2013

NCCR, IITM

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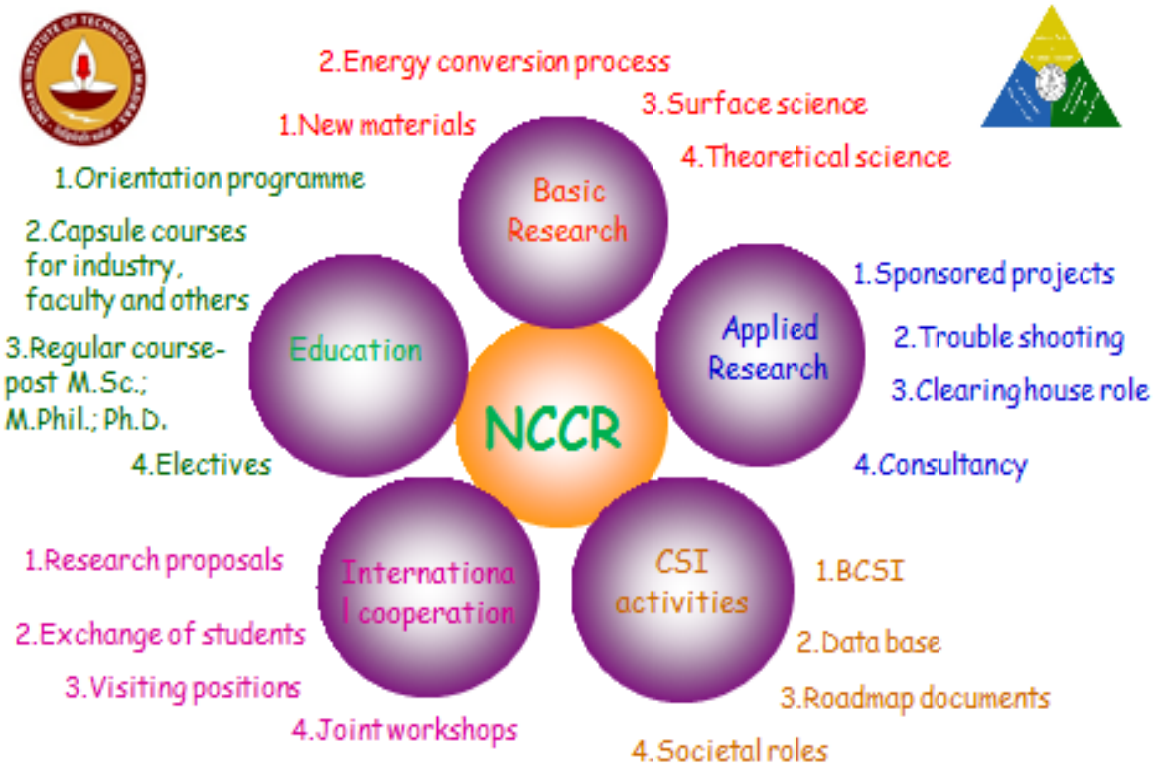
Progress report
[2011-2013]

National Centre forCatalysis Research
Indian Institute of Technology-Madras

Contents

Main activities of NCCR

In a nutshell



NCCR- Spheres of activity

I.Building Human resource in Catalysis

A. Educational courses and lectures

1. M.Tech. (Catalysis Technology)

NCCR offers an M Tech. course in Catalysis technology. The degree is offered by the Chemical Engineering Department of IITM. Two batches of M Tech. Catalysis Technology students have graduated during 2011 & 2012.

2. Orientation course in Catalysis

NCCR/IIT-M has been conducting Orientation courses for research students in Catalysis for the past many years. The course usually lasts for about 3 weeks, which includes about 200 hours of lectures, tutorials and discussions. The 12th and 13th Orientation Programs in Catalysis were conducted during the months of November and December in 2011 and 2012.

48 research scholars participated in 2011 and 43 in 2012. The participants were from all over India, like from ICT-Mumbai, NCL-Pune, IICT-Hyderabad, TezpurUniversity-Tezpur, Devi Ahalya University- Indore, PPISR- Bangalore, Loyola College- Chennai, Sacred Heart College-Tirupathur, IIT-Kanpur, IIP-Dehradun and CSMCRI-Bhavanagar. The names of persons who attended one of these courses are given in Annexure.2

3. Special lectures and academic courses.

i. The course on Fuel cell technology for MTech. Mechanical Engineering was shared by the faculty of NCCR with the faculty of Mechanical Engineering, IIT Madras during 2011 & 2012

ii. A number (at least 6) of on-line lectures were held in this period for the participants from various places in India like PPISR Bangalore, Defence laboratory, Delhi and a few other places in Mumbai like ICT and a private multinational company. A

number of lectures on-line lectures were also organized from Japan, Israel, and USA during this period.

iii. A number of lectures by the visiting scientists from other countries were arranged in the Centre during this period.

iv. The faculty members of the Centre delivered a large number of lectures in various academic meetings/workshops /courses.

v. A special course on Photo-Electrochemistry was conducted from December 15 to 19, 2012 with 40 participants from various parts of this country, like, Loyola College, Chennai, PPISR, Bangalore, IIT Kanpur, IIT Chennai from other departments. The actual list of the names of the participants is given in Annexure.3

vi. Short term courses on Analytical methods and Fuel cells were conducted by the Centre in the months of June-July, 2012.

vii. A special course on the Applications of Photo-Electrochemistry will be held for research scholars during July 2013.

viii. A Workshop on "Sustainable energy conversion and storage devices" will be held during September 2-8,2013 in collaboration with SRM University, Chennai

4. Training of students from other organizations

i) Three students were sponsored by Indian Science Academies to carry summer fellowships in NCCR. Two more will be participating in 2013 summer.

ii) Two students from the Department of Applied Chemistry, CUSAT, Cochin, will carry out their M Tech project in the Centre from June 2013.

iii) Three M.Sc students from A V V M Sri Pushpam College, Poondi, two M.Sc students from Thiagarajar College, Madurai, underwent training in the Centre during May-July 2012.

The names of the candidates are as follows:

1. Ms.N.Prabhavathy M Sc Chemistry, A V V M Sri Pushpam College
2. Ms.G Kalaiselvi, M Sc Chemistry A V V M Sri Pushpam College
3. Ms.S.Bhuvanya, M Sc Chemistry, A V V M Sri Pushpam College
4. Ms.P.Vidhyalakshmi, M Sc Chemistry, A V V M Sri Pushpam College
5. Mr.Karthick M Sc Chemistry Thiagarajar College, Madurai
6. Mr.R.Vijaya Kumar M Sc Chemistry Thiagarajar college, Madurai

iv) Several high school students underwent special courses (about 10 lectures by NCCR Ph.D. scholars) on recent developments in science during the summer months each year.

B. Ph .D/MTech Research/Degree in Catalysis

i) Ph D theses submitted to IIT Madras

1. B.Kuppan –Platinum supported ordered mesoporous carbons as electro-catalysts for direct methanol fuel cells (2013).(Supervisor: Professor. P. Selvam)
2. Two more Ph D theses (MrVamshi Krishna and MrRamanamurthiare under preparation and will be submitted in next few months (2013). (Supervisor Professor P Selvam)

ii) Ph D degree awarded/thesis submitted to other Universities

1. Dr. M. Banu,"Biomass Conversion and Utilization of polyhydric alcohols from Natural sources"- Thesis submitted to

BharathidasanUniversity,Trichy. Supervisor:Prof. S. Sivasanker – Degree awarded in January, 2013.

2. Dr. T.M. Sankaranarayan, "Trans-esterification and hydroprocessing of sunflower oil over heterogeneous catalysts"-Thesis submitted to Anna University, Chennai. Supervisor: Prof. S.Sivasanker-Degree awarded in March 2013.

3. Ms. GDeepa, "Hydrotreating reactions over different supported Ni-Mo(S) catalysts investigations using model compounds" Thesis submitted to Anna University, Chennai inNovember 2012. Supervisor: Prof. S. Sivasanker –Thesis is under evaluation.

4. Ms. K. Premalatha,"Studies on the catalytic oxidation of benzyl alcohol inhomogeneous and heterogeneous media: Role of the Reaction Environment" Thesis submitted to the University of Madras (with Madras Christian College) April 2012-Thesis under evaluation

iii) Students registered for Ph D degree in IIT-M and other universities

12 students have registered for Ph. D. either with IIT-M, Anna University, Bharathidasan University and Madurai University.

iv) M Tech (Catalysis Technology)- Theses submitted to IIT Madras

2013

1. Mr. Manish AMarode- Studies on self-condensation of ethanol-Influence of process parameters - [Supervisor: Prof. K R Krishnamurthy].
2. Mr.V.Surya Kumar - Selective hydrogenation of cinnamaldehyde to cinnamyl alcohol - [Supervisor: Prof. K R Krishnamurthy].

3. Mr. K. Veeraraghavulu - Synthesis of highly photoactive mesoporous TiO_2 for water splitting reaction [Supervisor: Prof P.Selvam].

2012

1. Mr. D. Sushil Kumar-Hydrotalcites as photo-catalysts for reduction of carbon dioxide [Supervisor: Prof. K. R. Krishnamurthy].

2. Mr. Aditya V. Ajgaonkar- Investigation of Ni-Mo/SBA15 as hydrotreating catalyst comparison wih Ni-Mo/Alumina catalyst, [Supervisor: Prof .S.Sivasanker].

3. Mr. Sunil, Mehla-Synthesis, characterization and evaluation of zeolites for hydro isomerization of model feed N-Hexadecane [Supervisor: Prof. K. R. Krishnamurthy].

4. Mr. MdMainakZaman- Noble metal supported porous carbon as oxygen reduction reaction catalyst for fuel cell applications [Supervisor: Prof. P.Selvam].

2011

1. Ms. K.Rajalakshmi- Photo catalytic reduction of CO_2 in conjunction with the decomposition of water on oxide semi-conductor surfaces [Supervisor: Prof. K. R. Krishnamurthy].

2. Ms. K.Devaki- Ordered porous carbon and nitrogen containing carbon supported nanoplatinumelectro-catalyst for direct methanol fuel cell applications [Supervisor:Prof P.Selvam].

3. Mr. Sanjay Kumar Soni-Bio-catalytic oxidation of primary and secondary alcohols by usingVandidaParapsilosis ATCC 7330 [Supervisor: Prof.AnjuChadha].

4. Mr. Sourav Khan- Synthesis and characterization of mesoporousCeria- Zirconia solid solution[Supervisor: Prof. P.Selvam].

5. Mr. Chaitanya Vijay Dhoke - Acylation of anisole with lauric acid over zeolite Beta.[Supervisor: Prof .S.Sivasanker].

C.Knowledge dissemination activities

1) Workshops and short-term courses

a. Indian

1. The 15thNational Workshop on Catalysis was organized by NCCR during the period December 11-13, 2011.

2. A Catalysis pre-school on Photo-catalysis was organized by the Centre during December 9-10, 2011. About 40 students and teachers benefitted from the pre-school.

3. A Special short term course on photo-catalysis and PEC from December 15 to December 19, 2012. About 40 participants from various parts of the country participated in this short course.

4. An in-house seminar on the research activities was held on 6th April 2013 wherein all the faculty and adjunct faculty of NCCR shared their research activities.

5. A half a day brain storming session was conducted in the Centre on 21st May 2012 on materials for PEC applications. ProfRajpala of IIT-K, Prof Ramnarayanan of IIT-M, Dr.Ramya of CFCT, Prof. PSelvam of Department of chemistry,NCCRand a few students from University of Madras and NCCR attended this session.

6. Two one day meetings of the research students of NCCR and Anna and Madras Universities, in which students presented their research activities, were conducted during this period.

7. A special course on the applications of Photo-electrochemistry will be held for research scholars in July 2013.

8. A workshop on Sustainable energy and Storage devices will be held during September 2-8, 2013 in collaboration with SRM University.

b. International

1. An Experts meeting between Russian Scientists and Indian Scientists (from all over India) was organized during December 14-15, 2011.

2.An Indo–AustralianSeminar on Bio mass utilization is being planned during the end of 2013.

2) Academic Assignments of NCCR faculty

1. Prof. P. Selvam, Member PAC (Physical Chemistry), DST, Government of India
2. Dr. S. Sivasanker, Member PAC (Chemical Engineering), DST, Government of India
3. Prof. P. Selvam, Editor, Journal Advanced porous materials.
4. Dr. S. Sivasanker, Editor, Catalysis Surveys from Asia,
5. Dr. K.R. Krishanamurthy, Member of RAC ofPoornaprajana Institute of Scientific Research (PPISR), Bangalore.
6. B. Viswanathan, (i)Editorial board member of Indian Journal of Chemistry, Eurasian Journal of Chemical Technology, Material Science an Indian Journal, Current Catalysis etc. (ii) PAC member of DST- PMAC on C sequestration, RAC member of: IOCL, R &D - Faridabad , CPCL- Chennai and CFCT (ARCI). Member of MNRE project Evaluation committee for major proposals.
7. Allthe faculty members of NCCR are academic reviewers for almost all the major scientific journals - the total number may exceed 50 Journals of all leading publishers in the world.
8. The faculty members of the Centre have delivered a number of lectures in various academic meetings and also have been in the advisory capacity to conferences organized by various institutions in India and abroad

IIResearch Activities

A. New Initiatives in Basic Research

1.Theoretical Studies

The theoretical studies carried out in the Centre aredirected towards a number of problems, such as:

a. How is the surface different from that of the bulk in terms of density of states and their wave functions?
b. Howcan theybe tuned for the molecular level transformation of substrates?

In this connection, the group has considered core shell configuration of TiO_2 as the reason for the better photo-catalytic/ photo-electrochemical activity of TiO_2.

c. The group is also investigating the stability of metallic clusters on supports and the reasons for a specific cluster being formed on a chosen support.
d. The group is also working on the reduction of CO_2 on various surfaces and the most probable pathway for the reduction and preferential formation of hydro-carbons or alcohols.

In a recent publication [1] the photosynthetic conversion of CO_2 to hydrocarbons (methane and other higher hydrocarbons) on Pd /TiO_2 in conjunction with nafion has been reported. However, the photo conversion efficiency of the process is very low because the activation of the thermo chemically most stable CO_2 requires highly energetic electrons. Since the one-electron reduction of CO_2 $_{+(}$the initial step in the reduction process) requires high potentials of the order of 2 Volt, a more favorable pathway is to reduce CO_2 though proton-coupled multiple-electron transfers (PCET). Nafion (per fluorinated polymer with sulfonate groups) coated Pd–TiO_2 particles (Nf/Pd–TiO_2) were prepared and their reactivity for the photo reduction of CO_2 was tested. The role of the Nafion layer is to enhance the local proton activity within the layer to facilitate PCET reactions and to stabilize intermediates and to inhibit the re-oxidation of the CO_2 reduction products. Nf/Pd–TiO_2 is more active than Pd–TiO_2 for the photo-production of hydrocarbons (e.g., methane, ethane, and propane). The photosynthetic activity of the Nf/Pd–TiO_2 catalyst was maintained through repeated cycles of photoreaction, which confirms the stability of the Nafion layer. The

proposed Nf/Pd–TiO_2 should serve as a model of more practical catalysts for the artificial photosynthesis that is based on PCET reactions.

The conceptual design of the catalyst system employed in this study is shown in Fig 1.

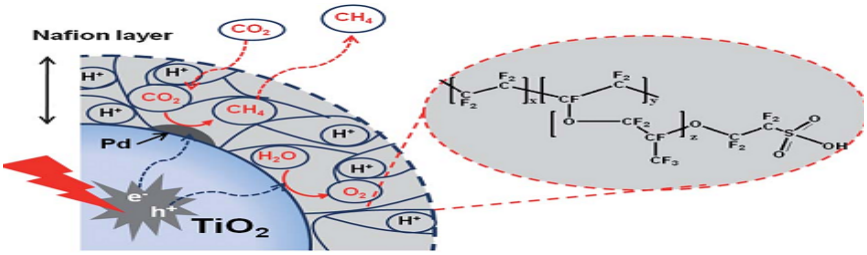


Fig.1 Pd/TiO_2 on Nafion catalyst system for the photochemical reduction of CO_2 [from ref 1]

In the light of this communication, the following is presented for conceptual analysis and possible adaptation. Essentially the points of relevance are:

(i) A direct proton source rather than from the decomposition of water is desirable so that the reduction of CO_2 is facilitated.

(ii) It must be ensured that the species employed for proton source should not undergo any electrochemical reaction within the potential range for CO_2 reduction reaction.

(iii) The reactivity of the proton should be as high as that in Nafion, where the Proton is in a highly electronegative environment of Fluorine atoms.

(iv) The available protons should be capable of reacting with carbon dioxide directly promoted by the light absorbed in TiO_2 and reduction reaction should be carried out on some reactive metal sites.

(v) In order to overcome the low solubility of CO_2 the source is any carbonate which can *in situ* generate CO_2 and thus can sustain the supply of CO_2.

Considering these aspects and also based on argumentative formulations it is possible that alternate PCET catalyst support systems which may sustain more acidic protons can be tried like heteropoly acids or super acids like sulphated zirconia.

Reference: [1] Wooyul Kim et al., Energy Environ. Sci., 5, 2012, 6066

2. Bio-mass conversion

The relevance of catalytic pyrolysis for the production of bio-fuels
(proposed joint work with NandanCleantech and NCCR)

The production of bio-fuels has assumed significant importance due to economic and environmental considerations[1].There are various process steps involved in this technology. One of the process steps that has received considerable attention is the fast (why and the need for fast?) pyrolysis that can yield high liquid yields with specific composition, but must be capable retaining majority of the energy content of the bio-fuel. These limitations are required simply to make bio-fuel to be compatible to the petroleum based fuels that are being extensively employed in the present days. The essential consideration in devising proper pyrolysis step is to remove selectively the oxygen component found in the bio-fuel. This oxygen removal can be achieved either by hydrogenation (conventionally known as hydro-treating) or by splitting the molecule (termed as cracking). Both these process steps are well known and practiced in oil industry today. Catalytic cracking for the production of biofuel is achieved by de-oxygenation through simultaneous dehydration, decarboxylation and decarbonylation reactions and these reactions have been shown to proceed in the presence of ordered micro-porous zeolites catalysts. Though the catalytic pyrolysis has been known, the search for appropriate catalyst system is still on since, it is necessary that one not only obtains the desired levels of conversion (which should be of the order of 90% or above), the hydrocarbon content should be optimum. This means the organic functional like carbonyls, acids, esters, phenols and ethers must be suitably handled so as to optimize the hydrocarbon content which provide the necessary fuel value. The literature is abundant[2-3] on these attempts especially with respect to finding appropriate catalyst system and also identifying suitable process formulation. There have been attempts to couple pyrolysis and catalytic cracking in a single flow without the intermediate separation of the cracked products from the points of view of economics of the process and also to avoid the possible catalytic deactivation by in situ coke formation or other condensed products. A variety of in situ techniques [4](like IR, XPS, TPD) have been adopted to identify the removal oxygenates especiallycarboxylic and ester functionalities since the presence of these functionalities will affect the hydrocarbon yield and thus reduce the fuel value. The type of studies that have been reported in literature are: (i) Evaluating various catalyst systems that will preferentially and selectively produce hydrocarbons thatcan be used as fuels or fuel blends. Though this can be achieved both by hydro-treating and cracking the latter is examined to a greater extent due to reasons like technology is well known and also process simplicity. In these studies the optimization has been focused on temperature, pressure, and adopting suitable analytical technique for unambiguous identification of the components of the product stream. Another major factor is to examine the exact ratio of catalyst to the biofuel content in a semi-continuous or continuous mode. In the following few lines, the recent research activity in this area is briefly summarized.

(i) Various types of catalysts systems have been evaluated for their performance and also to find guidelines for catalyst design. Not only conventional FCC (Fluid Cracking Catalysts) systems but also various types of modifications have also been evaluated. In addition, the recent meso-porous systems like MCM type with various types of substitutions have been evaluated with a view to optimize the hydrocarbon yield [5-10].
(ii) Various process variables mostly on laboratory scale reactors like super critical water method to increase heating value, effect of hydro-treatment to increase oxygen removal [11].
(iii)Another critical parameter that has been studies is the catalyst to bio-mass ratio [12].
(iv) Hydro-treating versus catalytic cracking[13].
(v) Reactor design and configuration

The following aspects have not been paid much attention

(i) Characterization of the fuel parameters produced by catalytic pyrolysis and thus optimizing the pyrolysis parameters. Only higher or lower yield is reported but the comparison with respect to petroleum based fuel has to be stipulated.(ii) The reactor design in detail is not yet available completely.[14]
(ii) The pretreatment procedures required for various catalyst system is not yet established.[15]
(iii) The selection of the appropriate catalyst has not yet been established though results on a number of catalyst systems are available.
(iii) The predictive capacity of bio-oil quality on the basis of input parameters is not yet shown.[16-17]

This summary note on the status of catalytic pyrolysis route shows that there are various gaps in our knowledge in transforming this technology into a viable technology. The teams are considering this possibility of transforming this laboratory based technology to a manufacturing matured technology.

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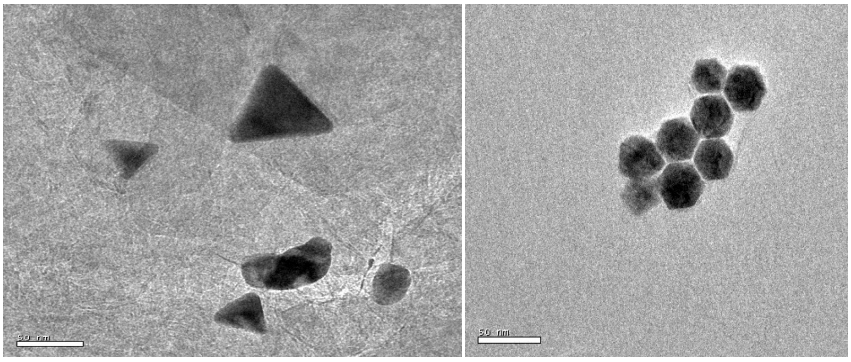
3 Studies on shape controlled supported metal nano particles

Nano sized supported metal catalysts have been extensively studied by virtue of their high activity, easy separation and the mild reaction conditions required in catalytic reactions. Several factors influence the performance of supported metal catalysts, including the metal loading, particle size, metal

surface morphology, nature of the support, and the metal–support interaction. Of these, the size and morphology of the metal particles are two important factors affecting the amount and nature of the active sites. Nano particles with different sizes and shapes have different degrees of dispersion, exposed facets and fractions of atoms located at different corners, edges, and defects (resulting from the loss of atoms at these locations). Thus, for a given reaction, the catalytic activity of particles with different morphology can vary quite dramatically Hence studies on the preparation, characterization and performance evaluation of shape controlled supported metal catalysts is considered as an area of tremendous importance both from fundamental as well as applied aspects of catalysis

In NCCR studies have been initiated on the preparation of shape controlled Pd particles. It is proposed toextendedsuch studies on other metals like Pt,Au,Ag, Co & Ni that have applications in different hydrocarbon conversion reactions.



Tetrahedral and Octahedral shaped Pdnano particles supported on Mg-Al hydrotalcite

B. Highlights of on-going research

a. Basic research

1. Platinum-supported Ordered Mesoporous Carbons as Electrocatalysts for Direct Methanol Fuel Cells

Ordered porous carbon materials with high surface areas and pore volumes prepared from porous inorganic templates are of current interest for energy storage, separation, catalysis, and many other applications. One of the most successful examples is the synthesis of OMCs using ordered mesoporous silica (OMSs) framework as hard-template (Ryooet al., 1999). This approach is based on a multi-step process *via* polymerization /carbonization of carbon precursors diffused within inorganic matrix followed by removal of the inorganic template by acid/alkali leaching thus replicating mesoporous structure. The general synthetic procedure for different types of carbons involves the following steps: a) preparation of carbon precursor/inorganic template composite, b) carbonization, and c) removal of the inorganic template. The typical methodology is followed for the preparation of mesoporous carbons such as NCCR-41 (hexagonal) and CMK-1 (cubic) employing OMSs, viz., MCM-41 and MCM-48, respectively.

2. Conversion of glycerol to value added product

In this project a variety of catalyst systems have been examined for the formation of value added products like 1,2 and 1,3 propandiol, acetone and other chemicals. The catalyst systems examined include oxides, heteropoly compounds, and other reported supported systems. The main objective is to optimize the yield of value added product.

3. Studies on the formation of gold nanoparticles and its reactivity

This study is mainly directed in the controlled formation of gold nano particles with various synthetic strategies and also on various supports. The aim of this work is to formulate synthetic methodologies for the formation of specified morphology, shape and size of gold nano-particles and to examine the catalytic properties. The size dependent activity and selectivity in the glycerol oxidation has been shown for Au supported on

carbon.

4.Design of materials for PEC applications and for hydrogen production from water decomposition and photo-catalytic activity.

Carbon substituted micro-porous anatase phase of Titanium dioxide was successfully synthesized. Meso-porous TiO_2 was synthesized using structure directing agents such as L31, P123 and F127, CTAB and CPBr. The calcined samples of meso-porous TiO_2 synthesized from L31, P123 and F127 were hydrogenated to increase the photo-catalytic activity. All the samples were characterized by powder XRD, UV-visible DRS spectroscopy, FT-Raman and TG-DTA. A variety of other photoactive morphologies were designed and their photo-catalytic activity for decontamination (Chloro-phenol decomposition) was tested.

5.Alternate concepts for photo-activity in oxide materials

The presence of non-native configuration over native configuration has been shown to be possible reasons for the activity exhibited by P25 –TiO_2. This postulate has been probed by the consideration of the Density of States (DOS) of a configuration with a core shell model and has been shown that the wave functions in this configuration are favourable for water decomposition.

6.Heteroatom substituted carbon materials – potential hydrogen storage Materials

Nano carbon materials have not shown promise as good hydrogen storage materials since the reports available shows that mostly zero percent storage though there are reports upto 67 weight % storage. None of these reports have been reproduced so far. Heteroatom substituted carbon materials have been shown to exhibit responsible sites for dissociation of molecular hydrogen and its spill-over to carbon surface. Theoretical and experimental results on hetero-atom substituted carbon materials have been assembled to verify this postulate. Phosphorus containing carbon materials have been prepared and its hydrogen storage capacity (~1 weight %) has been evaluated.

7 Photo-catalytic reduction of carbon dioxide Photo catalytic reduction of carbon dioxide by water on La modified sodium tantalate with different co-catalysts under UV-Visible radiation

Lanthanum doped sodium tantalate with different co-catalysts have been prepared, characterized and studied for photo catalytic reduction of carbon dioxide by water under UV-Visible radiation. Methanol and ethanol are the major products. Maximum CO_2 conversion is achieved with 0.2% NiO-$NaTaO_3$:La (2%) followed by 1% CuO-La:$NaTaO_3$. Coupling of the conduction bands of NiO&CuO with that of $NaTaO_3$ facilitates easy transfer of photo-generated electrons from $NaTaO_3$ to NiO/CuO, leading to effective charge separation and improved activity. Bicarbonate species in the medium undergo stage–wise reduction with active hydrogen from water splitting, to yield products, methanol/ethanol.

8.Electro-catalytic reduction of carbon dioxide

The conversion of carbon dioxide to useful chemicals has been pursued in many laboratories. The main issue is to overcome the high over voltage of the order of one volt. Another issue is to generate selective products in the conversion of carbon dioxide especially to hydrocarbons. In this work various configurations of metallic electrodes like bare copper, copper coated on copper and various other metallic electrodes have been examined for the preferential formation of hydrocarbons like methane and higher homologs.

9.Development of Fuel cell Electrode materials

The research on this topic centers around why platinum appears to be the best electrode material in fuel cell applications. The questions addressed are :i) How can the activity of the electrode can be increased even if it were still based on Pt? (ii) How to reduce the loading levels of Pt(at least one to two orders of magnitude) but still retain the same level of activity and stability? (iii) If there were to be alternate to Pt, which material (Perovskites?) is most preferred for fuel cell application?

10.Value addition of bio-mass: transformation of sorbitol:

The transformation of sorbitol into propylene and ethylene glycols is being investigated over Ni, Pt and Ru supported on Na-Y, activated carbon (AC), SBA-15 and C-coated SBA-15 (SBA-15-C), hydroxyapatite and fly-ash. The studies reveal that Ni is an excellent catalyst for the production of propylene glycol (1,2-PD) when supported on Na-Y. The catalyst was active and selective even at 6% Ni-loading. Similarly, Ru was a good catalyst when supported on AC or on SBA-15-C. It is found that 6% Ni-Na-Y is at least equivalent or better than expensive Ru catalysts reported in the literature.

11.Transesterification of vegetable oils over solid catalysts

The transesterification of a model vegetable oil (sunflower oil) over MoO_3 supported on alumina, silica and titania was investigated. The studies reveal that the performance of the catalyst is highly dependent on the support and the calcination temperature. Experiments have also been carried out in a continuous fixed-bed reactor. The studies reveal that MoO_3/Al_2O_3calcined at 950 K is a suitable catalyst for the reaction.

12. Hydroprocessing of diesel-vegetable oil blends

The conversion of vegetable oil-straight run diesel blends into value added diesel fuel was carried out over NiMo-supported on alumina-beta (zeolite) blends. Complete conversion of the oil into hydrocarbons (n-C_{17} and n-C_{18}) along with simultaneous desulfurization of the diesel feed takes place even under moderate reactions conditions normally used in diesel HDS. Thus, the process obviates the need for transesterification and subsequent blending of FAME.

b. Sponsored projects

1.Anchoring of stabilized metal nano particles on metal-oxide supports-Shell

- Synthesis and stabilization of metal nano particles in different size ranges in aqueous medium
- Choice of appropriate reducing/capping agents
- Anchoring of metal nano particles on different oxide supports
- Establishing calcination and reduction protocols to obtain mono dispersed metal nano particles anchored on the supports.

2. Anchoring of nickel nano particles on titania coated on SS-316-Shell

- Coating of high surface area titania on to SS-316 surface
- Developing suitable binder formulation
- Anchoring of Nickel nano particles on coated titania layer
- Establishing calcination and reduction protocols
- Ensuring the stability of (Ni nano+ Titania) coating under liquid phase hydrogenation conditions

3. Synthesis of higher carbon number alcohols form bio-ethanol and methanol- NFCL

- Conversion of bio-ethanol to higher alcohols using Guerbet chemistry
- Basic oxides catalysts like hydroxyapetites, hydrotalcites and mixed metal oxides based on rare-earth oxides to be explored
- Tuning the acidity-basicity of the catalysts
- Optimization of process conditions towards maximum yield

4. Improving nitrogen and phosphorous utilization efficiency-NFCL

- Exploring metal – urea complexes for slow release of N
- Solid state reaction between urea oxalate & phosphates of Fe &Al- Increase solubility of phosphate
- Incorporation of N &P in suitable matrix to enable slow release

5. Development of hydrocarbon trap materials- Nissan

- For application in auto exhaust control catalyst formulations
- Materials with facile hydrocarbon adsorption/desorption characteristics
- Stability under auto exhaust stream conditions

6. Electrode development for oxygen reduction reaction

- The oxygen reduction reaction is important for many electrochemical processes including water decomposition reaction.
- These studies are aimed at finding alternate to Pt electrode materials for this important reaction

III Collaborations

1. Strengthening of collaboration with industry

New projects sanctioned during 2011-13

1. Two projects, one on "Production of higher alcohols from bio- ethanol" (July 2012- July 2014) and the other on "Improving nitrogen utilization efficiency" (Oct.2012- March 2014) have been sponsored by NFCL Hyderabad

2. A project on "Stabilization of Co nano particles in aqueous media and anchoring on oxide supports" has been has sponsored by Shell (The Netherlands) April 2012- Sept 2014

3. Development of hydrocarbon trap materials by NissonJapan December 2012.

4. IOCL sponsored research fellowships to NCCR.- electro reduction of carbon dioxide this fellowship is continuing by IOCL (Grateful thanks to the management of IOCL for this generous grant)

5. Solar hydrogen project approved by DST for a consortium mode with IIT, Kanpur, BARC, DayalBagh Institute, Agra, NCCR, CECRI, Karaikudi and IIT Rajasthan. This project envisages the development of a commercially viable design and material for Photo-electrochemical/photo-catalytic production of hydrogen from the decomposition of water. The nodal institute is IIT, Kanpur.

6. MNRE has sanctioned a mission mode project for hydrogen storage in carbon materials with departments of Chemistry, Physics, Metallurgy and Material science, and CFCT, ARCI. The nodal unit is NCCR.

7. A proposal with Ms.NandanCleantec on the pyrolysis of biomass is under consideration by MNRE. This is a joint proposal with NandanCleantech, IIT B andNCCR. The coordinators from IITM are Prof P Selvam and Prof G RangaRao.

Projects under consideration/discussion

8. Discussions are on with Ms. Kothari Petrochemicals for a project on isomerization of C_4 hydrocarbons.

9. Chennai Petroleum Corporation Limited (CPCL) has initiated discussions on two projects and the MOU will be signed soon.

10. Tenneco Incorporated, USA has signed a non-disclosure agreement and is in the process of discussing with NCCR for possible cooperation.

11. University of Adelaide (Dr. David Lewis) for MOU with NCCR for bio-diesel project.MsAban will be the industry counter-part.

2. National/International Collaborative research

New MOUs were entered with the following organizations/academic Institutions during this period to carry out joint-research on various topics in catalysis and to impart training to the personnel/students from different organizations

i) National

New MOUs entered during this period

1. Poornaprajna Institute of Scientific Rsearch, a R and D institution in Bangalore

2. SRM Research Institute, SRM University, Kattankalathur

3. A V V M Sri Pushpam College, Poondi, Tamil Nadu

4. Department of Chemistry, Cresent Engineering College,B.S. Abdul Rahman University, Chennai

5. Department of Chemistry, Loyola college, Chennai

ii) International

1. South Africa: Discussion on research cooperation has been initiated with the University of Witwatersrand with Prof.Dr.NeilCoville.

2. Netherlands:University of Twente signed MOU with the IITM -One M.TechCatalysis Technology studentfrom NCCR to work in Univ. Twente as a part of Students Exchangeprogrammeduring 2013-14.

3. A MOU with the Department of Chemical Engineering University of Nevada and NCCR is under active consideration for exchange of research students between these two education centres.

4. An MOU is to be signed with the University of Adelaide (Dr David Lewis) for carrying out an algal-oil utilization project. M/s. Aban Industries will be the industrial partner

IV. Research contributions

A summary of the research out-put is given below:

1	No. of papers in journals	50
2	No. of presentations	~ 50
3	Books/Chapters	4/ 8
4	Patents	Four

A. Publications (March 2011-March 2013)

1)Premalatha, K., Raghavan P.S. and Viswanathan, B., Liquid phase oxidation of benzyl alcohol with molecular oxygen catalyzed by metal chromites, Applied Catalysis A,419-420 (2012) 203-209.

2) B. Viswanathan, Reflections on the Electrochemical Reduction of Carbon dioxide on Metallic Surfaces, Indian J Chem., 51A, 166-173 (2012).

3)KusumK.Bania, DipsikaBharali, B. Viswanathan and Ramesh C. Deka, Enhanced catalytic activity of zeolite encapsulated Fe(III) Schiff base complex for oxidative coupling of 2-naphthol, Inorganic Chemistry 2012, 51 (3), pp 1657–1674.

4) B. Viswanathan and K R Krishnamurthy, Reduction of carbon dioxide to useful chemicals by electro- and photo-chemical means, Proceedings of international conference on climate change and CO_2 management, Mitigation, separation and Utilization, Anna University, Feb 2-3, 2012.

5)KRajalakshmi, V Jeyalakshmi, K R Krishnamurthy & B Viswanathan, Photocatalytic reduction of carbon dioxide by water on titania: Role of photophysical and structural properties, Indian J Chem, 51 A 411-419 March 2012.

6) V.Jeyalakshmi, R.Mahalakshmy, K R Krishnamurthy and B.Viswanathan, Titania based catalysts for photoreduction of Carbon dioxide: Role of modifiers, Indian Journal of Chemistry, Section A 41A, 1263 (2012)

7). B.Viswanathan and K R Krishnamurthy, Nitrogen incorporation in TiO2 ¬- Does it make a visible light photo-active material?", International Journal of Photoenergy, Volume 2012 (2012), Article ID 269654, 10 pages; doi:10.1155/2012/269654

8)K.Joseph Anthony Raj, M.G.Prakash, T.Elangovan and B. Viswanathan, Selective hydro-genation of cinnamadehyde over cobalt supported on alumina, silica and titania, Catalysis Letters, 142, Issue 1 87-94 (2012).

9)VenkateswaraRao, C and B.Viswanathan, Microemulsion synthesis and electro-catalytic properties of carbon supported Pd-Co_Au alloy nanopartices, Journal of Colloid and Interface Science, 367, 337-341 (2012).

10)Kaviya, S, Santhanalakshmi, J., and B.Viswanathan, Biosynthesis of silver nano-flakes by CrossandraInfundibuliformis leaf extract, Materials Letters, 67, 64-66 (2012).

11) Kaviya, S, Santhanalakshmi, J., and B.Viswanathan, Green synthesis of silver nanoparticles using polyalthialongifolia leaf extract along with D-Sorbitor: Study of antibacterial activity Journal of Nanotechnology, art No 152970 (2011).

12) Raj, K.J.A., M.G.Prakash, and B.Viswanathan, Selective orthobutylation of phenol over sulfated Fe_2O_3-TiO_2 , Catalysis science and Technology, 1, 1182-1188 (2011)

13) K.J.A.Raj and B.Viswanathan, Synthesis of nickel nanoparticles with fcc and hcp crystal structures, Indian J Chem, 50A,176-179 (2011).

14)Kaviya, S, Santhanalakshmi, J., .Viswanathan,B Muthuswamy, J and Srinivasan,K., Biosynthesis of silver nanoparticles using citrus sinesnsis peel extract and its antibacterial activity, SpectroChimicaActa, Part A, Molecular and biomolecular spectroscopy, 79,594-598 (2011).

15) B.Viswanathan and G.Mahesh, Photocatalytic/electrochemical studies on cadmium stannates for water decomposition and pollution abatement, ACS national meeting book of abstract. : ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY Volume: 241 Meeting Abstract: 12-FUEL Published: MAR 27 2011.

16) Beck A, Mahesh G, Kuppan,B., Shay,Z.,Geszti, O.,Benko,T., Viswanath, R.P., Selvam, P., Viswanathan, B and Guczi,L., specific role of polymorphs of supporting titania in catalytic oxidation of CO,Catalysis Today, 164, 325-331 (2011).[cooperation with Hungarian Academy of Sciences]

17) K J A Raj, M G Prakash, R. Shanmugam, K.R. Krishnaurthy and B. Viswanathan, Surface acidic properties of sulphated Fe_2O_3-TiO_2, Indian J Chem.,50A, 1050-1055 (2011).

18) Du, H.-Y., Wang,C.-H., Hsu,H.-C., Chang,S.-T., Yen,S.-C., Chen L.-C., Viswanathan, B., Chen K.-H., High performance of catalysts by directly grown PTFE free micro-porous CNT layer in a proton exchange membrane fuel cell, Journal of Material Science, 21,2512-2516 (2011).{cooperation with Taiwan]

19) V.Udayakumar, S.Alexander, Gayathri, V, Shivakumaraiah, and B.Viswanathan, Study on the influence of substituents upon the hydrogenation of nitrobenzene using a polymer supported palladium-imidazole complex catalyst, Reaction Kinetics Mechanisms and Catalysis, 103,341-352 (2011).

20) K. Joseph Anthony Raj and B. Viswanathan, Synthesis of cobalt nanoparticles with vegetable oil as the stabilizing agent, Bulletin of the Catalysis Society of India, 10, 1-6 (2011).

21) S.Chandravathanam, B.Viswanathan and T.K.Varadarajan, Effect of citrate on the Pt state of Pt/Carbon black catalyst for methanol electro-Oxidation studies, Science of advanced materials, Vol 3, 1-7 (2011).

22) K.Joseph Antony Raj, M.G. Prakash, T. Elangovan and B. Viswanathan, Liquid phase hydrogenation of p-chloronitrobenzene on cobalt supported on various phases of titania, Bulletin of the Catalysis society of India, 11, 1-12 (2012).

23) K.Premalatha, P.S.Raghavan and B.Viswanathan, Sulpholane – A better co-solvent for the oxidation of benzyl alcohol, Bulletin of the catalysis society of India, 11, 13-21 (2012).

24) G.Deepa, T.M. Sankaranarayanan, K. Shanthi and B. Viswanathan, Hydrodenitrogenation of model N-compounds over NiO-MoO_3 supported on mesoporous materials, Catalysis Today198, 252-262 (2012).[cooperation with Anna University]

25). M. Banu, P. Venuvanalingam, R. Shanmugam, B. Viswanathan, S. Sivasanker, Sorbitol hydrogenolysis over Ni, Pt and Ru supported on Na-Y, TOPICS IN CATALYSIS Volume: 55 Issue: 11-13 Pages: 897-907 DOI: 10.1007/s11244-012-9864-5 [cooperationwithBharathidasan University]

26) Velu Jeyalakshmi , Rajaram Mahalakshmy, Konda Ramaswamy Krishnamurthy and BalasubramanianViswanathan, Sodium tantalate based catalysts for photo-catalytic reduction of carbon dioxide by water under UV-Visible radiation (communicated).

27) K. Joseph Antony Raj, M.G. Prakash, R. Mahalakshmy, T. Elangovan and B. Viswanathan, Liquid phase hydrogenation of nitrobenzene over nickel supported on titania, CHINESE JOURNAL OF

CATALYSIS Volume: 33 Issue: 8 Pages: 1299-1305 DOI: 10.1016/S1872-2067(11)60398-7. [cooperation with Thiagarajar College, Madurai]

28) *K Joseph Antony Raj, T Elangovan and B Viswanathan, Single-step synthesis and structural study of phosphate modified titania through seeding method', Indian J Chem.,51A,676 (2012)..*

29) *Navaladian, S., Viswanathan, B.Synthesis of different architectures like stars, multipods, ellipsoids and spikes of zinc oxide by surfactantless precipitation, Journal of Nanoscience and Nanotechnology 11 (11) , pp. 10219-10226.*

30) *S.Chandravathanam, B.Kavitha, B.Viswanathan and Y.Yesuthangam, Study of sulfonicacid functionalization of Vulcan XC-72 carbon black support of Pt/Vulcan XC-72 catalyst for methanol electro-oxidation Indian Journal of Chemistry A,51A, 704 (2012).*

31) *K.Anthony Joseph Raj, M.G.Prakash, R.Mahalakshmy, T.Elangovan and B.Viswanathan, Selective hydrogenation of acetophenone over nickel supported on titania, Catalysis Science and Technology, DOI: 10.1039/c2cy2013h (2012). [cooperation with Thiagarajar College, Madurai]*

32) *P.Selvam and B.Kuppan, Synthesis, characterization and electro-catalytic properties of nano-platinum-supported mesoporous carbon molecular sieves, Pt/NCCR-41, Catalysis Today, 198,85-91 (2012).*

33). *B.Kuppan and P Selvam, Platinum-supported mesoporous carbon (Pt/CMK-3) as anodic catalyst for direct methanol fuel cell applications: The effect of preparation and deposition method, Progress in Natural Science: Materials International 2012;22(6):616–624.*

34) *K.R.Krishnamurthy and B.Viswanathan, Catalysts for Trans-esterification, Chemical Industry Digest, PP.45, Feb 2013.*

35). *B.Viswanathan, Where does innovation in India fail to transform a viable process? Consulting Ahead, Vol 6,Issue 2, 1-9 (2012).*

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37). *.L.Himakumar, C.V.Rao and B.Viswanathan, Catalytic effect on nitrogen doped grapheme and carbon nanotubes additives on hydrogen storage properties of sodium alanate, J. Mater. Chem. A, 2013, 1, 3355-3361 DOI:10.1039/c0xx00000x*

38)..VenkateswaraRao,C and B.Viswanathan, Microemulsion synthesis and electro-catalytic properties of carbon supported Pd-Co_Au alloy nanopartices, Journal of colloid and Interface Science, 367, 337-341 (2012).

39). .NitulKakati, B.Viswanathan and et al. , Anode catalysis for direct methanol fuel cells in acid medium, chemical Reviews (in Preparation).[coopearation with south Korea]

40. Sankaranarayanan, T.M., M.Banu, Pandurangan and S. Sivasanker, Transesterification of sun flower oil over a solid catalyst, MoO_3 supported on alumina, Appl.Catal., A., 409-410,239-247 (2011).[cooperation with Anna University]

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44.) B.Viswanathan, M.Sankaran, A.Ariharan and KripalLakhi, Hetero atom substituted carbon – potential Hydrogen storage materials, Advanced Porous materials, 1, 122-128 (2013).

45) Carlos Caro, K Thirunavukkarasu, M. Anilkumar, N.R. Shiju and Gadi Rothenberg, Selective auto oxidation of ethanol over titania-supported molybdenum oxide catalysts: structure and reactivity, Advances in synthesis and catalysis, 354, 1327-1336 (2012).[cooperation with the Netherlands]

46)M. Banu, P. Venuvanalingam, R. Shanmugam, B. Viswanathan, S. Sivasanker, Sorbitol hydrogenolysis over Ni, Pt and Ru supported on Na-Y, (Communicated)

47) T.M. Sankaranarayanan, K. Tirunavukkarasu, S. Sivasanker, A. Pandurangam, Transesterification of vegetable oils over spinels (communicated).

48) K. Vijayashanthi, S. Sivasanker, Hydrogenolysis of sorbitol over supported metal catalysts (communicated)

49)Velu Jeyalakshmi ,Rajaram Mahalakshmy, Konda Ramaswamy Krishnamurthy and BalasubramanianViswanathan, Sodium tantalate based catalysts for photo-catalytic reduction of carbon dioxide by water under UV-Visible radiation (communicated).

50)K.R.Krishnamurthy, Sunil Mehla, ShivanandPai; Mathew Jhon; Kishore Kumar; YogeshNiwate;, n-Hexadecane Hydroisomerization over BTMACl / TEABr / MTEABrtemplated ZSM-12, Microporous&Mesoporous Materials (in press) [collaborative work with BPCL and NCCR]

B.Symposia/Conference presentations- (selected ones During1-4-11 to 31-3-2013).

Indian conferences

1. Sankaranarayanan, A.Pandurangan,,K.Thirunavukkarasu, and S.Sivasanker, Transesterification of sun flower oil over supported MoO_3 catalysts -15th national workshop pn the role of new materials in catalysis, NCCR, IITM, December 11-13, 2011.

2. Sankaranarayanan T.M. M.Banu, Pandurangan A and S.Sivasanker, Trans-esterification of triglycerides with alcohols over MoO_3-Al_2O_3 catalysts, 20th National symposium on catalysis for energy conversion and conservation of environment, NCCR, IITM December 19-22 (2010).

3. Sankaranarayan,T.M., Pandurangan A and S.Sivasanker, Hydro-processing of diesel and vegetable oil blends, National conference on advance in Nano-materials in catalysis, Loyola College, December18-19 (2010)

5. The role of material science in modern technology, presentation on 5th April 2013, in Saveetha College of Engineering, Chennai.

6. One dimensional nano materials for electrochemical applications 243rd ACS meeting at San Diego, March 25-29 (2012).

7. One dimensional nanomaaterials of Mo and W for electrocatalysis, at the 21st National symposium on catalysis ".at IICT, Feb 2013)

8. Developments in Fuel cells in sacred heart College, Thirupattur, Feb. 28,2013. "

9. Kuppan, B. Viswanathan, B. Selvam, P. (2008). "'Synthesis of Novel Nanoporous Carbon NCCR-41 NANO-2008, June 1-6, 2008, Rio-de-Janeiro, pp. 370. ",

10. Murthy, PalleR,Dissanayake, Aradhana, Milev, AdriyanKannangara, Kamali, SelvamParasuraman,Chemeca 2012: Quality of life through chemical engineering: 23-26 September 2012, Wellington, New Zealand Glycerol oxidation over nano-gold supported nano-graphite catalysts.

11. Selvam, P. Viswanathan, B. Kuppan, B. (2008). Nanoporous Carbon Supported Platinum (Pt/NCCR-41) Electrocatalyst for Methanol Oxidation, June 11-13, 2008, Porto, pp. 29.

12. Kuppan, B. Viswanathan, B. Selvam, P. (2009). Mesoporous Carbon Nitride Supported Platinum (Pt/NCMK-33) Electrocatalyst for Methanol Oxidation, CATSYMP-19, January 18-21, 2009, Pune, pp. OR-64.

13. Selvam, P. Viswanathan, B. Kuppan, B. (2009) "Platinum supported Nanoporous Carbon / Nitrogen containing Carbon Molecular Sieves: Promising Electrocatalyst for Methanol Fuel Cell Application, ICMAT-2009 - Symposium I, June 28-July 3, 2009, Singapore, pp. 9.

14. Kuppan, B. Viswanathan, B. Selvam, P. (2010). Platinum supported on Ordered Mesoporous Molecular sieves: Promising Electro Catalyst for Direct Methanol Fuel Cell Application, 20th National Symposium on Catalysis, December 19-22, 2010, Chennai, pp. 146.

15. Selvam, P. Viswanathan, B. Kuppan, B. Ramanamurthy, P. (2010). "Synthesis and characterization of gold supported mesoporous carbons, 20th National Symposium on Catalysis for Energy Conversion and Conservation of Environment", December 19-22, 2010, Chennai, pp. 147.

16. Kuppan, B. Viswanathan, B. Selvam, P. (2011). "Platinum supported on Ordered Mesoporous Carbon (Pt/CMK-n; NCCR-n) as Electrocatalyst for Direct Methanol Fuel Cell Applications, 15th National Workshop on the Role of Materials in Catalysis, December 11-13, 2011, Chennai, pp. 93.

17.Kuppan, B. Viswanathan, B. Selvam, P. (2012). "Platinum supported supported Nitrogen-containing Ordered Mesoporous Carbon (NCMK-33) asElectrocatalyst for Direct Methanol Fuel Cells, ACS 243rd National Meeting, March 25-29, Fuel Chemistry Division, San Diego, pp. 751.

18. Selvam, P. and Kuppan, B. (2012). "Platinum-supported Nanoporous Carbon (Pt/CMK-3) as Electrocatalyst for Methanol Fuel Cell, HKICEAS-2012, December 14-16, Hong Kong, pp. 68.

19. V.Jeyalakshmi, R.Mahalakshmy, K.R.KrishnamurthyandB.Viswanathan, Photo catalytic reduction of carbon dioxide by water on La modified sodium tantalate with different co-catalysts under UV-Visible radiation, Abstract submitted for APCAT 6 to be held at Taipai October, 2013.
20. B.Viswanathan, Lecture on Energy for the city science exhibition on 29th January, 2012 (Popular lecture in connection with the annual exhibition of State Council for Science and Technology).

International Conferences

1. 243rd ACS meeting at San Diego (March 2012) 1Dcompounds of Mo/W for electrochemcial applications, B.Viswanathan, J.Rajeswari and P.S.Kishore March (2012).

2. 241st ACS meeting at Anaheim (March 2011) The following presentations were made

   (i) Synthesis of O-isopropylidene derivatives from D-glucose using sulphated metal oxides by B Viswanathan, S Anuradha, and P Selvam,

   (ii) Photocatalytic activity of mesoporoustitania, byB.Viswanathan, A.Alagarasi and P Selvam

   (iii) Photocatalytic/electrochemical studies on Cadmium stannates for water decomposition and pollution abatement by B.Viswanathan and G.Mahesh

   (iv) Photo-electrochemical decomposition of water- selection of materials

3. 15th ICC was attended (in July 2012) by Professor S Sivasanker and B Viswanathan and presented one oral presentation and one poster presentation as follows

   (1) Transesterification of vegetable oils with methanol over spinels by T.M.Sankaranarayanan, B.Viswanathan, S.Sivasanker and A PanduranganI (poster)

   (2) Hydrogenolysis of sorbitol over supported metal catalysts, M Banu, B.Viswanathan, S.Sivasanker and P.Venuvanalingam (oral).

C. Contributions as book-chapters:

1. P.Selvam and A.Sakthivel "'Selective catalytic oxidation over ordered nanoporousmetallo-aluminophosphates in liquid phase oxidation in heterogeneous catalysis: Organic synthesis and applicaions, edited by M G Clerici and O.A.Kholdeeva Johan Wiley and Sons, 2013 pp.95-125 "
2. Selvam P and B.Kuppan "'Ordered mesoporous carbon and their applicaitons in direct methanol fuel cells, Micro and nano engineering of fuel cells (Ed Dennis Leung) CRC press in press ",
3. B. Viswanathan, Electro-catalytic reduction of carbon dioxide, chapter 11, New and future developments in catalysis, Edited by Prof Steven Suib, Elsevier, (in press).
4. M. AuliceScibioh and B. Viswanathan, The status of catalysts in PEMFC technology, chapter 9 "Catalysis for Alternative Energy Generation", Edited by L Guczi and A.Erdohelyi, Springer 2012.
5. B. Viswanathan, Electro-catalytic and electro-chemical applications of poly-oxo-metalates, a Chapter in the book edited by Anjali Patel, MS University, Baroda, Springer (in press).
6. V. Jeyalakshmi, R .Mahalakshmy, K R Krishnamurthy and B. Viswanathan, Photocatalytic reduction of carbon dioxide by water:- a step towards sustainable chemicals and fuels, Materials Science Forum, (Editor Rajesh J.Tayade) 734 pp. 1-62 (2013).
7. York Smith, R. Subrahmanian and B. Viswanathan, Photo-electrochemical and photocatalytic conversion of carbon dioxide – chapter 9 in Photo-electrochemistry and photo-biology for the sustainability, (Eds.S.Kaneco, B. Viswanathan and H .Katsumata, pp 217-242 (2010).
8. Vandavir, M, Lee,S., Viswanathan B, Subramanian, V, Harvesting solar energy using inexpensive and benign materials, Ed. Chen W.Y., Seiner, J., Suzuki T, and Lackner, M., Springer Publications, Amsterdam, 2012. [cooperation with the University of Nevada}

D. Books Prepared during this period

1. B.Viswanathan and M AuliceScibioh, Photoelectro-chemistry, Principles and Practice, Narosa Publishing House, (In press).
2. Kirpal Singh and B.Viswanathan, Chemical engineering A comprehensive Approach, Narosa Publishing House, (In press).
3. S.Kaneco, B.Viswanathan and H.Katsumata, Photoelectrochemistry and Photo biology for the Sustainability, Union press (2012).
4. B.Viswanathan, Thermal methods – Application to Catalysis-Monograph under preparation.

V.Augmentation of research facilities

The new analytical and other facilities added to the Centre in this period are listed below.

1) Transmission Electron Microscope

2) High pressure adsorption measurement unit

3) Low pressure micro reactor

4) Solar simulator

5) Electrochemical analyzer

6) Attachment for autoclaves for high temperature operation

7) Gas chromatographs-2

8) Gas analyzers

VI. Future plans

1. Fundamental Research

(a) Establishing the surface properties necessary for the activation of di-nitrogen and carbon dioxide at ambient conditions

(b) To formulate native non-native configuration as the possible reason for the surface reactivity (Theory)

(c) Core shell configurations its relevance in catalysis and the universality of this concept.(Theory)

(d) Bio-mass conversion to bio-fuels. The work will concentrate on lignocellulosic materials and algal oils

(e) Formulation and design of new semiconducting materials for hydrogen production from the photo-catalytic and photo-electrochemical decomposition of water.

(f) Hydrogen storage on variety of carbon materials like carbon from natural sources, nano-porous carbons and heteroatom substituted carbon (Both theory and experiment)

[All others are experimental based development]

2. Applied Research

(a) To respond to the needs of energy conversion processes for oil industry, like end point reduction, development of appropriate functional catalysts so as to improve fuel value of the feedstock.

(b) To develop high throughput catalysts so as to meet the future demands of chemical and oil processing industries.

(c) To formulate synthesis procedures for textured materials as required by the industry

(d) To exploit the newer nano-porous materials both carbon and oxide materials for appropriate catalytic applications.

3. On Human resource development activity

(a) NCCR will come up in addition to the Orientation program in catalysis, and other short courses new short courses on emerging areas of research like catalysis for energy conversion (both conventional and non-conventional), Catalysts for environmental protection, and other developments in the formulation of new catalyst systems.

(b) NCCR will evolve and strengthen its on line courses and lectures that they have initiated in the last two years

(c) NCCR will also come out state of art documents on various newer aspects of catalysis and also bring out appropriate monographs.

VII Other activities

A. Service to other institutions and training of students

1. NCCR has carried analytical services to many organizations for XPS, DRS, TPR, UV-Vis, XRF, and many other testing services. The total number will be over 1000 during this period. All these services are done free of charge to both academic and other organizations. The centre also has extended the analytical services to other departments in IIT, like chemical, civil, biotechnology, Physics and Chemistry departments. These services have been extended to other countries as well like the Netherlands, Australia, USA and a few other laboratories in the world.

2. In addition to the courses conducted by NCCR, it has provided academic input for various research scholars and other graduate students in nearby academic institutions. There will be around a hundred persons who would have benefitted by such an endeavor.

3. Ms. B. Kavitha, a MSc student of Periakulam did her master project work in the Centre during the summer of 2011.

4. The members of NCCR have participated in various short courses conducted by University of Madras, Anna University and a few other institutions in Tamil Nadu.

B. Catalysis Data Base

NCCR is maintaining a web site for the use by the catalysis community. The online service (Electronic Publishing Trust for Development)has considered this web site and came up with a write-up which is reproduced below to demonstrate the utility of the web site created by NCCR**.**

Monday, 1 August 2011

One man went to work* – a catalytic converter

News of a recently registered institutional repository (IR) has emerged. Called Catalysis Database, it uses the Eprints software and can be accessed at http://203.199.213.48/. It is hosted by the National Center for Catalysis Research (NCCR) at the Department of Chemistry, Indian Institute of Technology, Madras (IITM), and contains published research articles, unpublished concept articles, theses, reports, working papers, teaching resources and much more. There are currently over 1740 items archived, and the remarkable point to note is that this effort has been driven by a

single man, Professor B Viswanathan, and follows from his attendance at an open access workshop organized by EPT Trustee Professor Subbiah Arunachalam.

The professor has acknowledged that it would not have been possible without the help of a young IITM undergraduate student(Venkatasubramanian Viswanathan) with computer skills, who was able to set up the repository 'within days or hours' and who still helps resolve any technical problems that arise, 'though now working in the USA. But it is clear that the driving force was a single person who had the vision and open mind to understand the concept of open access as presented at a workshop, and to see the vast potential of such a repository. Most of the deposit of material has been carried out by Viswanathan himself as he found there were many inaccuracies when carried out direct by the authors, leading to failed searches. He has received no direct input from his institution, apart from registration of the domain name, carrying out the work himself. He describes the repository as an education and knowledge resource for catalysis since it also includes book chapters and other material of general relevance to this discipline.

And the cost? The server was purchased by the Catalysis Society of India for hosting its online journal and other catalysis purposes. The Institute covers the costs of direct online access and maintenances. Viswathan says, 'I would not say the cost was free, but hidden' as he was able to take advantage of the spare capacity within the ICT facilities at his institute. Since the resource is also a major contribution to his own work in many ways – allowing download of data in response to student class queries, for example - the time he exerted was also in the interest of the NCCR and part of his regular teaching and research work in the catalysis field.

He reports that the IR is used extensively on a global basis, and describes how he himself was able to prepare a lecture at short notice by downloading much information from the IR while attending an American Chemical Society meeting in March 2011. He had been ill-informed about his role as a main speaker, discovering the error only on the conference notice board on arrival.

It is good to know that he has benefited himself from his own efforts, but the value of the resource to the science of catalysis must be very substantial. One man and a student from the NCCR institute have achieved a catalytic impact on their discipline, though it is surely unlikely that the effort has left the 'agent' unchanged.

Our congratulations to Professor Viswanathan and the NCCR student – we hope all catalysis researchers appreciate their good fortune.

***Counting Nursery Song, 'One man went to mow'** - http://www.youtube.com/watch?v=h1TD95M8Fe4

Posted by Electronic Publishing Trust for Development

C.Catalysis Society of India

Contributions to the National Society – The Catalysis Society of India

The Centre is the head-quarters of the Catalysis Society of India. The following are the activities of the catalysis society of India during this period under review (mainly contributed by the members of NCCR)

1. On behalf of the Society, NCCR conducted the 19th National Symposium on catalysis and also the 15th National work shop on catalysis during December 2010 and 2011 respectively.
2. The Volume 10, 11 and 12 of the Bulletin of the Catalysis Society of India were brought out during this period.
3. The members of NCCR have contributed both academically and administratively to the awards of the Society for this period.
4. The administrative day to day functions of the Society and the finances of the Society were maintained by the members of NCCR during this period.
5. The members of NCCR have also contributed to forge links with other international societies and they also represent India in the International Congress on Catalysis and Asian Catalysis Congress.

ANNEXURES

Annexure 1

1. Personnel at NCCR

The following are directly working in NCCR at this point of time. (In addition there are a number of research fellows and students from other institutions who spend time in the Centre for various research activities)

1.B.Viswanathan
2.Professor Dr. P.Selvam
2.Prof.S.Sivasanker (Chair Professor)
3.Prof.K.R.Krishnamurthy (Chair Professor)
4.Dr.K.Thirunavukarasu (Research officer)
5.Mr B.Kuppan (Senior Research Fellow; MNRE)
6.Mr.Vamsi Krishna Senior Research Fellow; DST
7.Mr.P.Ramanamurthy Senior Research Fellow Institute
8.Mr.Anil Kumar Senior Research Fellow Institute
9.Mr.K.Suthagar Senior Research Fellow CSIR
10.Mr.S.Mahendran Senior Research Fellow Instittute
11.Ms.A.Alagarasi Senior Research Fellow
12.Mr.Sourav Khan Senior Research Fellow
13.Mr.P.Rajesh Kumar Research Fellow
14.Mr.Sanjeev Gupta Research Fellow
15.Mr.T.V.Ramamohan Research Fellow
16.Mr.Rajasekar Research Fellow

17.Mr.G.Prakash Senior Research Fellow CSIR
18.Mr.R.Shamugam Senior Research Fellow CSIR
19.Mr.A.Ariharan Senior Research Fellow MNRE
20.Ms.V.Jeyalakshmi Senior Research Fellow HPCL
21.Ms.Vijay Shanthi Senior Research Fellow
22.Ms.S.Lalitha Senior Research Fellow DST
23.Ms.A.Saranya Senior Research Fellow, Shell
24.Ms.K.Selvi Senior Research Fellow, NFCL
25.Ms.M.G.Meera Research Fellow
26.Mr.P.Jeyachandran Research Fellow, NFCL
27.Ms.G.Keerthiga Senior Research Fellow IOCL
Faculty from other departments associated with the centre.
1. Prof. Anju Chadha Department of Biotechnology
2. Prof G Ranga Rao Department of Chemistry
3. Prof. Debasgis Chakrabty, Department of Chemistry
4. Prof. Raghuram Chetty, Department of Chemical Engineering
5. Prof. Preeti, Department of Chemical Engineering
6. Prof. Ramnarayanan, Department of Chemical Engineering
7. Prof. K. Shanthi, Anna University
8. Prof. Kothandaraman, Department of Chemistry

Annexure.2

2.Names of participants of 13th Orientation course in catalysis

	Name	Institution
1	Pramod Dagajirao Patil	ICT, Mumbai
2	Rasal Kalidass B	ICT, Mumbai
3	Gawade Anil	ICT, Mumbai
4	Nilesh M Patil	ICT, Mumbai
5	Fr Theophil Anand	Sacred Heart College
6	Sr E.D.Sherley	Loyola College
7	C.Pasupathi	Loyola College
8	Fr P Suresh	Loyola College
9	Shivaji Bhanawase	ICT, Mumbai
10	Gunjam Deshmukh	ICT, Mumbai
11	Janardhan H.L.	PPIST, Bangalore
12	Priti Shrivastava	Devi Ahilya Univ
13	KamleshTayade	DDU, Nadiad
14	Debajyoti Bhattacharhee	Tezpur Univ
15	Dipshikha Bhstssli	Tezpur Univ
16	Rupesh Singh	IITK
17	Chandra Mohan	Anna Univ
18	S.Pitchaimuthu	AJA College
19	Atul S Nagpure	NCL
20	Hanmant R Gurau	NCL
21	Jayaram Moileti	ICT, Mumbai
22	Vilas Venunath Patil	ICT, Mumbai

23	Jeevan M Bhojane	ICT, Mumbai
24	Manohar A Bhosale	ICT, Mumbai
25	Sachin A Sarode	ICT, Mumbai
26	A.Saranya	NCCR
27	K.Selvi	NCCR
28	Jeyachandran	NCCR
29	Rajesh Kumar P	NCCR
30	Rajesh Khanna	Chemistry, IITM
31	Ms ShekeelaKhan	Chemistry, IITM
32	Kishore Wage	ICT
33	Silpi	IITK
34	Umesh Babu	
35	Hitesh	ICT,Mumbai
36	Kamalesh Tayade	ICT
37	Nithiya Arjunan	BIT
38	Mr Raghupathy	Loyola
39	Mr Jayaram Molleti	ICT
40	Mr Abhilash Sukhadeve	ICT
41	Mr Sandip T.Gadge	ICT
42	Sanmay Varma	
43	Soumya Gopi	
44	Deepak Nale	NCL

Annexure.3

3. Names of participants in special course on photo-electrocatalysis

	Name	Institution
1	A.Manikandan	IIT-H
2	Ajay Chahal	NCCR
3	Daya Mani Allumolu	IIT-H
4	Dr.L.J.Kennedy	Sacred Heart
5	Fr Theophil Anand	Loyola college
6	Mr Clement	Loyola college
7	Mr Harishankar	NCCR,IITM
8	Mr. Amal PradeepIITK	IITK
9	Mr. B.Dilip Kumar	IITK
10	Mr. C. Raghupathi	Loyola college
11	Mr. Deb Sankar De	IITK
12	Mr. Gyan Prakash	IITK
13	Mr. K.Kishor	IITK
14	Mr. Myilsamy	Anna Univ
15	Mr. R. Babu	Anna
16	Mr. Rajesh Khanna	IITM
17	Mr. Rokesh Karuppanan	
18	Mr. S.Chandra Mohan	Anna
19	Mr. S.Narayanan	Loyola college
20	Mr. S.Prabhu	Loyola College
21	Mr. Sajid Magal	Bharathiar Univ
22	Mr. Shaji Vaghese	
23	Mr. Sulay Saha	IITK
24	Mr. Thinesh Kumar	Loyola college
25	Mr. Vijaykumar Marakatti	PPST
26	Mr.T.Adinaveen	IITK
27	Ms Gopa Mishra	IIT H
28	Ms Lognamayee	IMMT

	Mohapatra	
29	Ms Udaya Aruldoss	Anna University
30	Ms. A. Daya Mani	VIT Chennai
31	Ms. E. Kavery	Anna Trichi
32	Rokesh K	IITM
33	S.Narayanan	IMMT
34	S.Prabhu	Loyola College
35	Santosh Kumar	Loyola College
36	Sowmyashree	
37	Sr.E D Sherly	Loyola college
38	Ushodaya	Anna University
39	Vichunath	Poornaprajgna
40	Vijay	Loyola college