a Board of Advisors during the year: Shri Harish Gandhi (Executive Director, Canaan Partners), Dr. Shailendra Vyakarnam (Director, Centre for Entrepreneurial Learning, University of Cambridge), and Shri. R R Abhyankar (Head, RDI & TPDU, Department of Scientific Industrial Research).

Businesses supported

Venture Center provided lab block, hot desk, hot lab, rent-an-address and other facilities to the following start-ups and clients and earned revenue of Rs. 27.13 lakhs.

- Abgenics-to commercialize the therapeutic potential of biotechnologically engineered antibodies for human and animal healthcare solutions.
- ANTfarm - a consumer robotics company.
- Automotive Robotics - a vehicle engineering and prototyping company.
- Biopore Surgicals - a company focused on ocular and maxillo-facial products.
- iTheme - a company offering services ranging from innovation and technology strategies to business and anagement consulting for the chemical industry.
- Revive Enterprises - a company that seeks to recycle electronic waste in India.
- Samir Gijre & Associates - a company that provides consulting, training and software products for chemical process optimization.
- Silicon Machines - a semiconductor technology start-up that develops hardware and software intellectual property for multimedia.

Business creation efforts

- Interns supported by the NCL Research Foundation conducted detailed analysis of scientific competencies at NCL, specifically in polymer sciences to identify a variety of product opportunities and presented these as opportunities for technology commercialization to an audience of about forty five entrepreneurs in Pune. This NCL Technology Showcase resulted in thirteen statements of interest from entrepreneurs, further resulting in one active opportunity for a spin-off, in the area of super-absorbing polymers.
- NCL-RF interns also worked on a detailed market research report on Poly-L-Lactic Acid (PLLA) in response to a request from Dr. Ashish Lele, NCL. This report identified a compelling opportunity for spin-offs in the area of bioabsorbables.
- Venture Center designed its flagship programme - Lab2Mkt - for commercialization of technology from NCL into new ventures (spin-offs). Venture Center discussed with various national and international experts in this domain to refine the model and adapt it to the Indian science and technology environment.

Resources for technology start-ups

- The Venture Center library launched in June 2009 has the collection relevant to technology entrepreneurs, techno-logists and inventors, technology managers and IP professionals. The library today has a collection of 1500+ books and periodicals and has over 140 members.
- Venture Center executed the acquisition, installation and commissioning of instruments/ equipment for the Lab Block.
- A variety of scientific support services were launched for entrepreneurs/start-ups in the material science and biotechnology domains.
- In FY2008-09, the Ministry of Micro, Small & Medium Enterprises (MoMSME) had approved a funding scheme for micro and small enterprises to be operated by Venture Center. As per the scheme, Venture Center identified ten technology entrepreneurs for grant

Venture CENTER

support. All proposals recommended by Venture Center to the MoMSME were approved.

- Venture Centre conceptualized, created and launched an online funding database, featuring over forty government schemes for technology entrepreneurs.

Events, Networks and Visibility

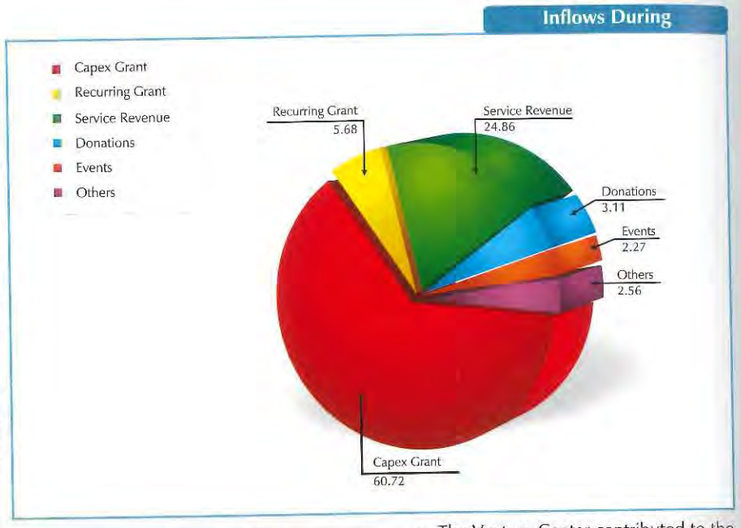
- Venture Center was featured on the national TV Channel ET-NOW in their entrepreneurship-focused programme Starting Up" on Feb 13, 2010.

- Co-hosted with NCL an event on Dec. 10, 2009 where technologies developed and commercialized at University of Toronto by students and other entrepreneurs were presented.

- Co-hosted with NCL in collaboration with Royal Society of Chemistry, UK an event on Nov. 30, 2009 to showcase UK and India best practices in commercializing scientific research, supporting academia-industry links and promoting innovation in the chemical sciences.

- Co-hosted with NCL a one-day event aimed at showcasing the commercial potential of some of the NCL technologies on Nov. 13, 2009.

- An article on "Government Funding for Technology Start-ups" based on Venture Center's funding database was published as cover story in November 2009 edition of DARE magazine.



Fund raising and utilisation

- The Venture Center continues to receive the donations under the following heads 1) NCL Technology and Entrepreneurship Club, 2) NCL Academy for School Children, 3) Venture Center Library and 4) unrestricted donations to Venture Center.

- Venture Center effectively managed a budget of Rs. 99 Lakhs.

- Venture Center also successfully deployed funds carried forward from the previous year; 1) Rs. 116 Lakhs of DST's first installment towards capital equipment and 2) Rs. 8 Lakhs from DST towards the Library project.

Infrastructure development and maintenance

Considerable effort went into development of the lab block, setting-up/installation of equipment/ instruments, developing SOPs and getting the lab block services operational

- The Venture Center contributed to the further development and maintenance of the NCL Innovation Park. The Venture Center worked with other stakeholders of the NCL Innovation Park to develop mechanisms for upkeep of the campus.

- The Venture Center added infrastructure resources (such as the Discussion Room) and operationalized campus facilities like the Cafeteria

Policies and systems

- Venture Center refined the following policies and systems during this fiscal: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 initiated monthly MIS reports and quarterly operational reports, both of which are shared with the board of directors.

- Venture Center refined and supervised contracts for general maintenance in and around the Center. Venture Center also insured the Lab block against fire and burglary and sought coverage for its employees in case of accidents.

Key challenges and risks

The Venture Center management has reviewed key challenges and risks to fully accomplishing its goals. Some important challenges are summarized below:

- Most R&D institutions do not have mechanisms for taking equity in lieu of intellectual property or research services. Past experiences in licensing have made several R&D institutions in India skeptical of deferred revenue models; risk aversion may result in a preference of cash-based technology transfer instead of equity stakes in start-ups and MSMEs. Furthermore, R&D institutions are very slow in executing tech transfer agreements given the lack of experience.

- Initiatives at the CSIR level (such as the CSIR-Tech) pose significant risks to Venture Center in the event that CSIR gives exclusive or wide ranging rights to knowhow/ IP to another entity and thus chooses not to commercialize technology via the Venture Center.

- Venture Center will have minimal managerial staff strength with very little redundancy. It is difficult to find and retain top-level managers for Venture Center who combine skills in science and entrepreneurship with a passion for business incubation and technology commercialization. Unless Venture Center finds creative ways of engagement and remuneration for such people, it runs a serious risk of becoming merely an infrastructural facility.

- Shortage of funding sources for the stages of technology validation, IP expansion and prototyping stages. Government grant funding options for these stages can take considerable time for decisions and release of funds.

- Identifying suitable entrepreneurs for spin-out companies is expected to pose challenges. At this time, the number of NCL scientists willing to start companies is very small. Students at NCL have also not shown significant interest in jumping into entrepreneurship at this stage of their careers.

- The continuing global economic weakness until late 2009 had a negative impact on potential incubatees due to financial constraints, constraints on expansion plans etc. Venture Center has seen a significant decrease in interest from international (esp. from US, UK) start-ups to incubate with us.

- Venture Center does not enjoy certain customs/excise tax and octroi benefits that NCL enjoys. Consequently, the Center's purchasing power has been reduced considerably. Venture Center had not anticipated these costs in its original proposal to the DST. Therefore, the Center expects that it will end up buying lesser equipment that originally projected.

- Uncertainties and delays in infrastructure development and improvements within the NCL Innovation Park pose a large threat to Venture Center - in particular, the unreliable power situation at the Park. The Park does not enjoy the special status enjoyed by NCL in terms of power availability and therefore, the Park has to bear with power cuts similar to other parts of the city. Furthermore, the Park has a legacy sub-station that is a continuous source of uncertainty.

- Venture Center still needs to demonstrate strong revenue streams to sustain operations at healthy levels and retain high-quality managerial staff. Currently, a large part of revenues is from the DST-NSTEDB. Venture Center needs to diversify its revenue sources as well as build a strong stream of revenue from services and sustained donations to thrive. Venture Center also needs to build a sufficiently deep reserve fund to help tide over cash flow problems that are expected as long as Venture Center is dependent on Government grants.

- The Venture Center's service revenues are in large measure dependant on the lab block revenues. Changes in the occupancy rates of the lab block pose a significant risk to service income.

- The Venture Center Library needs a considerable injection of funds to enable it to house resources for market research, technology foresight and patent information research. At this time, Venture Center does not have a commitment from a funding partner for the same. Venture Center also does not have a commitment from a funding partner for continuous replenishment of the Library's collection.

राजभाषा का कार्यान्वयन

राष्ट्रीय रासायनिक प्रयोगशाला में राजभाषा का कार्यान्वयन

राष्ट्रीय रासायनिक प्रयोगशाला वैज्ञानिक एवं औद्योगिक अनुसंधान परिषद (सीएसआईआर), नई दिल्ली के अधीन एक घटक प्रयोगशाला है।

सीएसआईआर विज्ञान एवं प्रौद्योगिकी विभाग, भारत सरकार की एक स्वायत्त इकाई है । अतः अन्य सभी केन्द्रीय सरकारी कार्यालयों के समान ही इस प्रयोगशाला में भी राजभाषा विभाग, भारत सरकार की राजभाषा नीति लागू है । प्रयोगशाला में राजभाषा कार्यान्वयन समिति का गठन किया गया है और इस समिति की बैठकें नियमित रूप से प्रत्येक तिमाही में निदेशक महोदय की अध्यक्षता में आयोजित की जाती हैं । प्रयोगशाला के 90 प्रतिशत से अधिक स्टाफ को हिन्दी का कार्यसाधक ज्ञान प्राप्त है, अतः इसे राजभाषा अधिनियम 10 (4) के अधीन अधिसूचित किया जा चुका है। राजभाषा विभाग, भारत सरकार की राजभाषा नीति के अनुसार प्रयोगशाला में राजभाषा के कार्यान्वयन हेतु सभी स्तरों पर हरसंभव प्रयास किए जा रहे हैं। इस दिशा में राजभाषा विभाग एवं सीएसआईआर मुख्यालय द्वारा समय-समय पर जारी किए गए सभी दिशानिर्देशों का अनुपालन किया जाता है।

प्रयोगशाला में राजभाषा के नियमों का कड़ाई से अनुपालन किया जाता है ।

अतः प्रयोगशाला में दैनंदिन कामकाज में प्रयोग में आनेवाली 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 । इसके अलावा दैनंदिन प्रयोग में आनेवाले द्विभाषी फार्मों एवं मानक मसौदों को कम्प्यूटरों में धीरे-धीरे अपलोड किया जा रहा है ताकि कर्मचारियों को हिन्दी में काम करने में आसानी हो ।

राजभाषा अधिनियम की धारा 3 (3) के अन्तर्गत जारी होने वाले अधिकाँश दस्तावेज अनिवार्य रूप से हिन्दी तथा अँग्रेजी दोनो 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 तिमाही बैठकों में प्रयोगशाला में हिन्दी के प्रगामी प्रयोग की समीक्षा की जाती है और तदनुसार कार्ययोजना बनाकर आगे की कार्रवाई की जाती है ।

प्रयोगशाला के स्टाफ में राजभाषा के प्रति रुचि निर्माण करने हेतु हरसंभव प्रयास किए जाते हैं। प्रयोगशाला के अतिथिगृह एवं स्टाफ मनोरंजन क्लब में हिन्दी समाचार पत्र एवं पत्रिकाएँ तथा पुस्तकें उपलब्ध करायी गई हैं। इसी प्रकार 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 । प्रशासन विभाग के अन्य अनुभागों में भी यथासंभव हिन्दी में कार्य होता है । 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 अँग्रेजी 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 और उन्हें प्रयोगशाला की वेबसाइट पर भी प्रदर्शित किया जाता है । प्रयोगशाला में आयोजित होने वाले सभी समारोहों, व्याख्यानों एवं संगोष्ठियों की रिपोर्टें सीएसआईआर समाचार एवं सीएसआईआर न्यूज में प्रकाशनार्थ क्रमशः हिन्दी और अँग्रेजी 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 हर स्तर पर प्रोत्साहित किया जाता है । प्रयोगशाला में राजभाषा के प्रगामी प्रयोग को बढ़ावा देने 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 भी किया जाता है । वर्तमान वित्तीय वर्ष में वैज्ञानिक, तकनीकी एवं प्रशासनिक स्टाफ के लिए कुल चार हिन्दी कार्यशालाओं का आयोजन किया गया जिनमें प्रतिभागियों को राजभाषा नियमों एवं संवैधानिक प्रावधानों से अवगत कराया गया। इसके अलावा उन्हें अपना दैनंदिन कामकाज हिन्दी में करने एवं कम्प्यूटर पर हिन्दी में कार्य करने का भी प्रशिक्षण दिया गया ।

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 (डॉक्युमेन्टरी फिल्म) का भी निर्माण किया है ।

प्रयोगशाला में राजभाषा सम्बन्धी सांविधिक प्रावधानों का समुचित रूप से अनुपालन करने के लिए प्रयास किए जाते हैं । 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। इस वर्ष सतर्कता बोध सप्ताह एवं शोधछात्रों के वार्षिक सम्मेलन के अवसर पर दो व्याख्यान हिन्दी में आयोजित किए गए थे जिनकी सम्पूर्ण कार्यवाही हिन्दी माध्यम से सम्पादित की गई। सीएसआईआर मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिन्तन लेखमाला आदि प्रोत्साहन योजनाएँ प्रयोगशाला में लागू हैं । इन योजनाओं में प्रयोगशाला के वैज्ञानिक एवं कर्मचारी भाग लेते हैं ।

राष्ट्रीय रासायनिक प्रयोगशाला एक वैज्ञानिक अनुसंधान प्रयोगशाला है । तथापि राजभाषा विभाग, भारत सरकार के निर्देशों को ध्यान में रखते हुए वैज्ञानिक अनुसंधान एवं हिन्दी के प्रयोग के बीच समन्वयन स्थापित करने के प्रयास किए जा रहे हैं । प्रयोगशाला के वैज्ञानिकगण स्टाफ के साथ हिन्दी और स्थानीय भाषा में ही बात करते हैं तथा छुट्टी आदि के आवेदन वे यथासंभव हिन्दी में प्रस्तुत करते हैं । 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 भी प्रस्तुत करते हैं ।

हिन्दी सप्ताह का आयोजन

राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में हिन्दी सप्ताह का आयोजन

राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में दि. 14 सितम्बर, 2009 से 18 सितम्बर, 2009 की अवधि में हिन्दी सप्ताह समारोह का आयोजन किया गया । इस अवधि में स्टाफ के लिए 3 प्रतियोगिताएँ आयोजित की गईं जिनमें वैज्ञानिकों/अधिकारियों/कर्मचारियों ने उत्साहपूर्वक भाग लिया। पहले दिन दि. 14 सितम्बर, 2009 को हिन्दी दिवस के अवसर पर प्रयोगशाला की वार्षिक राजभाषा पत्रिका **एनसीएल आलोक** का लोकार्पण किया गया । इस अवसर पर पत्रिका का विमोचन करते हुए मुख्य अतिथि के रूप में समारोह में उपस्थित प्रसिद्ध लेखक, समीक्षक, संपादक एवं राष्ट्रभाषा हिन्दी के पुरोधा श्री संजय भारद्वाज ने सरकारी कामकाज में राजभाषा हिन्दी के प्रयोग पर बल देते हुए कहा कि हिन्दी के माध्यम से हम अपना काम सरलता और सहजता से कर सकते हैं।

श्री भारद्वाज ने कहा कि हिन्दी का इतिहास बहुत पुराना है और सदियों से हिन्दी हमारे देश में बोली जाती रही है । उन्होंने हिन्दी की व्यापकता को स्पष्ट करते हुए कहा कि केवल हिन्दी ही हम भारतीयों को परस्पर जोड़े रख सकती है और यही हमारी राष्ट्रीयता की पहचान भी है । श्री भारद्वाज ने कर्मचारियों का आह्वान किया कि वे अपना सरकारी कामकाज राजभाषा में सम्पादित करके देश का गौरव बढ़ाएँ ।

अध्यक्ष के रूप में उपस्थित प्रयोगशाला के कार्यवाहक निदेशक डॉ. बी.डी. कुलकर्णी ने इस अवसर पर अपने सम्बोधन में हिन्दी की अपरिहार्यता को स्पष्ट किया और कहा कि हिन्दी अब केवल सरकारी कामकाज की भाषा न रहकर आम आदमी की भाषा बन गई है। उन्होंने आगे कहा कि आज हमारे देश में निजी एवं सरकारी क्षेत्रों में हिन्दी का प्रयोग बड़े पैमाने पर हो रहा है और सम्पर्क भाषा के रूप में हिन्दी का महत्त्व और भी बढ़ गया है ।

डॉ. कुलकर्णी ने स्टाफ के सदस्यों से अनुरोध किया कि वे अपने सरकारी कामकाज में हिन्दी का प्रयोग करके हिन्दी दिवस की सार्थकता को बनाए रखे। दि. 15 सितम्बर को स्टाफ के लिए हिन्दी निबन्ध प्रतियोगिता आयोजित की गई जिसमें प्रयोगशाला के 20 कर्मचारियों ने भाग लिया । दि. 16 सितम्बर को हिन्दी शब्दज्ञान प्रतियोगिता आयोजित की गई । इस प्रतियोगिता में 27 कर्मचारियों ने भाग लिया। दि. 17 सितम्बर को चतुर्थ श्रेणी स्टाफ हेतु हिन्दी शुद्ध लेखन प्रतियोगिता का आयोजन किया गया जिसमें 21 चतुर्थ श्रेणी कर्मचारियों ने भाग लिया। दि. 18 सितम्बर, 2009 को पूर्वाह्न में प्रयोगशाला की राजभाषा कार्यान्वयन समिति की तिमाही बैठक का भी आयोजन किया गया ।

हिन्दी सप्ताह समापन समारोह दि.18 सितम्बर, 2009 को अपराह्न 4.00 बजे प्रयोगशाला में सम्पन्न हुआ जिसकी अध्यक्षता प्रयोगशाला के उप निदेशक डॉ. गणेश पाण्डेय ने की। इस समापन समारोह में पुणे विश्वविद्यालय के हिन्दी विभाग के प्रोफेसर डॉ. तुकाराम पाटील मुख्य अतिथि के रूप में उपस्थित थे ।

डॉ. पाटील ने इस अवसर पर प्रयोगशाला के लगभग 15 कर्मचारियों को विभिन्न प्रतियोगिताओं में प्रथम, द्वितीय और तृतीय स्थान प्राप्त करने के लिए पुरस्कार प्रदान किए । इसके अलावा वर्ष 2008-2009 के दौरान अपना समस्त सरकारी कामकाज हिन्दी में करने हेतु प्रयोगशाला के 5 कर्मचारियों को नकद प्रोत्साहन पुरस्कार भी प्रदान किए गए ।

इस अवसर पर डॉ. पाटील ने कहा कि हिन्दी केवल राजभाषा या राष्ट्रभाषा ही नहीं है बल्कि हिन्दी हम सब की भाषा है । हिन्दी के वैश्विक रूप को स्पष्ट करते हुए उन्होंने कहा कि हिन्दी विश्व में सबसे अधिक लोगों द्वारा बोली जाने वाली भाषा है । केवल भारत में ही नही वरन् विश्व के अधिकांश भागों में हिन्दी का प्रयोग होता है । उन्होंने हिन्दी की सहजता और सरलता के सम्बन्ध में कहा कि अन्य भाषाओं की तुलना में हिन्दी इतनी आसान है कि इसे कोई भी बोल, लिख और पढ़ सकता है ।

डॉ. पाटील ने कर्मचारियों को सम्बोधित करते हुए कहा कि राजभाषा के रूप में हिन्दी को हमने ही कठिन बना लिया है । हमें सीधे एवं सरल शब्दों का प्रयोग करते हुए हिन्दी को प्रयोग में लाना चाहिए । इससे हिन्दी में काम करना आसान होगा। डॉ. पाटील ने आगे कहा कि हमें अपने मन में राष्ट्रीयता का बोध रखते हुए राजभाषा को उचित सम्मान दिलाना होगा ।

समारोह के अध्यक्ष के रूप में बोलते हुए प्रयोगशाला के उप निदेशक डॉ. गणेश पाण्डेय ने कहा कि अब यह एक वास्तविकता बन गई है कि राजभाषा हिन्दी का प्रयोग देश-विदेश में व्यापक स्तर पर हो रहा है । उन्होंने पुरस्कार प्राप्त कर्मचारियों से कहा कि वे आगामी वर्ष में अधिकाधिक हिन्दी में काम करते हुए पुरस्कारों को सार्थक बनाएँ । डॉ. पाण्डेय ने हिन्दी दिवस/सप्ताह के महत्त्व पर प्रकाश डालते हुए कहा कि इससे हम राजभाषा के प्रति अपने संकल्प को दोहराते हैं। यह संकल्प ही हमें हिन्दी में काम करने की प्रेरणा देता है ।

समारोह के आरंभ में डॉ. रमाशंकर व्यास, वरिष्ठ हिन्दी अधिकारी ने मुख्य अतिथि एवं कार्यवाहक निदेशक सहित सभी उपस्थित लोगों का स्वागत किया और हिन्दी सप्ताह की प्रासंगिकता की रूपरेखा प्रस्तुत की। समारोह की कार्यवाही का संचालन करते हुए श्री उमेश गुप्ता, हिन्दी अधिकारी ने अन्त में सभी के प्रति आभार व्यक्त किया ।

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 Disposal Committee	Dr. B.M. Khan

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

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