

**NATIONAL CENTRE FOR CATALYSIS RESEARCH  
INDIAN INSTITUTE OF TECHNOLOGY, MADRAS**

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**A National Centre sponsored and supported by**

**DEPARTMENT OF SCIENCE AND TECHNOLOGY  
GOVERNMENT OF INDIA, NEW DELHI**

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**PROGRESS REPORT  
SUBMITTED TO THE MAC MEETING  
June 22, 2009**

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## INTRODUCTION

The formation of the National Centre for Catalysis Research (NCCR) sponsored by DST, New Delhi was approved by the Board of Governors of IIT Madras, Chennai in July 2006. Since its formation, the members of the Centre have been striving hard to give it an organizational structure within IITM and make it a centre of excellence in the area of catalysis. The purpose of this document is to briefly outline the activities and achievements of the Centre during the period, July, 2008 to June 2009 and to present the same to the Management Advisory Committee (MAC) for its consideration.

It may be recalled that the Second MAC meeting was held on 7<sup>th</sup> July, 2008 under the chairmanship of Prof. M.M. Sharma. The minutes of this meeting and the recommendations of the MAC are enclosed. The action taken on each of the recommendations is presented along with this document. This forms **Part A** of this report.

The Centre has a mandate for contributing to education and development of human resource in the area of catalysis, as its primary function. **Part B** of this document gives a list of the man power at all levels at the Centre. A brief outline of the efforts taken by the Centre and the activities in education and human resource development are given in this part.

A number of experimental facilities have been installed during this period. The facilities created can be grouped as characterization facility, analytical tools and reactors for catalyst screening. A brief outline of the facilities created and the scope of their utility for research are outlined in **Part C** of this document.

The Centre has been active in carrying out sponsored projects for governmental organizations like CSIR, public sector undertakings (PSU) and also for multi-national industrial organizations. The necessary details of these projects are given in **Part D**.

The Centre has also established some international collaboration through government (DST) channels as well as through institutional contacts. The details of these collaborations are given in **Part E**.

The research output of NCCR in terms papers published, patents applied, books written and other tangible achievements are given in **Part F**.

The Centre is maintaining a catalysis data base (an open access system) and also conducting the affairs of the Catalysis Society of India, a national body. A brief report on these activities is given in **Part G**.

The Centre has participated in some other useful activities like the annual day (in August 2008), lectures by Scientists from other countries and also many internal seminars. A few selected ones are given in **Part H**

## NATIONAL CENTRE FOR CATALYSIS RESEARCH

### (A brief outline)

The National Centre for Catalysis Research at the Indian Institute of Technology, Madras is a Department of Science and Technology, Government of India sponsored research centre with the following objectives:

1. To create appropriate human resources in this technological area
2. To carry out research on some frontier areas of energy, materials and theory.

The Centre was established after approval of the Board of Governors of Indian Institute of Technology, Madras in July 2006. The centre will have a unique status of a National Centre within a national institution. The centre in this short period of three years has been growing into an internationally recognized centre for education and research. The centre has been recognized by various multinationals. The centre has won many sponsored projects from famous multinationals like Shell, Procter and Gamble, General Motors and IOC, (including CPCL). Discussions are also on at different stages with others like BASF, W R Grace, Dow Chemicals, Nissan, Tata Chemicals and Sri Ram Chemicals.

The centre conducts various educational programmes. The famous and popular one is the orientation for the research scholars of this country. Nine such programmes have already been conducted. The success of this programme has already been visible since the scientific and research out put of this country in this high technology area has shown considerable improvement in terms of the impact it had in the scientific community. The scholars who have attended this programme have greatly appreciated this programme and have been advocating for this programme among their juniors.

The centre has already been equipped with state of art facilities for research in this area and it is conceived that in the formation period this will evolve into a full fledged international centre for research in this area. The centre is housed in a building consisting of three floors with an area of approximately 40X50 feet in each floor.

International collaboration has already taken shape in bilateral programmes being evolved between NCCR and Hungary, Australia, Korea and Taiwan. More such international cooperation is expected to evolve soon. Discussions are already on with TU-München and TU-Delft.

The centre has attracted young and dynamic researchers and it has a number of post doctoral fellows and 25 research fellows and project assistants are working on various research projects in the centre.

The centre focuses on fundamental aspects of problems and the development of processes is mainly reflecting the needs of this country like adsorptive desulphurization, a process without any down stream processing of crude for obtaining directly diesel.

The centre, it is hoped will evolve as one of the leading Centres in the world in the area of catalysis. It is heartening to note that the work carried out in this centre has already been recognized in various international forums, like the International Congress on Catalysis ( in

the past ICC, there were two oral presentations and one invited presentation from the centre) and are also selected for special highlights in Nature India and other media.

## PART A

### **Minutes of the Second Management Advisory Committee Meeting of the National Centre for Catalysis Research at IIT Madras, Chennai**

The second MAC meeting of the National Centre for Catalysis Research, Indian Institute of Technology Madras was held on July 7, 2008 in the Board room of administrative building of the Institute.

#### **Members present:**

Prof M M Sharma (Chairman)  
Dr T Ramasami, Secretary, DST  
Prof V.G.Idichandy, Director-in-charge  
Dr.R.P.Verma, Member  
Dr R Brakaspathy, Advisor, DST

Dr Paul Ratnasamy, Dr T S R Prasada Rao, Dr S Sivaram, Dr M Subrahmanyam ((nominee of Dr J S Yadav of IICT) and Prof P Mannar Jawahar, VC of Anna University could not attend the meeting. Dr Paul Ratnasamy, however, sent his comments on the report submitted by the centre.

On behalf of the NCCR the following persons attended the meeting:

Prof B.Viswanathan  
Prof A.V.Ramaswamy  
Prof S.Sivasanker  
Prof P Selvam  
Prof R P Viswanath  
Prof T K Varadarajan  
Dr R Ramnarayanan.

Prof V Murugesan represented Anna University at the meeting.

Prof B.Viswanathan made a presentation on the activities of the centre and the facilities created since Feb 26, 2007 when the first MAC meeting was held. He also mentioned that a document outlining the constitution and administration of NCCR in line with that of SAIF had been prepared and submitted to the Dean (Admn.) of IIT M for approval.

Prof Sharma raised several issues during the presentation. Few of the important ones are:

- In the area of energy (which is one of the stated areas of research of the centre) the centre should also work on FT synthesis and syn gas production. He was of the opinion that the centre should generate new insights in this area.
- Prof Sharma also commented on the carbon materials developed by the centre. He said that uniform quality activated carbon was not available indigenously. The centre should be able to bring out a process for the production of high surface area activated carbon.

- He also said that the centre should give emphasis on the application of spectroscopy in catalysis.

The Secretary, DST also raised several points. The essential ones are:

- Capacity building is one of the mandates of the centre and the centre has not made progress in this respect so far. The centre should evolve specific courses and train at least 250 students (both Ph D and Masters) in five years to generate manpower in this important area.
- He also pointed out that no new faculty members have been recruited for the centre and suggested adoption of proactive approach by IIT to recruit faculty. Non appointment of Technical Officers was also pointed out during the discussion.
- Even though the centre has been adequately productive in terms of research publication, conduct of orientation programs, and collaboration with other institutions like Anna University, alliances with industries to be built up so that the centre can function as a self sustaining unit in five years. It is important that NCCR emerge as a nucleus for catalysis research activity in the country, he stressed.

Dr R P Verma, while appreciating the research activities of the centre, suggested carrying out some development work aiming at application in industry. He was of the opinion that 40% of the research activity of the centre should be application oriented.

The Director-in-charge, Prof V G Idichandy, mentioned that some space available at the annexure of the chemistry department has been allotted to the centre and it would be made available to the centre before the end of the year. He also assured that IIT would take expeditious steps in recruiting new faculty members, appointing technical officers, and introducing new courses as suggested by the committee

The following are the committee's recommendations. The committee also took note of Dr Paul Ratnasamy's views while making the recommendations.

### **Recommendations**

- (i) The Committee found the work done by the centre so far was laudable and it expects it to do much more to capture the spirit of NCCR in the years to come.
- (ii) The centre should recruit at least 2-3 new faculty members, and also appoint Technical Officers.
- (iii) The Centre should introduce new courses (such as M Tech in Catalysis) to train manpower in the area. It is suggested that the new courses be launched at the earliest, preferably, in the next academic session.
- (iv) IIT should provide adequate space for the centre.
- (v) The centre should also try to involve other institutions (apart from Anna University) in teaching and research. It should also interact with industry and generate projects so that it can function as a self-sustaining unit in five years time.

After the meeting was over, Prof Sharma met the research scholars and acquainted with the research activities of the centre.

The meeting ended with a vote of thanks to the Chair.

Action taken report on the recommendations and comments of the second MAC meeting. The relevant points are reproduced and the action taken is outlined below each of these points.

Chairman's (Prof M M Sharma) remarks:

Point 1: In the area of energy (which is one of the stated areas of research of the centre) the centre should also work on FT synthesis and syn gas production. He was of the opinion that the centre should generate new insights in this area.

The centre has attempted the following in the area of energy.

- A project proposal on FT has been evolved and it has been defended by presentation before CHT committee and it is learnt it is under consideration by CHT.
- The centre was associated and provided academic input for the development of "on-board hydrogen generation by a chemical route" and this has been directly used as fuel for Maruthi van. This vehicle was demonstrated for public on March, 20 in Hyderabad.
- Other details can be found in the details in the report.

Point 2: Prof Sharma also commented on the carbon materials developed by the centre. He said that uniform quality activated carbon was not available indigenously. The centre should be able to bring out a process for the production of high surface area activated carbon.

The centre has made considerable progress in the development of carbon materials. The Centre has produced three valuable documents in this area which will outline the efforts made in this area. These documents are:

- B. Viswanathan, P. Indra Neel and T. K. Varadarajan , The methods of activation of carbon materials and their specific applications - an e-book at the NCCR website <http://www.nccr.iitm.ac.in>.
- P. Indra Neel, B.Viswanathan and T.K.Varadarajan, The methods of activation of carbon materials and their electrochemical applications, submitted to Catalysis Surveys of Asia. (under consideration)
- P.Indraneel, B.Viswanathan and T.K.Varadarajan, The role of activation agents for the morphology of carbon materials from plant sources submitted to Carbon.

Point 3: Prof Sharma also said that the centre should give emphasis on the application of spectroscopy in catalysis.

As a consequence of this NCCR has produced a book on Surface analytical techniques in Catalysis. This book is now in print by M/s Narosa Publishing House, New Delhi. The orientation course conducted by NCCR has also included specific course content on this topic.

Points raised by the Secretary DST

Point 1: Capacity building is one of the mandates of the centre and the centre has not made progress in this respect so far. The centre should evolve specific courses and train at least 250 students (both Ph D and Masters) in five years to generate manpower in this important area.

NCCR has taken this suggestion with care and evolved a number of channels for capacity building:

- They have evolved an M Tech programme in Catalysis Technology and from the academic year 2009 this course will be offered by NCCR as a part of the programmes of the Chemical Engineering Department of IIT M.
- They have been accommodating many students from various institutions to carry out their project work ( for Ph D and also Masters and Bachelors programme) The details of such activities will be outlined in the report at appropriate places.

Point 2: The centre should also try to involve other institutions (apart from Anna University) in teaching and research. It should also interact with industry and generate projects so that it can function as a self-sustaining unit in five years time.

NCCR has taken this point for intensification of the effort. NCCR has established collaboration with Bharathidasan University, Trichy. NCCR has also signed MOU with the departments of Chemistry and Energy of Tezpur University in Assam and similar MOU is being considered with the University of Pune.

For all other points of the secretary, DST the appropriate action taken will be outlined in the report.

## **PART B**

### **EDUCATION AND CAPACITY BUILDING AT NCCR**

The family of NCCR consists of the following personnel:

#### **Faculty of NCCR**

1. Prof B Viswanathan, Emeritus Professor and Head
2. Dr AV Ramaswamy, Chair Professor
3. Dr S Sivasanker, Chair Professor
4. Prof P Selvam (Department of Chemistry, IITM)
5. Dr R Ramnarayanan (Department of Chemical Engineering, IITM)
6. Dr Raghuram Chetty (Department of Chemical Engineering, IITM)

#### **Associate Faculty**

1. Prof A Chaddha (Department of Biotechnology, IITM)
2. Dr D Chakrabarty (Department of Chemistry, IITM)
3. Prof R Dhamodaran (Department of Chemistry, IITM)
4. Prof. V Murugesan (Department of Chemistry, Anna University)
5. Dr G Ranga Rao (Department of Chemistry, IITM)
6. Prof T K Varadarajan (Department of Chemistry, IITM)
7. Prof M Velan (Department of Chemical Engineering, Anna University)

#### **Post Doctoral Fellows at NCCR**

1. Dr. K Joseph Antony, Shell Fellow
2. Dr. P.P. George, NCCR Fellow
3. DR Thirunavukarasu, NCCR Fellow
4. Dr. S.Navaladian, CCC fellow
5. Dr S.Anuradha, Indo-Australian Project fellow

#### **Ph D Students at NCCR**

1. Mr. P. Indraneel (Columbian Chemicals Scholar)
2. Ms. M. Helen (CSIR-SRF)
3. Ms. S. Chandravadanam (CSIR-SRF)
4. Mr. G. Magesh (CSIR-SRF)
5. Mr.B.Kuppan (IITM Scholar)
6. Mr. N. Vamsi Krishna (IITM Scholar)
7. Mr.Ramanamurthy (NMITLI Project Fellow)
8. Mr.Anil Kumar (NMITLI Project Fellow)
9. Mr. Mahendran (IOC Project Fellow)

#### **Project Assistants at NCCR**

1. Mr. T.M. Sankaranarayanan (CPCL Project Fellow)
2. Ms. M. Banu (CPCL Project Fellow )

3. Ms. R. Sumathi (CPCL Project Fellow )
4. Ms. T. Nithya (IOC Project Fellow)
5. Mr. K. Suthakar (NMITLI Project Fellow)
6. Mr. K. Polli Raju (IOC Project Fellow)
7. Mr. R.Kumaravel (GM Project Fellow)
8. Mr. P.R.Venkatesan (IOC Project Fellow)
9. Ms. A. Kiruba (NMITLI Project Fellow)
10. Mr. C.Bennet ( IOC Scientist)
11. Mr. P. Pachamuthu (Anna University Scholar)
12. Ms. Premlatha (Madras University Scholar)

Drs. Vidya Krishna, Mahalakshmi, Sabiah, and Sangeetha who were PDFs under various schemes have left for other assignments during the year. Research scholars, Ms Janet, Ms Rajeswari, Mr Kishore, Mr Himakumar, Mr Venkateswara Rao who have completed their Ph D during the year have left for PDF positions in USA. Few other project assistants like Mr Jude Vimal Michael and others left for other assignments. .

The following are some of the highlights of our efforts in Education and Capacity building in the area of catalysis:

### **1. The Orientation Program in Catalysis**

This program is the one of the unique educational endeavors of the Centre, conducted every year for the young research scholars of the country. The last such program (9<sup>th</sup> in the series) was conducted in the month of November -December 2008 for three weeks (November 25 to 13 December 2008). There were 40 participants from various institutions like IICT, University of Pune, UICT, CUSAT, Anna University, Defence laboratory at and IITM. This program is well structured and conforms to a syllabus, which is evolved and undergoes changes every year, depending on the trends and future scope of research in the area of catalysis. The fundamentals are stressed. The responses of the participants on the conduct of the course are available with Dr. R. Brakaspathy of DST.

### **2. Participation in Anna University Teaching Program**

The faculty of NCCR has handled two courses in the curriculum of the Department of Chemistry, Anna University during the first semester of 2008 (July - November 2008).

The courses are:

- (i) AC-086 INDUSTRIAL CATALYSIS for M.Sc. (Applied Chemistry) students (Prof S Sivasanker of NCCR)
- (ii) CY-073 CONCEPTS AND TECHNIQUES IN CATALSYIS for M Phil students.(part only - conducted by B Viswanathan)

These two courses were conducted by NCCR staff as per the syllabus and the time table provided by the Department of Chemistry, Anna University. Internal tests and final examinations were also conducted by faculty of NCCR. It may be mentioned that Part of the course for the M.Phil students of Anna University was conducted at NCCR.

Prof B Viswanathan conducted the course for the M Sc specialization in Catalysis at Tezpur University.

### **3. National Level Tutorial on Electron Spectroscopic Techniques in Catalysis**

NCCR took the initiative of conducting a two-day (16-17 January 2009) Tutorial on Electron Spectroscopic Methods in Catalysis (XPS, UPS, AES, EXAFS, XRF and other techniques for the research scholars from different organizations at the National Chemical Laboratory, Pune, prior to the National symposium on Catalysis (18-21 January 2009). Considering the importance of Electron spectroscopic techniques (Chairman himself has stressed this in his observations in the last year (2008) MAC meeting) in catalysis, the origin, theory and practice of this technique were illustrated with examples, problems and solutions. A practical demonstration and also details on the interpretation of the spectra obtained were also included. The course was conducted by Prof P Selvam and Prof B Viswanathan in coordination with Dr C S Gopinath of NCL.

### **4. Annual Children's Club programme**

NCCR also conducted this year's Children's Club summer programme on Pollution Control Strategies - A Chemists Perspective for two weeks. This course material is now available as e-book in the NCCR website.

### **5. Special Training Programme**

In addition, the faculty of the centre has participated in various educational and refresher programmes conducted by other institutions like Anna University (International School on Nano Materials, Tezpur University (Green Chemistry Summer School), Kalasalingam University, Krishnankovil, and many other schools and some of the details of these are available in the section on presentations.

Special training in catalysis was offered to number students of sister organizations like Christian college, Chennai, Loyola College and University of Madras. Prof S Sivasanker supervised four summer research fellows (two students and two lectures) sponsored by the Indian Academy of Sciences Bangalore for about 2 months. Prof Selvam supervised a summer fellow (under DST INPIRW scheme) from NISER, Bhubaneswar (Mr. Jayanth K Ajay). Also the following persons have been trained for their summer programme at NCCR.

1. Mr Abhishek Shiv Kumar MIT, Manipal
2. Mr Raghul Raghavan, NIT, Trichirapalli
3. Mr K T Vikesh, Thiagarajar college, Madurai
4. Mr.R.Shanmugam, Thiagarajar College, Madurai
5. S Esskiammal, Thiagarajar College, Madurai.

### **6. Ph D thesis work**

The centre has turned out 7 Ph D students in this year and has enlisted few new students for the Ph D programme. The centre has also initiated joint Ph.D students with Bharathidasan University, Tiruchirappalli in the new scheme. We have jointly registered

five students for Ph D programme with Anna University. Efforts are on for joint registration with University of Pune and Tezpur.

The titles of the Ph D theses that have been completed this year are:

1. Dr Ch Venkatewara Rao – On the search for efficient catalysts for oxygen reduction reaction.
2. Dr L Himakumar – On some challenging avenues in hydrogen storage.
3. Dr S Navaladian – Strategies for the synthesis of nano materials and their applications.
4. Dr J M Janet – Synthesis and characterization of materials for ammonia formation at atmospheric pressure.
5. Dr Satyananda Kishore – Catalytic and electrochemical exploitation of poly oxo metallates
6. Dr J Rajeswari – One dimensional nanoarchitected compounds of Mo/W for electrochemical applications
7. Ms M Helen – Development of hybrid membranes for application in Direct Methanol Fuel cells (DMFC)

The list of Ph D students jointly registered with other universities is as follows:

1. Ms Banu - Transformation of naturally occurring polyhydric alcohols into value added chemicals ( Bharathidasan University).
2. Mr Sankaranarayanan - Solid catalysts based on mixed metal oxides for biodiesel (Anna University).
3. Ms.Sumathilakshmi - Hydronitrogenation of model compounds over Ni-Mo supported on mesoporous composites (Anna University).
4. Mr Suthagar - Conversion of Glycerol to value added chemicals (Anna University).
5. Ms Nithya - The role of texture of supports on the catalytic activity (Anna University).

## **PART C**

### **FACILITIES CREATED AT NCCR**

The following facilities have been added at NCCR during the last one year. All the instruments have been installed tested and are being used.

- XRF facility
- Perkin Elmer GC
- UV Sources
- Thin film (dip) coating unit
- RDE facility
- Parr Auto claves ( Three numbers)
- A few other units are under process like GC-MS, NO<sub>x</sub>, CO and other detectors.

In addition, the following facilities created in the past are all in good working conditions and are being used for servicing a number of sister organizations.

#### **Structural and textural characterization**

- X-ray diffractometer (Rigaku)
- Surface area and pore volume distribution (Micromeritics ASAP 2030)
- Temperature-programmed technique TPR, TPD, etc., (Micromeritics)
- Thermal analytical instrument (TG/DTA) (Perkin Elmer)

#### **Spectral Characterization of solids**

- Spectrofluorometer (Perkin Elmer)
- FT-IR spectrometer (Bruker)
- UV-Vis spectrometer (Thermo Electron)
- All with attachments for in-situ studies at different temperatures and atmospheres.

#### **Catalyst screening and testing**

- High pressure Batch reactors (Parr Autoclaves: 100 and 300 ml)
- High pressure down flow reactor (Xytel: 100 ml reactor volume)
- Atmospheric/low pressure down flow reactors (Hi-Tech)
- High pressure micro reactor (Hi-Tech)

#### **Analytical facilities**

- 3 Gas chromatographs, including on-line analysis of reactor effluents
- Simulated distillation GC

### **Surface Analytical technique**

- X-ray photoelectron spectrometer (Omicron)
- With UVPS and Auger spectroscopy

### **Supporting equipment**

- Two oil free compressors (reciprocating and scroll type) along with refrigerated drying units
- One lab-scale extruder (manual) has been installed for preparing catalyst extrudates.

These facilities are now being routinely used by students for their research and maintained by the existing staff and students. These are also extended to other organizations (Anna University, Loyola college, Presidency college, other educational institutions in the south, CPCL, CLRI and many other institutions).

For the up-keep and maintenance of these instruments/facilities, the center will require the services of technical staff (technical assistant, technical officer) in future. Necessary steps will be taken to recruit such personnel for the centre.

## PART D

### 1. Some Highlights of Basic Research at NCCR

The basic research component of NCCR has various facets. The can be listed as follows:

1. Preparation of various kinds of meso-porous materials including carbon materials both synthetic and natural sources.
2. Exploitation of the synthetic strategies for preparation of new generation nano state materials for possible catalyst applications.
3. Examining the cluster compounds especially poly oxometallates for a variety of organic transformations.
4. Evolving suitable catalyst systems for specific reactions like conversion of glycerol to value added products like 1,2 or 1,3 propandiol or acrolin or esters.
5. Evolving strategies to increase the surface area of carbon with specific application in mind.
6. Fuel cell electro catalysts and membranes are the other areas of research in which the group is contributing considerably.

### 2. Industrial sponsored projects at NCCR

Eight sponsored projects are being carried out in NCCR at present. Out of these, seven have been sponsored by industries. These are briefly described below.

#### (i) Chennai Petroleum Corporation Limited

There are two on-going projects sponsored by Ms.CPCL, Chennai. Details of these projects have been given in our previous report. In short, these projects are:

- (a) Adsorptive Desulphurization: The aim of the project is to remove sulfur in the SR diesel fraction of Narimanam crude by an adsorptive desulfurization process for which suitable adsorbents have been developed, screened and selected. The process at the laboratory level has been demonstrated and the scale up studies is being pursued at CPCL R and D centre with the participation of NCCR. It is also proposed to convert the removed sulphur compounds into useful products. The process developed by NCCR has also been reproduced by and their results
- (b) End Point Reduction: The objective of this project is to bring down the T95 distillation point of straight run heavy diesel (T95 ~ 380°C) to less than 360°C without substantial yield loss. A number of catalysts have been screened and the most suitable catalyst has been selected and evaluated in detail.

#### (ii) Indian Oil Corporation :

IOC, R and D centre at Faridabad has sponsored two projects:

- (a) Development of alumina of certain specifications for the use of IOC in their catalyst formulations; (and this project has reached the stage, where the methodology for the

preparation of alumina with the specified characteristics has been successfully developed)

- (b) Basic understanding of the hydrotreating catalyst systems
- (c) IOC also has this year granted three fellowships for Ph D programme on topics of interest to them.

**(iii) Procter and Gamble**

This project involves development of specific catalysts for the conversion of long chain hydrocarbons into alcohols. The appropriate catalyst system has been identified and optimization studies are being carried out.

**(iv) Shell International Pvt. Ltd.,**

The project involves development of high throughput catalyst systems on stainless steel grids. On successful completion of this project, Shell International Private Limited has been considering another sponsored project on developing a specific catalyst system for high through put catalyst for their process

**(v) CSIR NMITLI Project**

Conversion of glycerol into 1,2 or 1,3 propanediol and acrolein (jointly with NCL, UICT and IICT)

**(vi) General Motors India Limited**

The project envisages the understanding of the kinetics of de -NOX reaction under SCR conditions.

**(vii) Tata Chemicals Limited –**

Tata chemicals have sponsored a project for the production of hydrogen through Photo-electrochemical route.

**3. Centre for High Technology:**

Presented a proposal on “**Monolith-based Fischer-Tropsch Catalysts**” to the Scientific Advisory committee of the Ministry of Petroleum (Centre for High technology, New Delhi) requesting a funding of Rs. 2.27 crores. Project is believed to be under consideration.

**4. Academic Research**

The Centre is involved in various types of academic research in fundamental areas. Only the main topics of research are listed here.

**(i) Preparation of mesoporous carbon:**

The mesoporous carbon have been synthesized or prepared in a variety of ways for applications like carbon supported electrodes for fuel cells and also as support for thermal catalytic reactions.

**(ii) Preparation of meso porous solids**

A variety of mesoporous solids are prepared in a variety of synthetic procedures. One of the works involves the preparation of aluminum containing SBA materials by pH adjusting method. These materials will be examined for a variety of organic transformations.

**(iii) Glycerol conversion to value chemicals**

This project has a broader scope than what has been carried out under NMITLI project. The selectivity optimization has been aimed at various products like propane diol, ethers with isopropyl alcohols and 5 or 6 ring compound formation. The catalytic systems that have been examined include, supported silver nano particles, substituted zeolites, and heteropoly compounds. These studies will give rise to some disclosure possibilities soon.

**(iv) Development of hybrid membranes**

New generation hybrid membranes have been developed which showed considerably lesser methanol cross over which is a major challenge encountered with Nafion membrane in direct methanol fuel cell application. These studies have given rise to some patents that have been filed.

**(vi) Electrode materials for Oxygen Reduction Reaction**

In addition to the conventional supported Pt and Pt alloy electrodes various chalcogenide based materials and Fe phthalocyanine and cobalt tetramethoxyphenylporphyrin complexes have been examined for this reaction.

**(vii) Hydrogen storage by alanates**

The exploitation of alanates for hydrogen storage is restricted due to slow kinetics. The work carried out examines the possibility of developing catalysts that can promote fast reaction kinetics in both ways for hydrogen sorption and desorption.

**(viii) Heteropoly acid based energy conversion devices**

A variety of systems have been examined for possible application in super capacitor applications and also as electrodes for a variety of energy conversion applications including as electrodes for direct methanol fuel cells.

**(ix) Nano Materials for fuel cell and water electrolysis**

Development of fuel cell electrodes and water electrolysis is still an area of interest. Variety one dimensional nano rods based on tungsten oxide or sulphide

or molybdenum sulphide electrodes (prepared in a simple cost effective manner) have been examined for these applications.

**(x) Metallic nano materials**

A variety of new methods including thermal decomposition and ultrasonics have been employed to prepare a variety of metallic nano particles and their behaviour has been examined.

**(xi) Examining basic catalysts**

Magnesium oxide based catalysts have been examined for a variety of reactions and also the possibility of atmospheric pressure synthesis of ammonia is being attempted.

In essence the centre has been working on a variety of studies in evolving fundamental understanding on catalytic processes.

## PART E

### INTERNATIONAL COLLABORATION

#### 1. Indo- Hungarian Program

This program deals with the application of nanoscience and nanotechnology in bi-metallic catalysts systems and is funded by DST, New Delhi. This two year program commenced in October 2007. Under this bilateral cooperation, Prof. Laszlo Guzzi and Dr. Zoltan Schay of the Department of Surface Chemistry and Catalysis, Institute of Isotopes, Budapest visited NCCR during 12-22 February 2008 to discuss the project details. They gave lectures at NCCR and also participated in the National Workshop on Catalysis held at IMMT, Bhubaneswar, where they delivered lectures on surface science.

Subsequently, with our XPS facility in place, Dr. Zoltan Paszti, who has expertise in surface analytical technique visited NCCR and spent two weeks in April 2008 working and training students on this technique.

One of our research fellows, Mr. G. Magesh has spent three months carrying out research at the Department of Surface Science and Catalysis, Budapest under the supervision of Prof. L. Guzzi.

In this year, Prof A V Ramaswamy and Prof B Viswanathan visited the Department of Surface Chemistry and Catalysis, Institute of Isotopes, Budapest and finalized their work on supported gold catalysts and a publication is being finalized.

Mr B Kuppan of the centre will visit Department of Surface Chemistry and Catalysis, Institute of Isotopes, Budapest for a period of five months and will carry out the research studies to be completed in this project.

#### 2. Indo-Australian Program

This program has just been approved by DST, New Delhi

The collaborative research involves strategies for conversion of bio-sources into valued chemicals.

The Australian team (Dr Jorge Beltramini and Dr Akshat Tanksale; ARC Centre for Functional Nanomaterials, The University of Queensland, Brisbane) visited NCCR and held discussions and the project is taking shape for production for platform chemicals from carbohydrates.

Prof Selvam and Prof Viswanathan shall be visiting the ARC Centre for Functional Nanomaterials, The University of Queensland, Brisbane during July 2009 to finalize experimental details of the project.

### **3. Indo-Taiwan Project**

A project for the development electrodes and hydrogen storage material has been approved and the development of materials already has been completed and evaluation is going on.

4. A MOU has been signed between NCCR and the New Chemistry Research Division, Korea Research Institute of Chemical Technology, for joint collaboration and exchange of research students.
5. Catalysis Research Centre, Technical University, Munich and NCCR has signed an MOU for mutual cooperation and also for joint research projects
6. A Confidentiality Agreement between Nissan Motor Company and NCCR has been entered for work on dry reforming and other aspects.
7. A MOU has been signed between International Centre for Materials, Nanoarchitectures, National Institute of Materials Science (NIMS), Japan for mutual cooperation and collaboration.
8. Efforts are being made to have MOU with Prof Sung Hwa Jhung, Department of Chemistry, Kyungpook National University, Daegu 702-701, Korea.

## PART F

### RESEARCH OUTPUT OF THE CENTRE FOR 2008-2009

The output of the centre for the period July 2008 - till day in terms of publications, books and patents are given in this part.

#### Research Publications

1. V. Krishna, V. S. Kamble, N. M. Gupta, and **P. Selvam** "Uranyl-Anchored MCM-41 as a Highly Efficient Photocatalyst in the Oxidative Destruction of Short Chain Linear Alkanes: An in situ FTIR Study", *J. Phys. Chem. C* **112** (2008) 15832
2. **P. Selvam** and S. Rajasekar "Synthesis, characterization and catalytic properties of Microporous cobalt aluminosilicate (CoLTL) molecular sieves, *Eurasian ChemTech Journal* **10** (2008).
3. **P. Selvam**, K. Vidya, A. Layek, "Synthesis of vanadium oxide nanoclusters in confined environment via a template-exchange method", *Stud. Surf. Sci. Catal.* **165** (2008) 179-186.
4. S. K. Badamali and P. Selvam, "Probing the Fe(III) sites in Mesoporous FeMCM-41", *Catal. Today* **141** (2009) 103.
5. M. Pandey, S.K. Ray, and P. Selvam, "The bonding configuration in a partially relaxed pseudomorphic epilayer of sige: evidence of the bc-8 phase of silicon", *J. Phys.: Condens. Matter*, **20** (2008) xxx.
6. N. Bhatt, P. Sharma, A. Pattel, and P. Selvam "Supported 12-tungstophosphoric acid: An efficient and selective solid acid catalyst for tert-butylation of phenol and cresols", *Catal. Commun.* **9** (2008) 1545.
7. P.Sangeetha, K.Shanthi, K.S. RamaRao, B.Viswanathan and P.Selvam, "Hydrogenation of nitrobenzene over palladium-supported catalysts -Effect of support", *Applied Catalysis A*, **353** (2009) 160-165.
8. K. Joseph Antony Raj, A.V. Ramaswamy and B. Viswanathan, Surface area, pore size and particle size engineering of titania with seeding technique and phosphate modification. *J.Phys.Chem.C* (Under revision).
9. K. Joseph Antony Raj, and B. Viswanathan, Single-step synthesis and structural study of phosphate modified titania through seeding method. *Materials Physics and Chemistry (Communicated)*.
10. K. Joseph Antony Raj, and B. Viswanathan, Effect of surface area, pore volume and particle size of P25 titania on the transformation of anatase to rutile. *Indian Journal of Chemistry Sec A, (Communicated)*
11. Veda Ramaswamy, Pallavi Shah, Karoly Lazar and A.V. Ramaswamy, Synthesis, Characterization and Catalytic activity of Sn-SBA-15 Mesoporous Molecular sieves, *Catal. Surv. Asia*, **12** (2008) 283.
12. B. Murugan and A.V. Ramaswamy, Chemical States and Redox Properties of Mn/CeO<sub>2</sub>-TiO<sub>2</sub> Nanocomposites prepared by Solution Combustion route, *J.Phys.Chem.C*, **112**, 2221-2224 (2008).
13. B. Viswanathan, and A V Ramaswamy, Selection of solid heterogeneous catalysts for transesterification reaction, *Chemistry Industry Digest* Pp 91-99 August 2008.
14. B.Viswanathan, Challenges in the development of Fuel cells Photo/ electrochemistry and photobiology for Energy fuel and environment, *Research Signpost*, 2008 to appear.

15. Ch. Subrahmanyam, S. Shanmugam, B. Viswanathan and T.K. Varadarajan Synthesis and Characterization of Thermally Stable Mesoporous Titania, Eurasian ChemTech Journal Volume 10 No 2 10(2008)1-31.
16. V.Chidambaram and B.Viswanathan "Single step liquid phase synthesis of methyl isobutyl ketone (MIBK) from acetone, Eurasian Chemico-Technological Journal Volume 10 No2 2008 to appear.
17. R.Mahalskshmy, P.Indraneel and B.Viswanathan "Functionality of carbon surfaces in Indian Journal of Chemistry section A 48A,352-356 (2009).
18. R. Ulaganathan, R. Mahalakshmy and B. Viswanathan "Identification of Active Phase of Sn-Sb-Mixed Oxide Partial Oxidation System A Combined MM/DFT Study, Bulletin of the Catalysis Society of India, 7, 50-55 (2008).
19. S.Sabiah and B. Viswanathan "Mo-aminoacid Complexes as Analogs for Mo based Enzymes: A DFT Approach, Indian Journal of Chemistry section A submitted (2009).
20. V.Venkatasubramanian, M Sankaran B. Viswanathan and V R Subramanian, Tungsten carbide as possible support for Pt in electrochemical Reactions, Bulletin of the Catalysis Society of India submitted 7,146-152(2008).
21. B. Viswanathan, and M Sankaran, "Hetero-atoms as activation centers for hydrogen absorption in carbon nanotubes, Diamond and Related Materials, 18, 429-432 (2009).
22. S.Arunachalam and B. Viswanathan, "South-South cooperation: The case of indo-Chinese collaboration in scientific research, Current Science, 95,311 (2008).
23. S.Arunachalam and B. Viswanathan "A historiographic analysis of fuel-cell research in Asia – China racing ahead, Current Science, 95, (2008) 36-49.
24. Anil Kumar, M P Maiya, S Srinivamurthy, and B.Viswanathan, Structural hydrogen storage and thermodynamic properties of some misch metal nickel alloys with partial substitutions for nickel in Journal of alloys and compounds 476, 92-97 (2009).
25. R.. Jothiramalingam, Wang and B.Viswanathan Heterogeneous catalysts for Transesterification reaction, Photo/electrochemistry and photobiology for Energy fuel and environment, Research Signpost, 2008 to appear.
26. P.S.Kishore, B.Viswanathan, and T K Varadarajan "Synthesis and characterization of metal nanoparticle embedded conducting polymer polyoxometalate composites, Nanoscale Res.Lett., 3, 14, 2008.
27. P.S.Kishore, B.Viswanathan and T. K.Varadarajan, "Electrochemical oxygen reduction reaction by Pt nanoparticles supported on carbon support stabilized by polyoxometalates, J Nanosci.Nanotech (In press).
28. P.S.Kishore, B.Viswanathan and T.K.Varadarajan, "Silicotungstic acid based carbon supported noble metal electrodes for energy conversion and storage applications, J.Phys.Chem (Accepted).
29. S.Shanmugam, B.Viswanathan and T.K.Varadarajan, " The preparation of metal oxygen molecular cluster embedded in organic inorganic nanocomposite and its rectifying behaviour, Materials chemistry and Physics, 112(2008) 863-868.
30. S. Navaladian, B. Viswanathan, T. K. Varadarajan and R.P. Viswanath, "A rapid synthesis of oriented palladium nanoparticles by UV irradiation Nanoscale Research Letters, Published online: 4 December 2008.
31. G.Vasu, A. Tangirala B. Viswanathan, K.S.Dhathatreyan, Continuous bubble humidification and control of relative humidity of H<sub>2</sub> for a PEMFC system International Journal of Hydrogen Energy, Volume 33, Issue 17, September 2008, Pages 4640-4648.
32. Ch.Subramanian, S.Shanmugam, B. Viswanathan, and T K Varadarajan, " Synthesis and Characterization of thermally stable mesoporous titania, Eurasian chem Tech Journal 10(2008)1-31.

33. J Rajeswari, P S Kishore, B. Viswanathan, and T K Varadarajan, One dimensional MoO<sub>2</sub> nanorods for supercapacitor applications “ Electrochemical communications (in press).
34. G Magesh, B. Viswanathan, R.P.Viswanath and T K Varadarajan, Photo catalytic behavior of CeO<sub>2</sub>-TiO<sub>2</sub> system for the degradation of methylene blue, Indian Journal of chemistry section A 48A, 480-488 (2009).
35. S. Navaladian, B. Viswanathan, T. K. Varadarajan and R.P. Viswanath, Microwave-assisted rapid synthesis of anisotropic Ag nanoparticles by solid state transformation, Nanotechnology, 19, 45603-45610 (2008).
36. L.Himakumar, B.Viswanathan and S.Srinivasa Murthy, Hydrogen storage by Mg<sub>2</sub>Ni prepared by polyol reduction, Journal of alloys and compounds, 461, 72-76 (2008).
37. S. Navaladian, B.Viswanathan, T.K. Varadarajan and R.P. Viswanath, "Fabrication of worm-like nanorods and ultrafine nanospheres of silver via solid state photochemical decomposition", Nanoscale Research Letters, 4 (2009) 471-479 .
38. M. Mapa, K. S. Thushara, B. Saha, P. Chakraborty, C.M. Janet, R. P. Viswanath, C. M. Nair, K. V. G. K. Murty and C. S. Gopinath, "Electronic Structure and Catalytic Study of Solid Solution of GaN in ZnO", Chemistry of Materials,(2009) ASAP article (available online).

#### **Papers communicated or under preparation.**

1. P.S.Kishore, B.Viswanathan and T.K.Varadarajan, “ Preparation of tungsten carbide from conducting polymer polyoxometalate composite and its selective role as supports for Pt nanoparticles in fuel cell applications ( in preparation).
1. P.S.Kishore, B.Viswanathan and T.K.Varadarajan, “Exploitation of Pt/WC for the facile hydrogen evolution reaction (in preparation.)
3. J Rajeswari, P S Kishore, B. Viswanathan, and T K Varadarajan, One dimensional MoS<sub>2</sub> nanorods for HER, Nanotechnology (communicated).
4. K. Joseph Antony Raj, and B. Viswanathan, Single-step synthesis and structural study of mesoporous sulphated titania nanopowder by controlled hydrolysis process. (*Manuscript under preparation*)
5. K. Joseph Antony Raj, and B. Viswanathan, Alkali titanates as an effective catalyst for combustion of diesel soot. (*Manuscript under preparation*)
6. , The methods of activation of carbon materials and their electrochemical applications, Submitted to Catalysis Surveys of Asia. (under consideration)
7. P.Indraneel, B.Viswanathan and T.K.Varadarajan, The role of activation agents for the morphology of carbon materials from plant sources submitted to Carbon

#### **1. Papers Presented**

1. P. Selvam, B. Viswanathan, and B. Kuppan, “Nanoporous Carbon Supported Platinum (Pt/NCCR-1) Electrocatalyst for Methanol Oxidation” XXI ENCONTRO NACIONAL SPQ, Porto, June 11-13, 2008.
2. B. Kuppan, B. Viswanathan, and P. Selvam, “Mesoporous Carbon Nitride Supported Platinum (Pt/MCN-1) Electrocatalyst for Methanol Oxidation” CATSYMP-19, Pune, January 18-21, 2009.

3. P. Selvam, B. Viswanathan and B. Kuppan, "Platinum supported Nanoporous Carbon / Nitrogen containing Carbon Molecular Sieves: Promising Electrocatalysts for Methanol Fuel Cell Application", ICMAT-2009, Singapore, June 28-July 3, 2009.
4. P. Selvam, "Uranyl-incorporated MCM-41: an efficient photocatalyst for the oxidation of volatile organic compounds" CATSYMP-19, Pune, January 18-21, 2009.
5. V. Kirishna, P. Selvam, and B. Viswanthan, "Chromium containing SBA-15: potential photocatalyst for the reduction of nitric oxide" CATSYMP-19, Pune, January 18-21, 2009.
6. S. Khaire and S. Sivasanker, "Phosphotungstic acid supported on SBA-15: catalyst for synthesis of fine chemicals", *14<sup>th</sup> International Congress on Catalysis, Seoul, Korea, July 13-18, 2008 (oral paper)*
7. T.M. Sankaranarayanan, M. Banu, R. Sumathi, J. Masih, G.Valavarasu<sup>b</sup>, A. Meenakshisundaram, B. Sairam and S. Sivasanker, "End point reduction of a straight run diesel fraction using zeolite catalysts", *19<sup>th</sup> National Symposium on Catalysis, Pune, Jan. 18-21, 2009 (oral paper)*.
8. P.S.Kishore, B.Viswanathan and T.K.Varadarajan, Silicotungstic Acid (STA) based carbon supported noble metal electrodes for energy conversion and storage applications, *14<sup>th</sup> International Congress on Catalysis, Seoul, Korea, July 13-18, 2008 (oral paper)*
9. B.Viswanathan, Some challenging avenues in the development of fuel cells, Hungarian Academy of Sciences on 5<sup>th</sup> November 2008 at CRC Budapest.
10. A.V.Ramaswamy, Chemical states and redox properties of Mn/CeO<sub>2</sub> – TiO<sub>2</sub> nano composites, Lecture at the Institute of Isotopes, Budapest, Hungary, 4<sup>th</sup> November 2008.
11. S.Sivasanker, "Zeolites – an overview, General Motors Research centre, Bangalore, 9<sup>th</sup> Sept 2008.
12. S.Sivasanker, "Nano-structures in heterogeneous catalysis" Workshop on Nanotechnology, SSN College, Chennai 20<sup>th</sup> March, 2009 (Chief guest lecture).
13. K. Joseph Antony Raj, A.V. Ramaswamy and B. Viswanathan, Synthesis and characterization of organic-free, phosphate-modified anatase titania with high surface area, CATSYMP-19, Pune, January 18-21, 2009.
14. B.Viswanathan, Photo electrochemical production of hydrogen a dream or reality, Dr K Swaminathan Endowment Lecture at Loyola College on December 10, 2008.
15. B.Viswanathan, Hydrogenstorage – Current Status, Energy Department, Tezpur University, 19<sup>th</sup> September 2008.
16. B.Viswanathan, Metal oxygen cluster compounds and their use in electrochemical devices, Presented in the International school on Nano Materials, Anna University, Feb 2009.

17. B.Viswanathan, Fuel cells and Spectro electrochemistry lectures at the department of chemical sciences, Tezpur university, September 2008.
18. B.Viswanathan, Chemical analysis by Photo electron spectroscopy, National student's symposium Horizon 08 NIT Trichi, 4th Oct 08.
19. B.Viswanathan, Photo-electrochemical methods - current status, Catalysis in Environmental Applications in ICT Hyderabad, 28th July 2008.
20. M Helen, B.Viswanathan and S.Srinivasa Murthy, Nanocomposite Membranes for DMFC Applications, Conference on Functional materials, IITM, November, 27-29 2008 ( best poster award).
21. B.Viswanathan, Techniques in Chemistry, at Stella Maris College on October 28, 2008.
22. P. Selvam, Synthesis of Novel Nanoporous Carbon: NCCR-1, 9<sup>th</sup> Int. Conf. on Nanostructured Materials (NANO-2008), Rio de Janeiro, June, 1-6, 2008, pp.370.
23. P.Selvam, Nanoporous Carbon Supported Platinum (Pt/NCCR-1): Electrocatalyst for Methanol Oxidation, XXI National Meeting of the Portuguese Chemical Society, Porto, June 11-13, 2008.
24. B.Viswanathan, delivered a total of 9 lectures in the summer school on Green chemistry at the Department of Chemical Sciences, Tezpur University during June4-9, (2009).
25. S.Chandravathanam, 'Enhanced utilization of Pt/C catalyst for methanol electrooxidation' in a National Seminar on 'Recent Trends in Chemistry, RTC-3' conducted at Jayaraj Annapackiam College for Women, Periakulam, 26-27 Feb., 2009.

#### **Book Chapters:**

1. S.Sivasanker, Catalysis – selected applications, Narosa Publishing house, (2009)  
Chapter 2 and chapter 3,  
(a) The Role of Catalysis in sustainable development  
(b) Acids and bases

#### **Books published by faculty of NCCR**

1. B.Viswanathan, (Editor) Catalysis some selected Applications (Narosa publishing House and in Production) (2008).
2. B.Viswanathan, (Editor) Surface characterization techniques (Submitted to Narosa Publishing house and in preparation (2008).
3. B.Viswanathan,(Editor) Nano materials (Narosa Publishing House)(2008)
4. . D.K.Chakrabarty and B.Viswanathan, Heterogeneous catalysis, International edition New Age Science Limited Kent TN1 1YS UK November 2008.

#### **e-books ((at the site <http://www.nccr.iitm.ac.in>)**

1. **Methods of activation and specific applications of carbon materials.**
2. **Pollution control – A chemists Perspective**

## **PATENTS-2008**

1. R P Viswanath and B.Viswanathan, water purification system (filed)
2. B.Viswanathan and M Helen, Membranes based on Heteropoly acid embedded polymer matrix
3. P. .Selvam, B. Viswantahan, and K. Suthagar, “Selective formation of 1,3 propane diol from glycerol” Submitted to our Dean IC and SR (To be filled).

## PART G

### THE CATALYSIS SOCIETY ACTIVITIES

The centre's contribution to the national body namely the Catalysis Society of India is outlined in this section.

1. The Catalysis society of India brings out a quarterly bulletin. For the year 2008 this bulletin had four issues with a total of 176 pages. **The Bulletin of the catalysis Society of India is fully available in electronic form.**
2. In addition, the catalysis Society conducted its National symposium in NCL, Pune.
3. B. Viswanathan is one of the editors for a special issue of Catalysis Today.
4. In January 2009, the catalysis society conducted a tutorial on electron spectroscopy techniques in catalysis during the national symposium on catalysis, This has been mentioned already in this report.
4. On behalf of the Catalysis society of India on open access Catalysis Data base has been continued to be maintained by NCCR. In this year, the data base has over **1300 full length** articles uploaded. More than 30 Ph D theses have also been uploaded. **The server was maintained without any down time during this year.**
5. B.Viswanathan has been elected as the president of the Catalysis Society of India for the term 2009-2010.
- 6.



## PART H

### Other Activities

(Only a few activities are only listed)

Date	Activity
January 16 and 17	Pre-school on Electron Spectroscopy conducted by P.Selvam and B.Viswanathan with others at NCL.
January 18-21	19th National Symposium on Catalysis
January 31	IOC hydrogen initiative meeting
Feb 5 to 8	Visit of Prof N Roesch and also signing of MOU for cooperation with CRC of the Technical University Munchen Prof N Rosch of CRC Technical university , Munich gave a seminar on  Hydrogen Activation by Transition Metal Species in Zeolites: A Density Functional Study
Feb 17	Prof.Ogura visited the centre and gave a seminar on 'Synthesis of new functional zeolites from mesoporous silica'
March 20	Demonstration of car by hydrogen fuel at Hyderabad
April 11	NCCR Anna university RS meet
April 29	Prof selvam submitted the indo Chinese research programme
May 15	Seminar by Dr Raghuram Chetty on Flexible fuel cells.

## **PART I**

### **Strengthening the collaboration with the Department of Chemistry, Anna University The activities for the year under review (2008-2009)**

- 1. NCCR conducted two Joint research scholars meet in august 2008 and April 2009. Third one is planned for August 2009.**
- 2. M SC (course of Anna University) one full course was conducted by Prof S Sivasanker during the odd semester of 2008.**
- 3. M Phil/Ph D course was conducted by NCCR partially during the odd semester of 2008.**
- 4. Ph D guidance is being strengthened. NCCR has been guiding some (5) students jointly with Anna University**
- 5. NCCR has provided laboratory and other facilities for work by Anna University students in NCCR ( two of them are working at NCCR at present)**
- 6. Visits by scientists from other countries are mutually coordinated.**

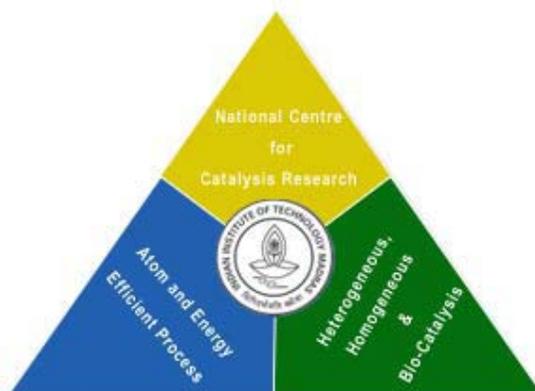
Annexure

Self Assessment Report for the year 2008

(The contents will overlap with the main report,

but this report is to show how the centre is evolving)

**NATIONAL CENTRE FOR CATALYSIS RESEARCH  
INDIAN INSTITUTE OF TECHNOLOGY MADRAS  
CHENNAI 600036**



**REPORT ON THE ACTIVITIES OF NCCR DURING 2008**

**NATIONAL CENTRE FOR CATALYSIS RESEARCH  
INDIAN INSTITUTE OF TECHNOLOGY MADRAS  
CHENNAI 600036**

**REPORT ON THE ACTIVITIES OF NCCR DURING 2008**

**A. Education, Capacity Building and Human Resource Development**

1. The following six research scholars of NCCR completed their Ph.D. thesis work during this year and have been awarded the degree by IITM:

**Mr. S. Navaladian  
Ms. C.M. Janet  
Mr. Ch. Venkateswara Rao  
Mr. L. Himakumar,  
Mr. P. S. Kishore and  
Ms. J. Rajeswari**

2. The following students have joined NCCR for research work and some of them have since been registered for their Ph.D. degree:

Mr. Anil Kumar  
Mr Ramanamurthy  
Mr. Mahendran  
Mr.P.R.Venkatesan  
Ms.Anandhakirupa

**New Research Associates** who have joined the centre during this year include:

1. Dr P P George
2. Dr Thirunavukarasu
3. Dr Anuradha
4. Dr Navaladian

Presently, the total number of research scholars and project associates at NCCR is **18** and Research associates (PDF) is **six**.

3. Detailed syllabus for an M.Tech course at IITM in Catalysis and Technology has been drawn and submitted to our administration for necessary action to enable us to offer this course from the next academic year.

4. The 9<sup>th</sup> Orientation program on catalysis for the research scholars in the country was conducted during 17<sup>th</sup> November – 8<sup>th</sup> December 2008 (21 days) in which 35 students from different institutions participated.

5. One of our NCCR faculty (Dr. S. Sivasanker) taught a regular course on industrial catalysis for the students of M.Sc. Applied Chemistry of Anna University (I semester), as a part of an academic cooperation between NCCR and Anna University.

6. A similar academic cooperation with Departments of Chemistry and Energy of Tezpur University has been established with an MOU. Prof. B.Viswanathan conducted a course on catalysis for the M.Sc. students of Tezpur University, as a part of their curriculum. He also delivered some special lectures on spectroelectro chemistry. (Dates: 10<sup>th</sup> September to 22<sup>nd</sup> September 2008)

7. For the students of M.Sc. Inorganic chemistry (3<sup>rd</sup> Semester) of Pune University, Dr. A.V. Ramaswamy gave a series of 12 lectures on homogeneous catalysis as a part of their course on organometallics (22<sup>nd</sup> to 27<sup>th</sup> September 2008).

8. A special one day course on catalysis, zeolites and characterization technique, with particular reference to deNO<sub>x</sub> systems was offered to a group of employees of General Motors, Bangalore on 9<sup>th</sup> September 2008 by NCCR faculty (Prof. B. Viswanathan, Dr. A.V. Ramaswamy and Dr. S. Sivasanker) under a research grant given by GM India Ltd., to NCCR.

9. The Annual Day of NCCR was observed on 2<sup>nd</sup> August 2008 with the participation of research scholars from Anna University, with four presentations on recent research work of the scholars and a special lecture by Prof. K. Shanthi of Anna University. For improving the general quality of research work, such joint programs will be conducted once in 6 months.

10. NCCR took the initiative to conduct a pre-workshop school (Tutorial) for selected research scholars, prior to the National Workshop on Catalysis held at IMMT, Bhubaneswar (15-16 February 2008). The subject was “Thermal Methods in Catalysis” and conducted very successfully by Prof. B. Viswanathan, Dr. A.V. Ramaswamy and Dr. C.V.V. Satyanarayana (NCL, Pune). The annual meetings of the Catalysis Society of India (a symposium and a workshop alternatively), henceforth, will include such 2-day intensive tutorials (schools) for in-depth training of research scholars on a particular subject or technique in catalysis.

11. As a part of course work for research scholars in catalysis of National Chemical Laboratory, Pune, Dr. A.V. Ramaswamy gave a series of lectures at NCL, Pune during 24<sup>th</sup> to 28<sup>th</sup> November 2008.

12. Steps have been taken to enter into an MOU with some international institutions, including the Centre of Catalysis of the Technische Universität München, Germany.

13. A book entitled “Heterogeneous Catalysis” authored by Prof. D.K. Chakrabarty and Prof. B. Viswanathan has come out as an international edition, published by New Age Science Limited Kent TN1 1YS, UK.

14. Our annual program for Children’s Club on “Synthetic Strategies in Chemistry” has been placed as an e-book in our Centre’s web site. Our E-prints server has crossed over a 1000 documents this year in the area of catalysis.

## **B. Basic Research/Outcome**

1. NCCR’s focus on basic research has been in four areas, viz., catalysis in energy conversion, new materials and environmental catalysis, surface science and theoretical studies and modeling of catalysts and surfaces. The pursuit of research by the Ph.D. scholars

and post-doctoral fellows in these areas and the research output are reflected in the research publications, presentations at national and international conferences, reviews and status documents of NCCR faculty and the research scholars. During 2008, we have published more than 30 research papers (list to be appended), 20 or more of papers presented at conferences (list to be appended) and special lectures delivered by the faculty.

<b>Name</b>	<b>Title of the presentation</b>	<b>Details of presentation conference with date</b>
A.V. Ramaswamy	Designing Functional Ceria Materials by Nanoarchitecture	Plenary lecture at International Catalysis Conference, Tehran, Iran, 28-30 April, 2008
A.V. Ramaswamy	Chemical States and Redox properties of Mn/CeO <sub>2</sub> -TiO <sub>2</sub> Nano composites	Lecture at Institute of Isotopes, Budapest, Hungary, 4 November, 2008
A V Ramaswamy		Rev Fr L M Yeddanapalli memorial oration award lecture March 25, 2009
	<b>Others details are given at the end of this document under presentations 2008</b>	

2. We have submitted a patent application for a novel membrane material based on composite polymers for filing in India.

### **C. Industry supported projects/Industry-Academy interactions**

1. The following projects sponsored by Chennai Petroleum Corporation Limited, Chennai have been completed and final reports have been submitted:

- a) Adsorptive desulphurization of diesel fraction and
- b) End point reduction of diesel fuel.

2. The following projects are under progress:

- a) **Deposition of ceramic oxides on SS surfaces (under Shell Fellowship)**
- b) **IOC (Preparation of alumina support)**
- c) **NMITLI, CSIR (Glycerol to value added products)**
- d) **P&G (Oxidation at terminal position in alkanes)**
- e) **GM Research Grant for studies on deNO<sub>x</sub> reactions**

3. With General Motors India Ltd., Bangalore, a project proposal on the mechanistic aspects of SCR of NO<sub>x</sub> has been filed and is under consideration for funding.

4. Following the interactions with BASF, USA personnel and their visit to NCCR earlier, an agreement for sponsoring of projects by BASF at NCCR is being signed.

5. We had two interactive sessions with researchers of Nissan Motors for possible areas of collaboration and research projects to be undertaken at NCCR.

6. A research proposal for MNRE, as per their request in Hydrogen energy program, with multiple institutional involvement has been submitted.

7. The following new proposals are under consideration:

- a) Consultancy work for Sri Ram Fibers Ltd.,
- b) Consultancy work for Tamil Nadu Petro-products Ltd.,

#### **D. International Collaboration**

1. Under the Indo-Hungarian joint research project on metal clusters and surface Studies, exchange visits and discussions had taken place. Three of the Hungarian Scientists visited NCCR, and reciprocal visits by two professors from NCCR to Budapest and a long term (3 months' visit) of one of the research scholars from NCCR to Institute of Isotopes, Budapest for working on the project have been completed. The details are given below:

<b>Name</b>	<b>Organization</b>	<b>Name Details of the visit and dates</b>
Prof. Laszlo Guzzi and Dr. Zoltan Schay	Department of surface chemistry and catalysis, Hungarian academy of sciences	12-24, February 2008 Also participated and gave lectures at the National Workshop on Catalysis, IMMT, Bhubaneswar
Dr. Zoltan Paszti	Same as above	To work on Centre's XPS machine
Mr. G. Magesh	Research Scholar, NCCR, IITM –visited Hungary	April to July 2008 to carry out research
Prof. B. Viswanathan and Dr. A.V. Ramaswamy	NCCR to visit Budapest laboratory	Lectures and also research 31 October to 8 November 2008

2. Indo-Taiwan (Project on development of fuel cells and membranes)

3. Indo-Australian (Carbohydrates to chemicals)

#### **D. Activities related to Catalysis Society of India:**

1. NCCR brought out four issues of the Bulletin of the Catalysis Society of India in time during this year. The other activities of CSI are coordinated from the Centre.

#### **E. Other Events and Activities:**

1. New analytical instruments installed this year include, HPLC (With a number of detectors) (Shimadzu, Japan) and XRF (wave-length dispersive) (Rigaku, Japan).

2. The annual MAC meeting was held on 7<sup>th</sup> July 2008, chaired by Prof. M.M. Sharma and attended by among other members, Dr. T. Ramasamy, Secretary, DST, New Delhi.

3. Our centre finds a place in the documents prepared by the British High Commission for Fuel cell opportunities in India and for Fuel Cell today. These two documents refer to our efforts in the research on fuel cells.

5. Ms. M. Helen (research scholar) won the best poster award at the recent International Conference on Functional Materials, held at IITM during November 2008.

6. The PAC meeting of the Physical Chemistry of DST was organized by the Centre on March 2008 to include an interactive session with PIs of new proposal for quality improvement of their project proposals.

7. Our Centre was formally declared open by Mr. Kabil Sibal, the Minister of Science and Technology, Government of India on in a glittering ceremony to mark the golden Jubilee of IITM and the Indo-German cooperation.