NATIONAL CENTRE FOR CATALYSIS RESEARCH

INDIAN INSTITUTE OF TECHNOLOGY, MADRAS

(Book let of abstracts presented on January 26,2020)





PROGRAM FOR THE SEMINAR ON 26TH JANUARY 2020 AT NCCR

9.30 **Introduction Presented by**

9.55 **Release of the Catalogue of books in NCCR by Mr. Hariprasad Narayanan**

10.00 **Dr.Aparna on line presentation on**

10.30 **Rathinasamy Vinayagamoorthi Sathish on** Catalytic upgrading of ethanol to n-butanol over Ni-Cu bimetallic catalyst supported on CeO2-Al2O3

11.00 Coffee Break

11.15 **Mr. K. Shivaraj Kumar on** **Selective catalytic reduction of NOx over γ-Al2O3 supported Ag and Au catalysts in automotive exhaust emissions**

11.45 Concluding Remarks

**PREFACE**

The national holidays have been celebrated in scientific discussions by the academic community in Chennai for a number of years. It is necessary that the younger generation continues all these practices in the years to come and hand-over to the next generation to emulate. Though the Madras chemists were organizing this traditional-meetings, NCCR has taken the role of the distinguished chemists of the city of Madras.

This year’s Republic day seminar is based on the contributions by the fellow scientists of NCCR. NCCR is grateful to all those who agreed to make presentations during this half day seminar. The theme of the presentation is based on search for catalysts relevant today’s context.

NCCR will like to utilize all the three national holidays (January 26, August 15 and October 2) in rededicating ourselves to the service among ourselves and it is hoped that the members will agree to this and also carry on this legacy in the coming years. This year we will have some presentations from our research scholars and hope these presentations are useful to all of us including the person who is presenting the same.

On this occasion, NCCR is happy to release the Catalogue of Recent Books that NCCR possession by the efforts of Mr.Hariprasad and one can access the catalogue on line. NCCR is grateful to Mr.Hariprasad for his efforts.

NCCR wishes to thank all its members for their cooperation and support all these 13 years.

January 26, 2020

**A Library of e-books in catalysis and related subjects**

We all know there is a boom in publishing books in recent years die to various reasons including the development of the digital era. The world known publishers are bringing out on daily basis books on various topics and it is hard to keep track of all of them.

NCCR with the great effort of Mr.Hariprasad made a collection of 1000 or more books and in order to make them available to any one who needs them NCCR again with the great effort of Mr.Hariprasad made a catalogue and this is available to any one in the following web site

<https://sites.google.com/view/library-catalogue-2020/home>

This is supposed to be accessible at any internet connections and one can browse them at any time and can ask for a hard copy or soft copy whichever is available, NCCR will try to provide them.

This site will be formally released on this 26th January in the half a day seminar at NCCR by Mr. Hariprasad Narayanan and this will be happy occasion for those who belong to NCCR. I am sure the members of NCCR will be proud of this unique attempt and will appreciate the efforts of Mr.Hariprasad and few others who were responsible for this initiative.

NCCR will be happy to receive feedback from all those who visited this on line catalogue and also will be grateful for any suggestions to improve the services rendered by NCCR to development of science in particular in the field of catalysis.

Finally, NCCR is grateful to all of you for all the support provided all these years

**Registered List of Participants**

**Name Organization**

1. **Mr Surya Kumar ……………. NCCR**
2. **B.Viswanathan NCCR**
3. **Mr.K.Shivaraj Kumar Chem Engg, NCCR**
4. **Mr. Rathinasamy Vinayagamoorthi NCCR**
5. **Dr. Aparna IIT(ISM) on line**
6. **Mr. Hariprasad NCCR, CUSAT**

**Catalytic upgrading of ethanol to n-butanol over Ni-Cu bimetallic catalyst supported on CeO2-Al­2O3**

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**Abstract**

The direct conversion of ethanol to higher value 1-butanol is a catalytic transformation of great interest in light of the expected wide availability of bioethanol originating from the fermentation of renewable resources. n-Butanol (BuOH) often has superior properties as a bio-fuel compared to ethanol (EtOH). Amongst many types of catalysts under investigation, alumina supported nickel catalysts are highly effective for conversion of ethanol to butanol and higher alcohols. In order to improve the selectivity towards butanol, we have modified the alumina support, with ceria (5% w/w of alumina) and added copper as the second metal. Bimetallic Ni-Cu catalysts with varying proportions of the metals, bi-metallic 5.5% Cu-2.5% Ni, 4% Cu-4% Ni and 2% Cu-6% Ni and 8% Cu, 8% Ni mono metallic catalysts, supported on CeO2-Al2O3 have been prepared by wet impregnation and characterized by XRD, BET, TEM, NH3-TPD, CO2-TPD, H2-TPR and XPS. Condensation of ethanol on these catalysts has been carried out in Parr reactor in batch mode at 200°C up to 8hrs, after pressurization with nitrogen up to 10 bar. Mono metallic Ni displays ethanol conversion of 41%, with a selectivity of 48.6% towards butanol. Substitution of Ni with Cu up to2% increases ethanol conversion to 45% with butanol selectivity of 44%. On increasing Cu loading to 4%, conversion decreases to 37% and butanol selectivity increases to 46.4%. Further increase of Cu loading to 5.5% results in higher butanol selectivity of 55.6 % with conversion at 32.2%. Whereas mono metallic Cu catalyst under identical reaction conditions displays high butanol selectivity, (64%) but very low ethanol conversion (18%). Thus, by optimization of Cu & butanol selectivity, (64%) but very low ethanol conversion (18%). Thus, by optimization of Cu & Ni composition, it is possible to maximize butanol selectivity with optimum conversion level. XPS and TPR studies indicate Ni-Cu alloy formation, especially in the compositions, 4% Ni-4% Cu, and 2.5% Ni-5.5% Cu. Ethanol to butanol process involves initial dehydrogenation of ethanol to acetaldehyde, its condensation to crotonaldehyde, which gets hydrogenated to yield buanol. Ni-Cu alloys facilitate the dehydrogenation and hydrogenation steps, thereby improving activity and selectivity to butanol. Sun et al (5) have reported ethanol conversion of 56% and butanol yield of 22% on Ni-Cu supported on Mg-Al hydrotalcite at higher temperature (320°C) in batch mode. In the present work Ni-Cu catalysts supported on CeO2-Al2O3display comparable performance at lower temperature (200°C)

Table 1. Catalytic performance of Ni-Cu/CeO2-Al2O3 catalysts for the upgrading ethanol to n-butanol

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Catalysts** | **Temp. (°C)** | **Conv. (%)** | **H A**  **Selec. (%)** | **Butanol**  **Selec. (%)** | **HA**  **yield (%)** |
| 8%Cu/5%CeO2-Al2O3 | 200 | 18.0 | 81.8 | 64.1 | 14.7 |
| 2%Cu-6%Ni/ 5%CeO2-Al2O3 | 200 | 45.1 | 62.4 | 44.1 | 28.1 |
| 4%Cu-4%Ni/ 5%CeO2-Al2O3 | 200 | 37.0 | 62.8 | 46.4 | 23.2 |
| 5.5%Cu-2.5Ni/5%CeO2-Al2O3 | 200 | 32.2 | 77.3 | 55.6 | 24.9 |
| 8% Ni/ CeO2-Al2O3 | 200 | 41.1 | 81.0 | 48.6 | 35.0 |

**References**

1. Efficient Catalytic Conversion of Ethanol to 1-Butanol via the Guerbet Reaction over Copper- and Nickel-Doped Porous ACS Sustainable Chem. Eng. 2017, 5, 1738−1746.

2) Continuous Catalytic Upgrading of Ethanol to n-Butanol and >C4 Products over Cu/CeO2 Catalysts in Supercritical CO2 DOI: 10.1039/C4GC00219A

3) Catalytic upgrading of ethanol to n-butanol over M-CeO2/AC (M =Cu, Fe, Co, Ni and Pd) catalysts Catalysis Communications 100 (2017) 15–18.

) Continuous catalytic upgrading of ethanol to n-butanol over Cu–CeO2/AC catalysts *Chem. Commun.,* 2016, 52, 13749—13752.

5) Butanol synthesis from ethanol over CuMgAl mixed oxides modified with palladium (II) and indium (III) Fuel Processing Technology 177 (2018) 353–357.

6) Continuous liquid-phase valorization of bio-ethanol towards bio-butanol over metal modified alumina Renewable Energy 74 (2015) 369-378.

7) Catalytic Conversion of Ethanol into Butanol over M–Mg–Al Mixed Oxide Catalysts (M = Pd, Ag, Mn, Fe, Cu, Sm, Yb) Obtained from LDH Precursors Catal. Lett (2013) 143:23–30

**Selective catalytic reduction of NOx over γ-Al2O3 supported Ag and Au catalysts in automotive exhaust emissions**

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NOx emissions adversely impact the environment and human health. Necessary action is needed to control and monitor the emission of NOx from automotive exhausts. Three-way automotive catalyst has been highly successful in controlling exhaust emissions from the conventional gasoline engines which operate close to stoichiometric conditions, but this catalyst is not effective in NOx reduction in excess oxygen environment. i.e., it is not applicable for diesel and lean-burn exhaust NOx emission reduction. So, a catalytic system is needed such that, it should reduce NOx even in excess of O2, in the presence of a suitable reducing agent. In our work, γ-Al2O3 supported Ag and Au-based catalysts prepared by different techniques are developed for NOx reduction applications.

The packed bed reactor experiments were performed with all the catalysts (Ag/, Au/, and Ag-Au/γ-Al2O3) which are prepared by three method of preparation techniques. Those techniques are (1) co-precipitation method, (2) single-step sol-gel method, and (3) impregnation method. The experimental results of NOx reduction observed are; the bare-boehmite is showing very good NOx conversion and catalytic activity is increased monotonically with respect to temperature. The boehmite phase is transformed into γ-Al2O3 phase after the first cycle of reaction. Ag/Alumina catalysts prepared by coprecipitation method are shown low performance of activity than the catalysts prepared by other methods. Monometallic Au catalyst is shown less NOx conversion and adding gold to the silver catalysts is giving negative synergetic effect with detrimental decrease in NOx conversion. Finally, monometallic silver catalyst prepared by both single step sol-gel and impregnation catalyst is providing the best activity for NOx reduction by propene, under the conditions studied.

<https://sites.google.com/view/library-catalogue-2020/home>