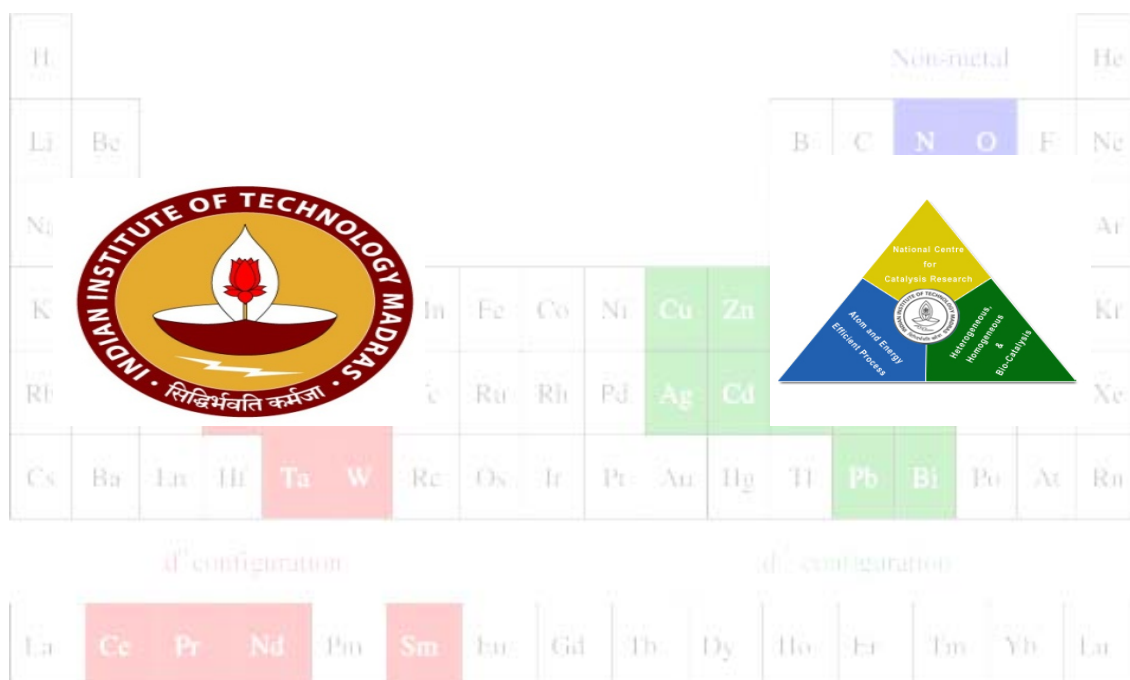


# NATIONAL CENTRE FOR CATALYSIS RESEARCH

Indian Institute of Technology - Madras



The image shows a periodic table with several elements highlighted in colored boxes. The highlighted elements are: N, O, Cu, Zn, Ag, Cd, Ta, W, Pb, Bi, Po, Ce, Pr, Nd, Pm, and Sm. The IIT Madras logo is on the left, and the NCCR logo is on the right. The NCCR logo is a triangle with three sections: yellow (top) for 'National Centre for Catalysis Research', blue (bottom left) for 'Atoms and Energy Efficient Process', and green (bottom right) for 'Heterogeneous Homogeneous & Biocatalysis'. Below the main table, there are two rows of lanthanide and actinide elements, with 'd configuration' written above them. The lanthanide row highlights Ce, Pr, Nd, Pm, and Sm. The actinide row highlights Pu and Am.

H																	He
Li	Be											B	C	N	O	F	Ne
Ni																	Ar
K			In	Fe	Co	Ni	Cu	Zn									Kr
Rb			Sn	Ru	Rh	Pd	Ag	Cd									Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
d configuration								d configuration									
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Th	Dy	Ho	Er	Tm	Yb	Lu			

*Fifth Annual Day – 2011 (Saturday, 30<sup>th</sup> July)*

*At*

*M V C Sastri Hall, NCCR, IITM*

## PREFACE

The National centre for catalysis Research was established in Indian Institute of Technology, Madras by the Department of Science and Technology, Government of India in July 2006. The centre has completed five years of its existence. During the five year period the centre has carried out the following activities in essence:

1. Conducting orientation programme in catalysis for research scholars of this country every year
2. Carrying out research in some frontier areas.
3. Has facilitated the educational programmes of sister institutions in variety of ways including housing some of the research scholars in NCCR
4. Establishing international collaborations with a variety of organizations
5. Creating and maintaining data base and also bringing out variety of text books, monographs and other educational materials.

These are only indications and if any one of you wish to know the full range of activities of the centre they are kindly requested to visit our data base and download the document of our report.

We do realize that we can do better in many other spheres and this will be possible only when our fellow scientists of this country can kindly indicate and demand from NCCR.

This research scholars meet is routine one usually conducted in the last week of July every year in the last five years with the participation from our neighbouring institutions like Anna and Madras University and it is our desire to expand this to neighbouring cities. We are also in a position to broadcast some of the presentations in other institutions if they have the simple facilities for projection. This possibility can be exploited by all of us to our mutual benefit.

Our colleagues who have left NCCR in the past five years have done a great service to us and it is our duty to thank them all on this day.

NCCR wishes to place on record its grateful thanks to all those who have helped in building this centre in the formative five years.

NCCR will also be grateful for any feedback any one of us can offer and it is assured that every feedback will be carefully examined and implemented to the extent possible.

30<sup>th</sup> July 2011

Present Members of NCCR

**PROGRAMME FOR THE 5<sup>TH</sup> ANNUAL DAY ON 30<sup>TH</sup> JULY 2011**

<b>TIME</b>	<b>NAME OF THE SPEAKER</b>	<b>TITLE</b>
09.00-09.20	Prof Dr S Sivasanker	Inaugural Address
09.20-09-40	Dr L Himakumar, OSU, USA	Ammonia Borane - synthesis properties and applications.
09.40-10.00	Ms Jeyalakshmi	Photocatalysis by modified titania
10.00-10.20	Mr S Naidu	Hybrid materials and their applications with G Ranga Rao
10.20-10.40	Ms.G.Keerthiga	Electroreduction of carbon dioxide to hydrocarbons on copper electrodes
10.40 -11.10	Break and poster	Poster
11.10-11.40	Prof R Kothandaraman	CH <sub>3</sub> OH oxidation activities of an unsupported Pt <sub>x</sub> Ru <sub>y</sub> powder catalyst before and after different electrochemical treatments with C. Bock, and B. MacDougall
11.40-12.00	Mr T M Sankaranarayanan	Transesterification of triglycerides with alcohols over MoO <sub>3</sub> – Al <sub>2</sub> O <sub>3</sub> catalysts with A Pandurangan and S Sivasanker
12.00-12.20	Ms R Vijayashanthi	Acylation of anisole with n-dodecanoic acid over Zeolite beta
12.20-12.40	Prof R Ramnaryanan	Not another research talk
12.40-12.50	Prof K R Krishnamurthy	Concluding remarks

The background image shows a portion of the periodic table with d-orbital configurations highlighted. The d<sup>0</sup> configuration is highlighted in red, and the d<sup>10</sup> configuration is highlighted in green. The elements shown include Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, and the lanthanide series (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu).

## 5<sup>th</sup> Annual day 30<sup>th</sup> July 2011 List of participants and other details.

S.No	Name and organisation	Oral	Poster	Participate	Initial
1	B.Viswanathan	No	No	Yes	
2	Mr Vamshi Krishna	No	No	Yes	
3	Ms V Jeyalakshmi	Yes	No	Yes	
4	Ms G Keerthiga	yes	No	yes	
5	Ms Alagarasi	No	No	yes	
6	Mr R Shanmugam	No	No	yes	
7	Mr Ariharan	No	No	yes	
8	Mr Mahendran	No	No	yes	
9	Dr Himakumar FROM USA	net	No	No	
10	Prof K R Krishnamurthy	No	No	yes	
11	Prof S Sivasanker	yes	No	yes	
12	K. Thirunavukkarasu	No	No	Yes	
13	M G Prakash	No	No	yes	
14	P.Ramanamurthy	No	No	Yes	
15	P.Pachamuthu	No	No	yes	
16	Sourav Khan	No	No	yes	
17	Dr S Parimala	No	No	yes	
18	Dr D Naresh	No	No	yes	
19	Ms Vijaya Shanthi	No	No	yes	
20	Ms G Deepa	No	No	yes	
21	Ms M Banu	No	No	No	
22	Mr T V Ramamohan	No	No	yes	
23	Prof A Pandurangan ,Anna U	No	Yes	Yes	
24	Mr Anil kumar	No	No	Yes	
25	Mr Satya Chinnama Naidu	Yes	No	yes	
26	Prof G Ranga Rao, Chy	No	No	yes	
27	Prof GRR student1	No	No	yes	
28	Prof GRR student2	No	No	yes	
29	Prof GRR student3	No	No	yes	
30	Prof GRR student4	No	No	yes	
31	K Suthagar	No	No	yes	
32	Mr Santharaj. D Anna Uni	No	No	Yes	
33	Mr Selvaraj. M Anna Uni	No	No	Yes	
34	Mr Selvamani. A Anna Uni	No	No	Yes	
35	Mr Suresh. C Anna Uni	No	No	Yes	
36	Dr R Kothandaraman Chy	Yes	No	Yes	
37	Prof R Ramnarayanan Ch E	yes	No	Yes/No	
38	Prof P Selvam	NA	NA	NA	
39	Mr. Anthuvan Rajesh Anna U	No	Yes	Yes	
40	Mr. G.Karthikeyan,Anna	No	Yes	Yes	
41	Mr J Balamurugan, Anna	No	Yes	Yes	
42	Ms Shrine Maria Nithya,J	No	Yes	Yes	
43	Mr T M Sangaranarayanan	Yes	No	Yes	
44	Malarvizhi Naganathan,Anna	No	Yes	Yes	

## HYBRID MATERIALS AND THEIR APPLICATIONS

Satya Chinnama Naidu and G. Ranga Rao

Department of Chemistry, IIT Madras

Synthesis and application of new type of hybrid materials based on ionic liquid and heteropoly acid are interesting areas of research. These hybrid materials are effective for carrying out organic conversions like esterification, epoxidation and lactonization and involve the peroxo bridging bond between atoms like W or Mo. There is good example of using these hybrid materials for ascorbic acid oxidation. They also act as fast proton conductors and solid electrolytes. Some of these aspects will be presented.

H																			Non-metal	He		
Li	Be											B	C	N	O	F	Ne					
Na	Mg											Al	Si	P	S	Cl	Ar					
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr					
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe					
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn					
			$d^f$ configuration										$d^f$ configuration									
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Th	Dy	Ho	Er	Tm	Yb	Lu								

# CH<sub>3</sub>OH oxidation activities of an unsupported Pt<sub>x</sub>Ru<sub>y</sub> powder catalyst before and after different electrochemical treatments

R. Kothandaraman<sup>a</sup>, C. Bock<sup>b</sup>, and B. MacDougall<sup>b</sup>

<sup>a</sup>Indian Institute of Technology Madras, Chennai 600036, India

<sup>b</sup>Institute for Chemical Process and Environmental Technology, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada

An unsupported Pt<sub>75</sub>Ru<sub>25</sub> powder was synthesized by co-reducing the corresponding precursor salts rapidly. An alloy powder of Pt<sub>75</sub>Ru<sub>25</sub> composition was formed in this manner. The catalyst powders were subjected to various electrochemical treatments in either 0.5 M H<sub>2</sub>SO<sub>4</sub> or 0.5 M CH<sub>3</sub>OH + 0.5 M H<sub>2</sub>SO<sub>4</sub> solutions. Applying specific electrochemical treatments in respect to time (e.g., the potential cycling number) relative to the E+ value result in either a decrease or increase in the CH<sub>3</sub>OH oxidation activity of this catalyst. The differently treated catalyst powders were further studied using EDX, XPS and CO adsorbed (CO<sub>ads</sub>) stripping voltamograms and transients. The results suggest that removal of surface Ru-oxides result in an increase in CH<sub>3</sub>OH electro-oxidation activity, while extensive loss of Ru from the catalyst surface results in a decrease in CH<sub>3</sub>OH oxidation activity. Refluxing this as-prepared catalyst powder in an excess of boiling 0.5 M H<sub>2</sub>SO<sub>4</sub> did neither result in the removal of the surface Ru-oxides nor improve the CH<sub>3</sub>OH oxidation activity.

H																	He	
Li	Be																F	Ne
Na	Mg																Cl	Ar
K	Ca																Br	Kr
Rb	Sr																I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
d configuration													d configuration					
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				



## Acylation of anisole with n-dodecanoic acid over zeolite beta

C. Dhoke, R. Vijayashanthi, S. Sivasanker

NCCR, IIT-M, Chennai – 600 036

Friedel-Crafts acylation of aromatic compounds is used in the production of many pharmaceutical, agrochemical, and fragrance compounds. The present industrial practice involves the use of stoichiometric (or more) amounts of metal halides (Lewis acids, like  $\text{AlCl}_3$ ,  $\text{FeCl}_3$ ) as the catalysts and acyl chlorides as acylating agents, which results in substantial by-product formation besides operational difficulties due to the corrosive nature of the acids and halides. To eliminate corrosion and environmental problems, the replacement of the conventional mineral acids by solid acid catalysts has become a necessity. There are many types of solid acids, such as zeolites, heteropolyacids, sulfonated resins and sulfated metal oxides that possess different acidities.

In this work, the Friedel-Crafts acylation of anisole with a long chain carboxylic acid (lauric acid) over zeolite beta (BEA) and its modified forms is reported. The  $\text{SiO}_2/\text{Al}_2\text{O}_3$  ratio (SAR = 25) of the parent BEA was altered by dealumination with  $\text{HNO}_3$  and by desilication with tetrapropyl ammonium hydroxide (TPAOH). The parent  $\text{NH}_4$ -form of the zeolite was also ion-exchanged with  $\text{Ce}^{3+}$ ,  $\text{Zn}^{2+}$  and  $\text{Fe}^{3+}$  - ions, and the samples used in the acylation reaction. The parent beta and the modified samples were characterized by powder X-ray diffraction (XRD),  $\text{N}_2$  adsorption and temperature programmed desorption (TPD) of ammonia. XRD results showed that the BEA structure was maintained after the various treatments. The Friedel-Crafts acylation of anisole with lauric acid was carried out at  $155^\circ\text{C}$  and atmospheric pressure in two necked RB flask under reflux conditions. Gas Chromatographic analysis of the products revealed the formation of mainly the para isomer of the ketone a [1-(4-methoxyphenyl)dodecane-1-one] as the product. The o- and m- isomers were formed in much smaller amounts. The by-products of the reaction were small amounts of phenol, methanol and esters. While mild dealumination increased the activity, severe dealumination decreased the activity. Similarly, desilication and ion-exchange treatments also increased the activity of the zeolite. The activity was highest for Zn-exchanged BEA. Likely reasons for the observed changes in activity on dealumination, desilication and ion-exchange treatments are presented.



# Photocatalysis by modified Titania

V. Jeyalakshmi

National Centre for Catalysis Research, IITM, Chennai 600 036

Titania as an effective photocatalyst has been extensively studied, due to its stable chemical structure, biocompatibility, physical, optical and electrical properties. One of the drawbacks that limit its application in the visible region is its inherent bandgap energy, that makes it active in UV region only. In order to extend the light absorption beyond UV region, modification of titania with metals, non-metals and metal oxides have been attempted that alter its energy level characteristics. An account of studies on such modifications of titania and its effects on photo-physical properties and activity will be discussed.

## Reference:

1. Amy L. Linsebigler, Guangquan Lu, and John T. Yates, Jr, *Chem. Rev.*, **1995**, *95*, 735-758
2. Tracy L. Thompson and John T. Yates, Jr, *Chem. Rev.*, **2006**, *106*, 4428-4453.
3. Umar Ibrahim Gaya, Abdul Halim Abdullah, *Journal of Photochemistry and Photobiology C: Photochemistry Reviews*, **2008**, *9*, 1-12.
4. Pengfei Ji, Masato Takeuchi, Tran-Manh Cuong, Jinlong Zhang, Masaya Matsuoka, Masakazu Anpo, *Res, Chem Intermed*, **2010** *36*:327-347.
5. Ying Yang, Hui Zhong, Congxue Tian, *Res Chem Intermed*, **2011** *37*:91-102.
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# Electroreduction of CO<sub>2</sub> to hydrocarbons on Cu electrode

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National Centre for Catalysis Research, and

Department of Chemical Engineering, IITM, Chennai 600 036

Globally, environmental problems due to greenhouse gases are ought to be mainly caused by CO<sub>2</sub>. Nevertheless, CO<sub>2</sub> is an abundant raw material for the production of value added chemicals. Among the numerous methods available for its utilization, electrochemical method appears to be promising in activating and building of CO<sub>2</sub> to hydrocarbons. The reaction rate and the products formed are dependent on several variables, such as the type of working electrode, potential applied, type and concentration of the electrolyte, pH, mass transport effects and purity of reactants. Hence, to start with, the electro reduction of CO<sub>2</sub> was studied in KCl and KHCO<sub>3</sub> as the supporting electrolyte on Cu electrode and the faradaic efficiency of the products were estimated. Ethane and methane is the major product formed when the potential was varied form -0.9 to -2 V vs. Ag/AgCl electrode. Ethane was likely to be formed in KCl while methane was observed in the rest. The reduction of CO<sub>2</sub> in KCl medium yields higher efficiency than compared with KHCO<sub>3</sub> motivates to look deeper into its kinetics.

Rh	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

d<sup>0</sup> configuration

d<sup>10</sup> configuration

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
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# HYBRID MATERIALS AND THEIR APPLICATIONS Ammonia borane – Synthesis, Properties and Applications

**Dr. Hima Kumar Lingam**

Postdoctoral Researcher

Department Of Chemistry, The Ohio State University

Columbus OH 43220

H	Non-metal																He
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Ammonia borane a Lewis acid-base adduct with both protic N-H and hydridic B-H bonds is a potential material with broad range of properties. The properties and synthetic utility of various amine-borane complexes have been adopted and exploited in various applications. In the recent years it has been considered as potential candidate for hydrogen storage applications because of its low molecular weight and high gravimetric, volumetric energy densities. In this perspective synthesis, properties and applications of ammonia borane will be discussed in the presentation.

Reference:

1. S. G. Shore and R. W. Parry, *Journal of American Chemical Society*, **77**, 1955, 6084
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4. D.J. Heldebrant, A. Karkamkar, J.C. Linehan and T.Autrey, *Energy & Environmental Science*, **1**, 2008, 156.