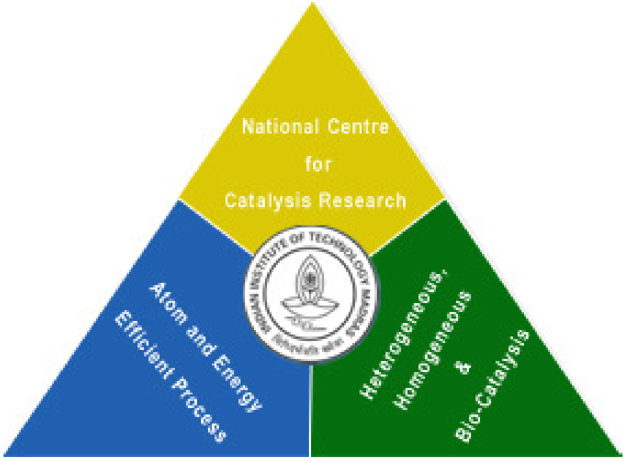
NATIONAL CENTRE FOR CATALYSIS RESEARCH
INDIAN INSTITUTE OF TECHNOLOGY
4TH ANNUAL DAY (1ST AUGUST 2010)



Programme
&
Abstracts of the presentations
M V C SASTRI HALLL
(9.00 a.m. to 12.45 p.m.)

PROGRAMME FOR THE ANNUAL DAY ON 1ST August 2010

9.00 to 9.10 am	Introduction	Prof S Sivasanker
9.10 to 9.30 am	Presentation I	Mr.Vamsi Krishna
9.30to 9.50 am	Presentation II	
9.50 to 10.10 am	Presentation III	Ms A.Alagarasi
10.10 to 10.40am	Special presentation	Dr Sathish (on line)
10.40 to 11.00am	Coffee Break	
11.00 to11.20 am	Presentation IV	
11.20 to 11.40am	Presentations V	Mr.P.Ramanamurthy
11.40 to12.00 am	Presentation VI	Ms.M.Banu
12 to12.20 noon	Presentation VII	Ms.V.Anadha Kiruba
12.20 to 12.40pm	Presentation VIII	
12.45 pm	LUNCH	

Synthesis and Characterization of Novel Mesoporous Silicates

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Mesoporous molecular sieves are special class of materials with ordered arrays of uniform pores, high surface areas and large pore volumes. These periodic silica/silica-based materials are promising for variety applications including catalysis, adsorption and separation processes [1,2]. Two most common types involve MCM-41 and SBA-15 has ordered structures consisting of two dimensional hexagonal arrays of uniform mesoporous. SBA-15 materials have been prepared in acidic conditions with poly (alkylene oxide) tri-block co-polymer (Pluronic P-123) as template. SBA-15, which possesses larger pores, thicker walls and higher thermal stability as compared other mesoporous silicas including MCM-41 [3]. However, it is of interest to make materials with a combination of moderate pore size and thicker wall structure. Therefore, in this investigation, an attempt has been made to prepare materials with desired characteristics using oligomeric alkyl poly ethylene oxide (Brij-56) surfactant template. We report here, for the first time, a novel mesoporous silicate material, designated as IITM-56, with a (moderate) pore size of 38.4 Å and a wall thickness of 21 Å. Fig. 1 depicts the XRD pattern of IITM-56 which is typical characteristics of MCM-41/SBA-15 type structure. TG studies of IITM-56 show a 47 % weight loss in conjunction with exothermic transition (DTA) suggestive of mesoporous nature of the material [4]. This further confirmed by N_2 sorption measurements (Fig.3), which indicate type IV isotherm with capillary condensation at 0.3-0.4 (P/P_o).

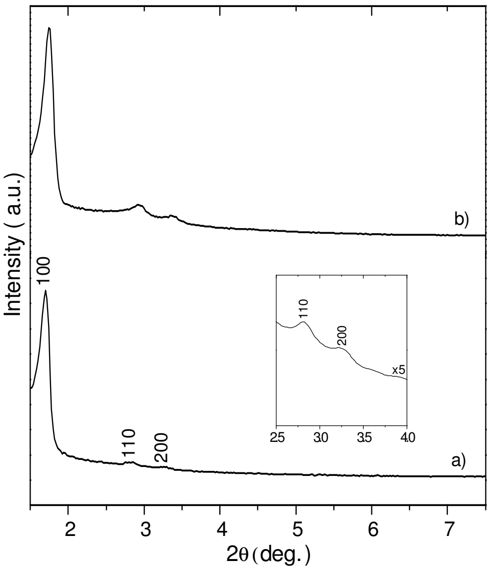

Fig.1. XRD patterns of IITM-56:
a) Synthesized; b) Calcined.

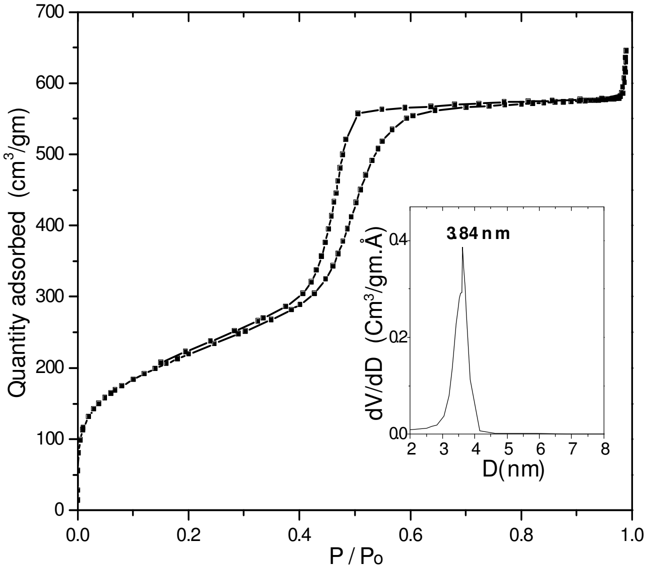

Fig.2. N_2 sorption isotherm and pore size distribution of IITM-56.

REFRENCES

[1] Selvam, P.; Bhatia, S.K.; Sonwane, C.G. *Ind. Eng. Chem. Res.* 40, *2001,* 3237.
[2] Taguchi, A.; Schuth, F. *Micropor. Mesopor. Mater.* 77, *2005*, 1.
[3] Zhao, D.; Huo, Q.; Feng, J.; Chmelka, B. F.; Stucky G. D. *J. Am. Chem. Soc.* 120, *1998*, 6024.
[4] Kruk, M.; Jaroniec, M. *Chem. Mater.* 12, *2000*, 1961.

Synthesis and Characterization of Ordered Mesoporous Titania and Alumina

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Ordered mesoporous siliceous materials are extensively studied in recent years, and this generated considerable interest on mesoporous metal oxides because of their potential application in the fields of catalysis, separation technology, polymerization and nano electronics. Among the various metal oxides, the mesoporous titania (TiO_2) has received significant attention owing to the distinguished mesostructure and the outstanding photocatalytic activity for the complete destruction of organic pollutants. In the case of mesoporous alumina, the textural property plays a vital role on its performance in applications like catalyst, catalyst support and adsorbent. The conventional bulk alumina and titania have distinct disadvantages like lower surface area, broad pore size distribution and pore volume. Hence, in this investigation, we focus our attention to synthesize organized mesoporous materials with improved textural properties. For example, mesoporous TiO_2 was synthesized using neutral (Brij-56 and P-123) as well as cationic (CTAB) surfactants by hydrothermal technique while mesoporous alumina was prepared using lauric acid as a template by sol-gel method. All the samples were systematically characterized by various analytical and spectroscopic techniques. Table 1 summarizes the structure and textural properties of these metal oxides.

Table 1. Physico-chemical properties of various samples.

Sample	Surfactant	S_{BET} [a] (m^2/g)	V [b] (cm^3/g)	D_{BJH} [c] (Å)	t [d] (nm)	E_g (eV)
Mesoporous TiO_2	Brij-56	119	0.24	80	7.1	3.25
	P-123	126	0.25	88	7.0	3.17
	CTAB	333	0.37	41	5.7	3.16
Mesoporous Al_2O_3	Lauric acid	478	0.56	47	2.9	-

[a] BET surface area; [b] Total pore volume; [c] Average pore size estimated from N_2 adsorption-desorption; [d] Average anatase crystallite size evaluated from Scherrer equation.

References

[1] X. Wang, J. C. Yu, C. Ho, Y. Hou, X. Fu, *Langmuir* 21 (2005) 2552.

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[3] L. Chen, B. Yao, Y. Cao, K. Fan, *J. Phys. Chem. C* 111 (2007) 11849.

[4] Q. Liu, A. Wang, X. Wang, T. Zhang, *Micropor. Mesopor. Mater.* 92 (2006) 10.

Synthesis, characterization and catalytic properties of gold supported mesoporous carbons

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Mesoporous carbon with its uniform pore channels and high surface area leads to well dispersion of noble metal catalysts than microporous carbon. Generally, mesoporous carbons (CMK-3, CMK-1) are prepared using ordered mesoporous silica (SBA-15, MCM-48) as replica [1]. Gold catalysts are mild oxidation catalysts and they won't get poisoned leading to its higher active life compared to other catalysts [2]. We have synthesized mesoporous carbons CMK-3 and NCCR-56 using SBA-15 and IITM-56, loaded gold on these and characterized them. In Fig.1, low angle XRD of CMK-3 shows peak corresponding to 100,110 and 200 planes and NCCR-56 show 100 peak indicating proper replication of 2D hexagonal silicas. TEM of gold loaded mesoporous carbon shows well dispersion of gold particles due to its uniform pores which prevents agglomeration. We have studied glycerol oxidation reaction by using Au supported mesoporous carbons.

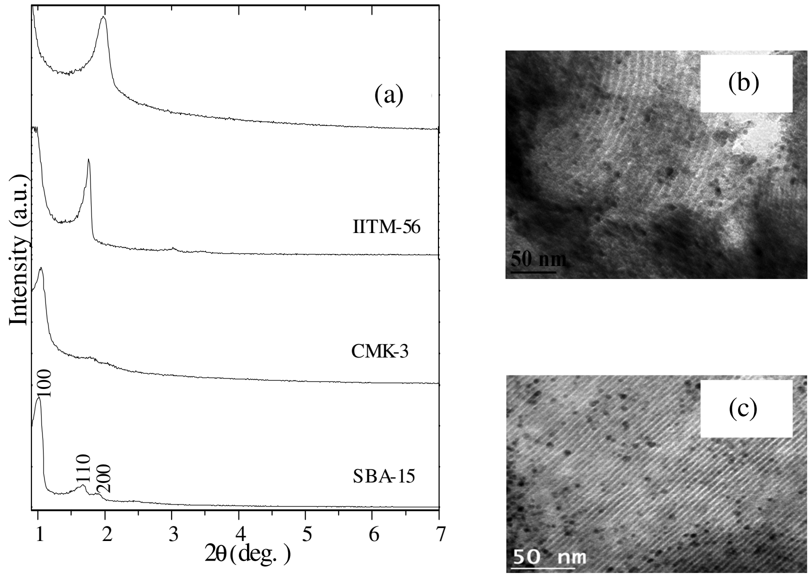

Fig.1. (a) Low angle XRD patterns of SBA-15, CMK-3, IITM-56 and NCCR-56. (b) TEM of 1 wt% Au/CMK-3. (c) TEM of 1 wt% Au/NCCR-56.

References

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Hydrogenolysis of sorbitol over Ni and Pt loaded on NaY

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Biomass is the most abundant organic material on earth and is therefore an ideal renewable feedstock for the production of chemicals. For example, the hydrogenolysis of sorbitol obtained from glucose made by the hydrolysis of cellusose (biomass) can be used to produce valuable di and polyhydric alcohols like ethylene glycol, propanediols and glycerol, which are generally produced by multi-step transformations from non-renewable petroleum based feed-stocks (olefins). In this communication, we report the use of Ni and Pt loaded on NaY as catalysts for the hydrogenolysis of sorbitol. We have investigated the influence of the mode of preparation of the Ni catalyst, the effect of Pt addition and the role of basic promoters like $Ca(OH)_2$.

The hydrogenolysis of sorbitol (15 % aqueous solution) was carried out at 60 bar pressure at 220 ºC in a stirred batch reactor using Ni-NaY (2, 4, 6 wt% Ni) with and without added Pt (1 wt%). 1,2-Propanediol was the major product over Ni-NaY and the addition of 1 wt% Pt to the Ni-catalysts did not alter conversion or selectivity of the catalysts to any significant extent. Glycerol was the main product over Pt(1 wt%)-NaY. Addition of $Ca(OH)_2$ as the promoter to both Ni and Pt catalysts increased the conversion marginally. The studies reveal Ni-NaY to be a suitable catalyst for the conversion of sorbitol to 1,2-propanediol; Over 6 % Ni-NaY, sorbitol conversion and selectivity for 1,2-propanediol was, 68 % and 62 % respectively, 75 % and 69 % in the presence of $Ca(OH)_2$. Reasons for the difference in the over Ni and products obtained Pt catalysts are examined.

Dehydration of glycerol over CuO-ZnO catalyst

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Supported copper oxide was an effective catalyst for the dehydration of glycerol to produce hydroxyl acetone under inert conditions [1]. Vapour phase dehydration of glycerol was performed over a series of CuO–ZnO catalysts prepared by sol-gel method [2] with varying Cu/Zn mole ratios in a fixed-bed down-flow reactor at atmospheric pressure (N_2) and temperatures between 275 and 330°C. The prepared catalysts were characterized systematically by various analytical and spectroscopic techniques. The XRF results of the calcined catalysts (CuO-ZnO) are in good agreement with the calculated (Cu/Zn = 0.33-1) values. The XRD pattern of the spent catalyst showed the presence of metallic Cu, and no CuO as was observed in the fresh catalyst. Among the catalysts with different Cu/Zn composition, the one with Cu/Zn ration of 0.33 shows higher glycerol conversion and selectivity towards hydroxyl acetone suggesting a compositional dependence of catalytic activity (Fig. 1).

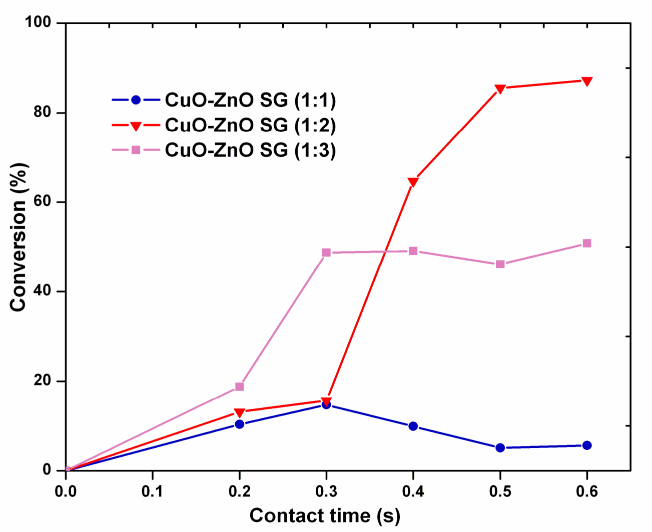

Fig. 1. Effect of contact time on glycerol conversion in dehydration of glycerol.

References

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(Optional presentation)

Lithium Ion Batteries (LIB) – Do they stand a chance to be the near future energy conversion devices?

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A Lithium ion battery (Li-Ion battery or LIB) is a family of rechargeable battery types in which Lithium ions move from the negative electrode to the positive electrode during discharge and back during charging. These batteries (different from lithium primary batteries) are common in consumer electronics. They are one of the most popular energy devices for portable electronics with one of the best energy to weight ratios, no memory effect and a slow loss of charge when not in use.

The purpose of this presentation is to examine some critical aspects like the chemistry of the electrochemical reactions, the choice of materials, supporting electrolyte employed and the possible effects of the use of ethylene carbonate and other carbonates as electrolytes. The safety aspects of this class of batteries have been considered at various times in the past and hence this aspect will not be considered .

The electrolyte typically is a mixture of organic carbonates such as ethylene carbonate or diethyl carbonate containing complexes of Li-ions. This situation can lead to the formation of lithium carbonate and the whole of the electrochemistry of this type of rechargeable batteries can be different from what have been conceived so far.

The set of cathode and anode materials employed in the LIB are given in the following table.

Cathode material	**Average voltage (V)**	**Anode Material**	**Average Voltage (V)**
$LiCoO_3$	**3.7**	**Graphite (LiC_6)**	**0.1 – 0.2**
$LiMn_2O_4$	**4.0**	Hard carbon (LiC_6)	**?**
$LiNiO_2$	**3.5**	Titanate ($Li_4Ti_5O_{12}$)	**1-2**
$LiFePO_4$	**3.3**	Si($Li_{4.4}Si$)	**0.5 -1**
Li_2FePO_4F	**3.6**	$\mathrm{Li}\vert 4.4\vert\mathrm{Ge}$	**0.7 – 1.2**
$LiCo_{1/3}Ni_{1/3}Mn_{1/3}O_2$	**3.6**		
$Li(Li_a Ni_x Mn_y Co_z)O_2$	**4.1**		

The questions that one faces today are:

(i) **Can lithium batteries be the appropriate substitutes for the energy conversion devices especially when the deployment of Fuel cell appears to be a long term dream?**

(ii) **Do we have any other alternatives for electrode and electrolytes in LIB?**