



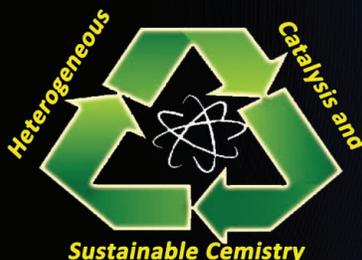
RSC-NIT Symposium

on

Heterogeneous Catalysis and sustainable Chemistry

November-05, 2016

Venue:EEE Auditorium



Abstract Book

Combinely Organized by

NIT,Trichy

IIT, Madras

&

Royal Society of Chemistry

RSC-NIT SYMPOSIUM

Title: Heterogeneous Catalysis and Sustainable Chemistry

Venue: NIT, Trichy

Date: November 5, 2016

Organisers: National Institute of Technology, Trichy and Royal Society of Chemistry.

Background:

The Royal Society of Chemistry and NIT Trichy organise a scientific symposium on Heterogeneous catalysis and sustainable chemistry on November 5, 2016.

The symposium aims to highlight new trends and developments in Heterogeneous catalysis and explore research collaborations between the UK and India.

A special session will be conducted by the Royal Society of Chemistry on how to publish in high impact journals for students and early career researchers. This apart, a poster session will also be held.

The symposium will appeal to academics, students and industrial scientists and is free to attend.

Speakers:

- Sankar Meenakshisundaram, Cardiff University
- Thomas Chamberlien Leeds University
- Xubein Ke, University of Hull
- Francisco Garcia-Garcia, Edinburg University
- Mark Symes, Glasgow University
- Andrew Logsdail, University College London
- P. Selvam, IIT Madras,
- A. Chandra Bose, NIT Trichy
- S. Velmathi, NIT Trichy

Scientific Committee:

- P Selvam, IIT Madras
- S Velmathi, NIT Trichy
- Deeksha Gupta , RSC
- Abhiram Prabhu, RSC

Program Schedule

 DEPARTMENT OF CHEMISTRY NATIONAL INSTITUTE OF TECHNOLOGY, TRICHY. RSC-NITT Symposium on Heterogeneous catalysis and sustainable chemistry November 05, 2016	
Venue-EEE Auditorium, Programme Schedule	
Time	Event
05.11.2016	
09.30 - 9.45 am	Inauguration
	Session-I
9.45-10.05 am	Lecture I Prof. Dr. P. Selvam, National Centre for Catalysis Research, IIT Madras- Sustainability through catalysis
10.05-10.25 am	Lecture II Dr. M. Sankar, Cardiff Catalysis Institute, Cardiff University, United Kingdom -Supported bimetallic catalysts for selective oxidation
10.25-10.45 am	Lecture III Dr. Thomas Chamberlein, Leeds University -Controlling the structure of carbon nanoreactor supported metal nanoparticles for heterogeneous catalysis in continuous flow
10.45-11.00 am	Interaction with speakers of session I
11.00-11.15 am	Tea Break
	Session-II
11.15-11.35 am	Lecture IV Dr. Xuebin Ke- University of Hull, Light-driven chemical synthesis with surface plasmon resonance effect
11.35-11.55am	Lecture V Dr. A. Chandra Bose-Department of Physics, NITT Findings on visible light driven photocatalysis
11.55am-12.15 pm	Lecture VI Dr. Mark Symes, University of Glasgow -Materials for the electrochemical production of chemical feedstocks
12.15-12.30 pm	RSC-Lecture
12.30-12.45 pm	Interaction with speakers of session -II
12.45-1.45 pm	Lunch
1.45 -2.45 pm	Poster session
	Session-III
2.45-3.05 pm	Lecture VII Dr. Francisco R Garcia Garcia, Department of Chemical Engineering, University of Edinburg, Scotland, UK-New Approaches for Reforming: Chemical Looping
3.05-3.25pm	Lecture VIII Dr. Stefano Leoni, Cardiff University- Advanced methods for materials simulations
3.25-3.45 pm	Lecture IX Dr. Andrew J Logsdail-Department of Chemistry, University College London, London, UK - Elucidating the Properties of Catalytic Materials using QM/MM Computational Methods
3.45-4.05pm	Lecture X Dr. S. Velmathi, Department of Chemistry, NITT - Catalytic applications of mesoporous materials
4.05-4.25pm	Interaction with speakers of session -III followed by Tea Break
4.45 pm	Concluding remarks and poster prize announcements

Invited Lectures

Supported Bimetallic Nanoalloy Catalysts for a Green and Sustainable Future

M. Sankar

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United Kingdom.*

Supported bimetallic nanoalloys have significantly different properties compared to their monometallic analogues, especially as catalysts. Recent advances in spectroscopic and microscopic techniques have enabled us to study the structural properties of these bimetallic nanoalloys in greater detail. In this presentation, emphasis will be given to the importance of tuning the structural properties of these materials by designing appropriate synthesis strategies to exploit the exceptional catalytic activities of these nanoalloys. The strategies to tune the activity, selectivity and stability of supported bimetallic catalysts for different reactions are presented. For this purpose, I will discuss three examples (a) gold–palladium nanoalloy supported on TiO_2 catalysts for the direct synthesis of hydrogen peroxide from hydrogen and oxygen. This example will demonstrate the importance of designing correct synthesis strategy to make an active and stable catalyst by controlling the size, composition and nanostructure of the bimetallic nanoparticles (b) gold palladium nanoalloys supported on different supports (TiO_2 , Nb_2O_5 , C, MgO & ZnO) for the selective aerobic oxidation of benzyl alcohol. This example demonstrates that by tuning the active site responsible for the by-product (toluene) formation we can switch-off its production and increase the selectivity of the desired product (benzaldehyde) to >99% and finally (c) supported gold–palladium and ruthenium–palladium nanoalloys for the hydrogenation of levulinic acid (LA) to g-valerolactone (GVL). This final example will demonstrate that by alloying two catalytically inactive metals (gold and palladium) at a nanoscale we can design an active catalyst and in another case the selectivity of the monometallic ruthenium catalyst can be increased dramatically by alloying it with palladium at a nanoscale.

Controlling the structure of carbon nanoreactor supported metal nanoparticles for heterogeneous catalysis in continuous flow

Thomas Chamberlain

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Preparation of catalytic nanomaterials with a desired structure and properties requires strict control of their size, shape and composition. We utilise a new universal approach for the formation of quasi one dimensional materials inside CNTs via the sequential encapsulation of molecular precursors which contain the appropriate elemental building blocks and subsequent reaction. The chemically inert nature of such nanosized containers makes CNTs ideal candidates for use as both reaction vessels, in which the precursors can be combined, and 1D templates which can direct the formation of products which are unfavoured or impossible to synthesise in the bulk phase.¹ Our methodology has enabled a wide variety of CNS supported materials to be fabricated, including metallic and bimetallic systems, e.g. NiRu and PtRu nanoparticles, metal oxides, e.g. Fe₂O₃ and Co₃O₄, and inorganic materials, e.g. MoS₂, PtI₂.^{2,3} It also enables different metal loadings to be achieved, as well as, control over nanoparticle size and location.

I am particularly interested in understanding the structure of catalytic materials down at the atomic level and using solid state analytical techniques including aberration corrected high resolution electron microscopies (AC-HRTEM and STEM),⁴ X-ray absorption⁵ and diffraction and gas adsorption to elucidate the exact structure of materials. By monitoring both the formation of heterogeneous catalysts from metallic precursors and the structure of the catalyst during chemical reactions using a combination of *in situ* HRTEM and near edge X-ray absorption fine structure (NEXAFS) experiments it is possible to reveal atomic level structural information and mechanistic details of how the catalysts function.

The supported materials are explored in heterogeneous catalysis using an efficient continuous process scheme involving scCO₂ in packed bed continuous flow and electrochemical reactor systems.^{6,7} The hydrogenation of biomass derived platform chemicals, e.g. furfural, readily available via the dehydration of renewable feedstocks including rice husks and oats, to 2-MeTHF, a bulk chemical used as fuel additive and solvent for a variety of chemical transformations, has been used as a model system. Such reactions are typically limited by the stability of the catalyst, however, the high thermal stability of CNS support materials makes them ideal candidates for this chemistry. Incorporating in-line analysis coupled to evolutionary algorithms enables rapid screening of reaction conditions and maximise yield and/or throughput.

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Elucidating the Properties of Catalytic Materials using QM/MM Computational Chemistry Methods

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As consumer desire for affordable, clean, renewable energy continues to grow, despite increasingly stringent environmental legislation, heterogeneous catalysis is vital to ensure environmental viability. In many cases, progressively more efficient heterogeneous catalysts have been produced and tested experimentally, but a fundamental understanding of the reaction mechanisms and material properties that make these catalytic processes effective remains elusive.

To aid our understanding in this field, computational chemistry has become a necessary tool for providing accurate descriptions at a molecular level, particularly due to the recent theoretical improvements in fields such as electronic structure theory, as well as from the continued growth in accessible computational resources. We present our work developing and applying computational chemistry techniques, in particular the embedded-cluster QM/MM methodology, [1, 2] in the context of heterogeneous catalysis. Particular focus is towards elucidating catalytic mechanisms, understanding the effects of reaction environments, and characterizing the underlying properties of important materials, such as TiO₂, at the atomic level (Figure 1). [3]

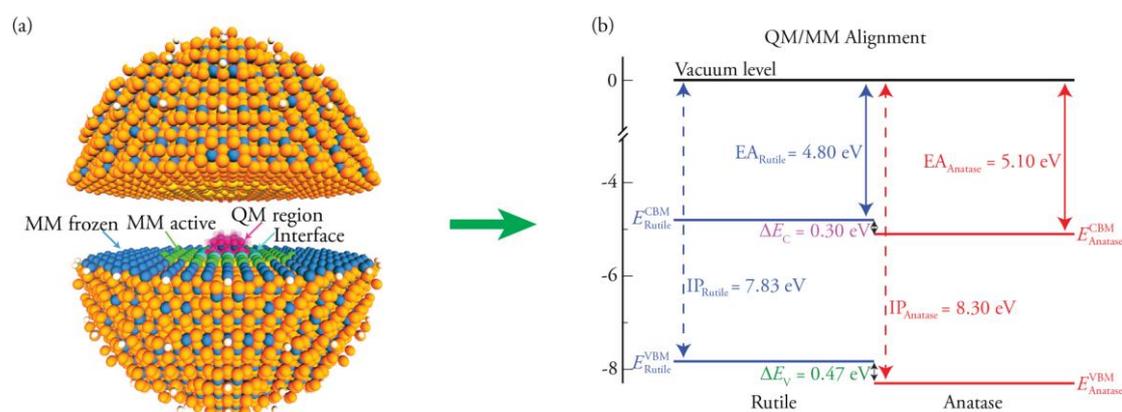


Figure 1: **(a)** Graphic of a hybrid QM/MM embedded cluster as used for rutile TiO₂. The cluster is divided into hemispheres to highlight the different regions in the model. Hole density iso-surfaces are shown (semi-transparent purple) in the QM region. **(b)** Schematic of the QM/MM alignment of rutile and anatase TiO₂. IP and EA denote ionization potential and electron affinity, respectively. The electron affinity is calculated by adding the experimental bandgaps to the calculated ionization potentials. ΔE_V and ΔE_C are the valence band offsets and conduction band offsets, respectively and E^{CBM} and E^{VBM} denote the positions of the conduction band and valence band respectively.

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New Approaches for Reforming: Chemical Looping

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My research seeks sustainable solutions to today's energy production challenges by mimicking biological cell strategies. Biological cells can be seen as enhanced multifunctional reactors specifically designed to solve fundamental chemical engineering issues such as thermodynamic limitations, catalyst deactivation, and product separation. For example, cells can overcome the thermodynamic limitations because the reaction sites are enclosed within the cell membrane, which is permeable to some of the reaction products. Likewise, cyclic vs linear pathways allow a quick and economic solution to chemical problems. While these approaches are common in cells, they are only sporadically applied technologically in a purposeful manner. The aim of my research group is to design, develop and fabricate multifunctional catalytic reactors inspired by how biological cells work, which allows the integration of multi-processes in a single device. So far the difficulty of combining chemistry, materials science and engineering knowledge in a single unit has prevented the full development of this concept.

Light-driven chemical synthesis with surface plasmon resonance effect.**Xuebin Ke***School of Engineering and Computer Science**University of Hull, Hull, UK*X.ke@hull.ac.uk

With diminishing of finite fossil reserves and increasing concern about environmental issues, cellulose conversion becomes attractive for the production of fuels and chemicals. An innovative material structure is presented to develop light-enhanced green process, combining porous zeolites, metal oxide nanofibres and metal nanoparticles. The directional growth of porous materials is designed to sufficiently expose the active surface. The new nanostructure will facilitate mass diffusion and thus enhance processing efficiency. Moreover, plasmonic metal nanoparticles loaded on the surface will efficiently absorb renewable solar energy and drive the transformation of biomass into useful chemicals/fuels. The surface plasmon effect of gold nanoparticles is a physical absorption to visible light, which plays a key role in influencing the polarized electronic-magnetic field of zeolites. With the light on, the conversion of cellulose can be up to 60% and main products are glucose and 5-hydroxymethylfurfural (HMF) with a high selectivity above 95%. The outcomes would significantly decrease processing costs, reduce energy consumption, and contribute to the utilisation of broad biomass resources.

Materials for the electrochemical production of chemical feedstocks

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There has been much interest recently in using electrocatalytic water splitting (driven by renewable inputs such as solar power) to produce hydrogen as a chemical feedstock and energy vector. In this talk, I will give an overview of the research in the Symes group that works towards the overall objective of renewably-driven electrocatalytic water splitting. In particular, we shall explore the role of trace impurities in the electrolyte as a potential source of significant electrocatalytic activity for water oxidation¹ and proton reduction,² and steps that can be taken to prevent such adventitious contaminants from giving false positive results for electrocatalysis. We will also examine ternary metal chalcogenides as highly active proton reduction electrocatalysts, touching on methods by which these catalysts can be prepared and their electrochemical performance.³ Emphasis will be placed throughout on the expertise that the Symes group possesses and areas in which we hope there will be scope for collaboration, especially as we move beyond hydrogen to the electrocatalytic production of other feedstocks such as ammonia.⁴

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Advanced methods for materials simulations

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The Leoni group focuses on the study of activated processes in the solid state by means of advanced computational tools. Structural and electronic phase transitions, chemical reactions, formation mechanisms, reactive intermediates, structure prediction and the rules behind polymorphism in general are relevant research areas. Understanding processes like crystallization, nucleation and growth, diffusion of impurities or defects, or electrochemical reactions are crucial factors for the development of better materials. Despite major advances in device resolution, experiments can only provide a coarse-grained view of such processes. Theory can now integrate the experimental data by implementing the missing length and time resolution, thanks to novel strategies of numerical simulations. At the interface of inorganic and material sciences, theoretical chemistry, computational chemistry and physics, physical chemistry, materials for energy and sustainability, this area offers fascinating opportunities to leverage computational tools in the design of innovative materials.

Catalytic Applications of Mesoporous Materials

S. Velmathi

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Highly ordered mesoporous materials like SBA-15, KIT-6 were synthesised by hydrothermal method. The ordered nature of the synthesised materials were analyzed by low angle X-ray diffraction. The high surface area, pore diameter and mesoporous nature of the materials was confirmed by BET surface area analyzer. Si-O-Si, Si-OH and Metal-Si bonds in the framework was verified by FTIR spectroscopy. The morphology of the synthesized materials and percentage of metal present in the material were analyzed by HR-SEM-EDAX. The catalytic activity of synthesized materials were explored for various reactions like catalytic hydride transfer reduction of aromatic nitro compounds to amines, hydroxylation of benzene with 30% aqueous H₂O₂, Friedel- Crafts alkylation of benzene and styrene epoxidation reactions. The optimization studies of catalyst amount, reaction time, temperature etc., were done. Photocatalytic applications of the metal doped mesoporous materials will also be discussed. The salient features of the work will be presented in the lecture.

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Findings on visible light driven photocatalysis

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The field of photocatalysis has expanded rapidly within the last four decades, having undergone various developments especially in relation to energy and the environment. Photocatalysis is the efficient way to degrade the organic toxic dye. In recent years, interest in photocatalysis has focused on the use of semiconductor materials as photocatalysts for the removal of ambient concentrations of organic and inorganic species from aqueous system in environmental clean-up, drinking water treatment, industrial and health applications. In the last few decades, many literature report the usage of TiO_2 as an effective photocatalyst to degrade the organic pollutants, but facilitate the degradation only in the UV region. Thus, the research interest continues to search for an active visible light driven photocatalyst for the maximum utilization of solar energy. Hence the presentation focused on investigating the photocatalytic activities of hexagonal MoO_3 and the effects of experimental conditions such as catalyst loading, initial dye concentration, light intensity, and operating temperature on methylene blue degradation [1-3]. We also worked on Ag_3PO_4 as a photocatalyst material to oxidize water and decompose the organic contaminants in aqueous solutions under visible light irradiation. However, the conduction band potential of Ag_3PO_4 is more positive than that of $\text{H}_2\text{-H}^+$ which limits its application in hydrogen production from water splitting. Hence, Ag_3PO_4 composites have been developed by coupling with wide bandgap semiconductors. Herein, we developed a highly stable and novel $\text{Ag}_2\text{MoO}_4/\text{Ag}_3\text{PO}_4$ composite photocatalyst which are going to be discussed in the presentation [4].

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2. Preparation of h- MoO_3 and a- MoO_3 nanocrystals: comparative study on photocatalytic degradation of methylene blue under visible light irradiation, A. Chithambararaj, N. S. Sanjini, S. Velmathi and **A. Chandra Bose**, *Physical Chemistry Chemical Physics* 15 (2013) 14761
3. Role of synthesis variables on controlled nucleation and growth of hexagonal molybdenum oxide nanocrystals: Investigation on thermal and optical properties, A. Chithambararaj and **A. Chandra Bose** *Crystal Engineering Communications* **2014**, **16 (2014) 6175**
4. High Efficiency new Visible Light Driven $\text{Ag}_2\text{MoO}_4\text{-Ag}_3\text{PO}_4$ Composite Photocatalyst towards Degradation of Industrial Dyes, R. Dhanabal, A. Chithambararaj, S. Velmathi, **A. Chandra Bose**, *Catalysis Science & Technology*, 2016 (In Press)

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There is significant interest in the ordered porous materials due to their varied applications in organic transformations. Among different classes of ordered porous materials, e.g., microporous and mesoporous materials are extensively investigated. The microporous zeolites such as ZSM-5, zeolite-Y and zeolite- β are favourably considered for very many applications. However, the activity of catalyst is low for bulky molecules owing to smaller pore sizes and inherent limitations of the products diffusion. On the other hand, the discovery of ordered mesoporous aluminosilicates, e.g., M41S-family or SBA-family, with mild acidities have shown promise. However, poor thermal stability of the materials makes the process undesirable for large scale applications. Hence, in recent years, attempts have been made to induce mesoporosity into zeolite framework or prepare mesoporous materials with zeolitic merits; however, only very few groups have succeeded in synthesizing the so-called "hierarchical/mesoporous zeolites". This presentation outlines our efforts to synthesize such materials (Meso-ZSM-5) via dual templating strategy. In addition, a novel ionic templating as well as intrinsic hydrolysis methods were also employed for the synthesis of mesoporous aluminosilicates, viz., AllITM-56 and AISBA-15, respectively. In this talk, synthesis of zeolites *via* organic template-free hydrothermal route will also be discussed.

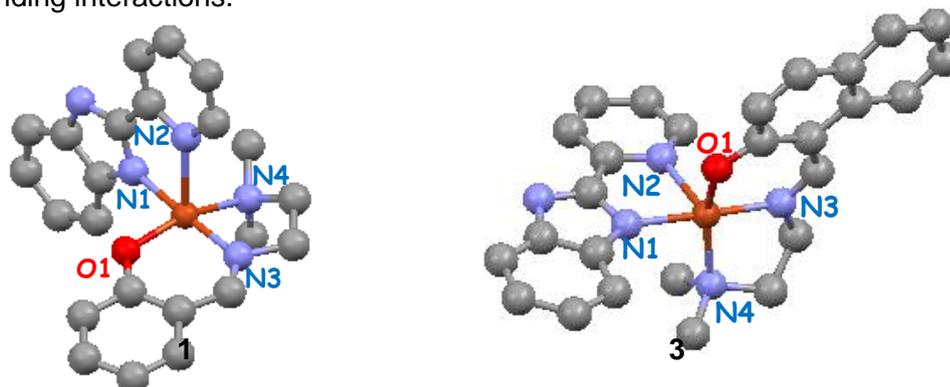
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POSTER PRESENTATIONS

PP-01 Functional Mimics for Copper Oxidases: Structure Spectra and Catalytic Properties of Mononuclear Copper(II) Complexes*Somasundaram Sangeetha, Velusamy Sathya and Mariappan Murali***Department of Chemistry, National College (Autonomous), Tiruchirappalli 620 001**e-mail: ma66mu@gmail.com and murali@nct.ac.in*

Proteins containing copper ions at their active site are usually involved as redox catalysts in a range of biological processes, such as electron transfer or oxidation of various organic substrates. In particular, ascorbate oxidase (AO), dopamine β -hydroxylase (D β H) and amine oxidase (AmO) (type-2) and Catechol oxidase (CO) (type-3) [1,2]. The primary role of type-2 copper center is electron transfer, in which ascorbate under physiological reaction conditions act as an electron donor and catalyze a two electron oxidation of primary amines to aldehydes. The type-3 copper enzyme, which was found to be EPR-silent, assigned to an antiferromagnetically spin-coupled Cu(II)-Cu(II) pair [3] and catalyze the oxidation of catechols to *o*-quinone. Mononuclear copper(II) complexes provide a distorted square-pyramidal (4+1) coordination geometry with labile binding site(s) are of great importance for modeling sites of copper oxidases [4-6]. Thus, copper(II) complexes of the type [Cu(1, L1/2, L2/3, L3/4, L4)(pybzim)]ClO₄ (where HL1-HL4 are tridentate Schiff base ligands derived from the condensation of salicylaldehyde (HL1/HL2) or 2-hydroxy-1-naphthaldehyde (HL3/HL4) and N,N-dimethylethylenediamine or N,N-diethylethylenediamine and pybzim is 2-(2-pyridyl)benzimidazole) have been synthesized. The crystal structures of **1** and **3** consist of mononuclear copper(II) species display a distorted square-pyramidal (4+1) coordination geometry. The degree of distortion (τ) calculated as 0.25 (**1**) and 0.30 (**3**). In addition, these complexes show intermolecular π - π stacking interactions and chemically significant hydrogen bonding interactions.



The complexes exhibit d-d and charge transfer transitions as well as show quasi-reversible Cu^{II}/Cu^I redox couple. Both polycrystalline and cryogenic EPR spectra are axial indicating a $d_{x^2-y^2}$ ground state. The complexes are catalytically active in the oxidation of ascorbic acid (AO and D β H), benzylamine (AmO) and catechol (CO) (**3**>**4**>**1**>**2**). Complexes display two types of non-covalent interactions, which play an important role in determining the catalytic activity.

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PP-02**PRODUCTION OF ELECTRICITY FROM LIVING PLANTS**S.Yuvaraj^{1*}, G.Suthakar²*Lecturer, Department of Chemical Engineering, Kongu Polytechnic College,
Perundurai, Erode – 638052.***Corresponding author's mail id: yuvachem08@gmail.com*

The Electricity from living plants concept is based on the cooperation of plants and microorganisms to produce electricity. The aim our project is to enhance the productivity of the Plant Power concept such that it becomes competitive with other bio energy systems. Plants take up carbon dioxide and water and capture light energy as food. This energy is stored in the chemical bonds of sugars produced, using carbon dioxide and water. Part of this chemically stored energy is transferred to the roots of the plants. This energy present in the root zone can then be captured by the electro-chemical active bacteria. These organisms are capable to oxidize the organic matter present in the root zone and transfer the energy rich electrons to an electrode. The energy carried by the electrons can be used as electrical energy, after which the electrons react at another electrode with oxygen to form water. Via photosynthesis a plant produces organic matter. Part of this organic matter is used for plant-growth, but a large part can't be used by the plant and is excreted into the soil via the roots. Around the roots naturally occurring micro-organisms break down the organic compounds to gain energy from. In this process, electrons are released as a waste product. By providing an electrode for the micro-organisms to donate their electrons to, the electrons can be harvested as electricity. Research has shown that plant-growth isn't compromised by harvesting electricity, so plants keep on growing while electricity is concurrently produced.

KEYWORDS: micro-organism, photosynthesis, metabolism, electricity

PP-03**Investigations on pure and Zinc doped Copper oxide nanoparticles: An antibacterial agent**L. Guru Prasad¹, R. Ganapathi Raman²¹*Department of Science & Humanities, M. Kumarasamy College of Engineering, Karur*²*Department of Physics, Noorul Islam University, Kumaracoil, Thuckalay 629 175, India*

Nanomaterials are used in numerous marketable and technological applications, including environmental, drug delivery and electronic, optical and mechanical devices. Many new nanomaterials have been developed in order to meet the demands in various fields. Among the available materials, metal oxide receives much attention due to its potential applications in opto-electronic devices. Most of metal obtains its lowest free energy states when it becomes metal oxides and these metal oxides demonstrate its property ranging from semiconductor to insulators. Copper oxide (CuO) is one of the simple oxide with an unfilled 3d-shell and it has fascinated applications when they prepared as nano. Most of the transition metal oxides having heat transfer applications. The uniqueness of CuO nanoparticles is even though they are metallic in bulk they behave like semiconductors when they are in nanosized. In this view, we attempt to synthesis and to characterize the pure and Zn doped copper oxide (CuO) nanoparticles.

Pure and zinc doped CuO nanoparticles have been prepared by co-precipitation method. XRD pattern of the prepared samples demonstrates the monoclinic structure of CuO and the presence of dopant. Band gap was calculated for the prepared materials by using UV-VIS spectrum and it confirms the band gap energy values gets increase while increasing the dopant concentrations. SEM image of the pure CuO shows the higher tendency of agglomerations of CuO nanoparticles and Zn doped CuO nanoparticles appears nearly spherical in shape with homogeneous size distribution. Pure CuO and Zn doped CuO nanoparticles were subjected to antibacterial activity for two pathogenic bacteria and it confirms the antibacterial nature of the prepared materials.

Keywords: Metal oxide; Doping; XRD; Antibacterial activity

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PP-04**UNPROTECTED D/L-ALANINE DERIVED THIOUREA LIGANDS AND THEIR WATER SOLUBLE Ru(II)-*p*-CYMENE COMPLEXES FOR ASYMMETRIC REDUCTION OF PRO-CHIRAL KETONES**

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Water is an eco-friendly solvent in catalysis and also, diverse interactions are possible among water, catalyst and substrate, which make the catalytic system homogeneous and effective. The development of water soluble chiral catalysts is a crucial area of green chemistry. The newfangled chiral aroylthiourea ligands (*R*)/(*S*)-2-(3-benzoylthioureido)propanoic acid (L1/L2), (*R*)/(*S*)-2-(3-(thiophene-2-carbonyl)thioureido)propanoic acid (L3/L4), (*R*)/(*S*)-2-(3-(furan-2-carbonyl)thioureido)propanoic acid (L5/L6) were produced from unprotected D/L-alanine and their water soluble Ru(II) complexes (**1-6**) were synthesized from their reaction with $[\text{RuCl}_2(\eta^6\text{-}p\text{-cymene})]_2$. The analytical and spectral methods were used to confirm the structure of the ligands and complexes. The solid state structure of L1, **5** and **6** was confirmed by single crystal XRD. Chiral alcohols are one of the utmost essential key chiral building blocks for various single enantiomer pharmaceuticals.^{1,2} Asymmetric reduction of pro-chiral ketones is a powerful method for the production of chiral alcohols. The complexes (**1-6**) catalyzed the asymmetric reduction of aromatic ketones to yield chiral secondary alcohols with admirable conversions (up to 99 %) and attractive enantiomeric excesses (ee up to 98 %), in presence of formic acid and triethylamine in water medium.

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PP-05**Synthesis, Characterization, Antimicrobial Activity and docking Analysis of Mannich bases derivatives****S. Veeramankandan¹, H. Benita Sherine^{1*}**

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The new Mannich base 3-(2,6-dichlorophenyl)-3-morpholino-1-phenylpropane-1-one and N-((2,6-dichlorophenyl)(morpholino)methyl)benzamide were synthesized from Morpholine, 2,6-dichlorobenzaldehyde and acetophenone or benzamide using Mannich synthetic route. The compounds were synthesized and characterized by various spectral techniques such as FT-IR, ¹H NMR, ¹³C NMR and Mass spectral analysis. The biological activities for the synthesized compounds were screened *in vitro* against five bacterial pathogens species: *B. Polymyxa*, *B. Megaterium*, *V. Cholera*, *P. Alkalifaciens* and *F. antarctium* and also against two fungal species: *C. Albicans* and *A. fumigates* by disc diffusion technique, using agar nutrient as medium, Chloramphenicol and Fucanazole as standard. *In vitro* molecular docking analysis was carried out for synthesized compounds on *Mycobacterium tuberculosis* (*Mtb*) strain by discover studio 2.1 version.

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PP-06

HALF-SANDWICH RUTHENIUM(II) ARENE COMPLEXES FOR TRANSFER HYDROGENATION OF KETONES

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The four new dibenzosuberene substituted thiourea ligands were synthesized, characterized and used to prepare novel Ru(II) piano stool complexes (**1-8**). These Ru(II) complexes were obtained from the reaction of $[\text{RuCl}_2(\eta^6\text{-arene})]_2$ (arene = *p*-cymene/benzene) with dibenzosuberene substituted thiourea ligands. All the Ru(II)-arene complexes were characterized by analytical, spectral (UV-Vis, FT-IR, ^1H NMR, and ^{13}C NMR) and single crystal X-ray diffraction studies. The molecular structure of all the ligands and the complexes (**1**, **3**, **6** and **7**) were confirmed by single crystal X-ray crystallography. All the synthesized complexes exhibit pseudo octahedral half-sandwich "piano-stool" geometry, with the chloride as a "leaving group" and unreactive arene as a "spectator ligand" in the metal coordination sphere. All the complexes were successfully screened out as catalysts for transfer hydrogenation of ketones using 2-propanol as the hydrogen source in the presence KOH. Among the different hydride sources available, 2-propanol/KOH finds more attraction because of its stability, easy accessibility, nontoxicity, inexpensive and environmentally benign nature. The mechanism probably involves the formation of Ru-Hydride intermediate. The transfer hydrogenation reactions proceeded with excellent yields up to 99%. The scope of this catalytic system was extended with substituted aromatic ketones and hetero aromatic ketones. In the transfer hydrogenation reactions, the catalytic activity of Ru-benzene complexes with a dibenzosuberene unit containing thioureas was significantly higher activity compared to monodentate analogues of similar complexes.

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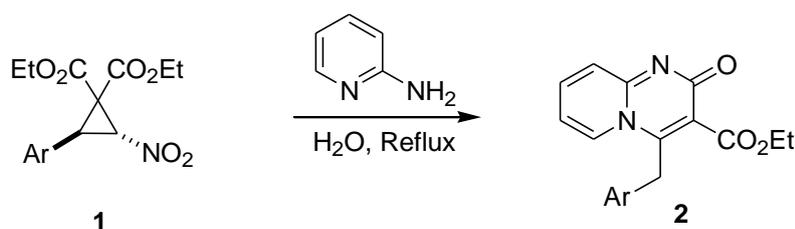
PP-07

Ring-opening cyclisation of *trans*-2-aryl-3-nitro-cyclopropane-1,1-dicarboxylates with 2-aminopyridine in water: A facile access to pyridopyrimidines

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Water is rarely used as a solvent for organic transformations despite being the de facto solvent for biochemical transformations. In recent years, with a growing interest to impart greenness in organic synthesis a great deal of efforts have been directed towards carrying out organic reactions in water.¹ Donor-acceptor cyclopropanes, especially those with nitro substituents have emerged as versatile building blocks in organic synthesis.² In continuation of our interest in donor-acceptor cyclopropane chemistry,^{2,3} we became interested in the investigation of the reactions of *trans*-2-aryl-3-nitro-cyclopropane-1,1-dicarboxylates **1** in water. We found that when cyclopropane dicarboxylates **1** were heated under reflux with 2-aminopyridine in water, they afforded pyridopyrimidines **2** in high yields. It may be noted that the pyridopyrimidine core is found in many pharmaceutically important compounds such as *pemirolast* (antiasthmatic agent), *pirenperone* (tranquilizer) and *barmastine* (antiallergen).⁴ The scope, mechanism and other details of the present investigation will be discussed in the poster.

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PP-08**Selective condensation reactions catalyzed by heterogeneous catalyst****Oxovanadium(IV) complex of 2-thiophenecarba benzhydrazone****Jyothy G Vijayan and N M Nanje Gowda***Department of Chemistry, Christ University, Bengaluru-29*

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The hydrazone ligand obtained from 2-Thiophene carboxaldehyde and benzhydrazide react with equimolar mixture of vanadyl acetyl acetonate in methanol to yield Oxovanadium(IV) complexes of 2-thiophenecarba benzhydrazone. Oxovanadium(IV) complexes of 2-thiophenecarba benzhydrazone is used as the catalyst in the system. The catalytic process was carried under room temperature. The major products were 2,3 -di (furan-2-yl) quinoxaline, 2,3 -di (furan-2-yl)-6-methyl quinoxaline, 2,3 -diphenyl pyrido [2,3-b] pyrazine, and 6-methyl - 2,3 -diphenyl quinoxaline. The influence of solvent and quantity of catalyst has been studied. Oxovanadium(IV) complex of 2-thiophenecarba benzhydrazone shows significantly higher catalytic activity. The catalyst can also be reused for several times. It is an efficient and inexpensive method for condensation reactions.

Keyword: Oxovanadium complex, 2- Thiophenecarba benzhydrazone , and catalytic activity

PP-09

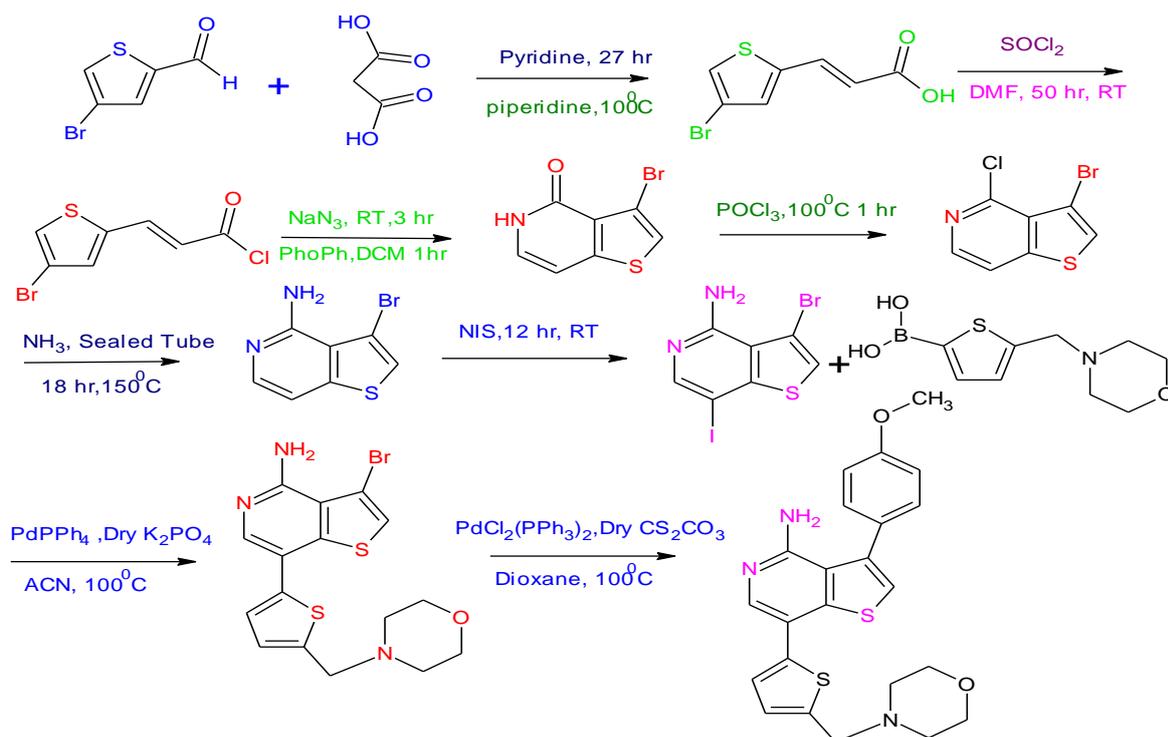
Synthesis of Newer thiopyridine derivatives and their biological evaluation**P.Muthuraja, P.Manisankar****Department of Industrial Chemistry, Alagappa University, Karaikudi – 630 003 Tamilnadu, India.*

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In present study, new scaffolds of 5-bromo-4-[5-(morpholin-4-ylmethyl)thiophen-2-yl]-5h-cyclopenta[c]pyridin -1-amine functionalized with different aromatic boronic acid were synthesized and computationally evaluated using cheminformatic tools. Six newer thiophene derivatives obeyed Lipinski's rule of five with good biological activity. Six targets among one showed lesser drug likeness and drug score values compared to other thiophene derivatives using OSIRIS property explorer. Except these one derivatives, all other synthesized targets act as drugs.

Key words: Thiophene derivatives, Libinskis rule, OSIRIS Property Explorer, Molinspiration software.



PP-10**A green and efficient methodology for the synthesis of 1,3,5 triazines:
Microwave assisted cyclization of Aldehydes with Amidines.**

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Microwave assisted methodology for the synthesis of 2,4,6- tri aryl- 1,3,5- triazine from aldehydes with amidines in a green and bio friendly solvent system has been developed (Scheme-1). This cost effective method is giving an excellent yield for a wide range of substituted s-triazines. The use of microwave irradiation has made this protocol energy economic and rapid. Various 1,3,5-triazines were synthesized in good to excellent yields. The developed methodology was trailed with non-aqueous work up, shorter reaction time and higher yield. This protocol offers an excellent chance to avoid toxic solvents, and catalysts. Moreover, after extraction with ether, PEG-600 was recovered and could be reused. Highly fluorescent compound 2,4-diphenyl-6-(pyren-1-yl)-1,3,5-triazine has been synthesized using this method and its spectroscopic behaviors studied.

Scheme-1 Synthesis of Triazines

PP-11**Boehmite - An efficient and recyclable acid-base bifunctional catalyst for aldol condensation reaction**

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In this work, boehmite was used as an acid-base bifunctional catalyst for aldol condensation reactions of aromatic aldehydes and ketones (Scheme-1). The catalyst was prepared by simple sol-gel method using $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and NH_4OH as precursors. The catalyst has been characterized by X-Ray diffraction (XRD), Fourier Transform Infrared (FTIR), Scanning Electron Microscopy (SEM), UV-Visible spectroscopy (DRS), BET surface area and Temperature Programmed Desorption (TPD) analyses. Boehmite is successfully applied for the condensation reaction between 4-nitrobenzaldehyde and acetone giving α - β unsaturated ketones without any side product. A probable mechanism has been suggested to explain the cooperative behavior of the acidic and basic sites. The catalyst is environmentally friendly and easily recovered from the reaction mixture and it is reusable up to 3 cycles.

Scheme 1: Aldol reaction using boehmite

PP-12**New Zinc functionalized metal organic Framework for selective sensing of chromate ion**

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Metal organic framework have been prepared by the solvothermal process of 2-(4-carboxyphenyl)-1, 3-dioxoisindoline-5-carboxylic acid with $\text{Zn}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (Scheme-1). The framework has a PtS - type net. The obtained porous material has been characterized by X-ray diffraction, Scanning electron microscopy, UV-vis spectroscopy, FTIR spectroscopy and BET surface area analysis. The BET surface area was $757\text{m}^2/\text{g}^{-1}$. The synthesized MOF exhibits reasonably good fluorescence characteristics. The luminescent studies indicates that the obtained Zn MOF could be an efficient material for high sensitivity anion especially CrO_4^{2-} . The mechanism of sensing is also studied in detail. The Zn-MOF senses the anion without altering its structural integrity. This post-synthesis route can be used for synthesis of isomorphous metal-organic frameworks that cannot be obtained by direct synthesis.

Scheme 1- Synthesis of ligand

Keywords: Metal organic frameworks; Zeolites; Zn-MOF; Trimellitimide; Fluorescence Quenching; Metal ion exchange.

PP-13**Selective hydrogenation of cinnamaldehyde over Co-Ni bimetallic catalysts****A.Saranya^{a,b}, G.Vivekanandan^b, K.R.Krishnamurthy^a and B.Viswanathan^a**^a National Centre for Catalysis Research, Indian Institute of Technology, Madras, Chennai-600036,^b Department of Chemistry, A.V.C College, Bharathidasan university, Tiruchirappalli-620024,

Selective hydrogenation of cinnamaldehyde to cinnamyl alcohol is an important reaction with respect to industrial and academic point of view. It has applications in pharmaceutical industries, mainly in field of flavor and fragrance industry and agrochemicals. Cinnamyl alcohol is raw material for cinnamates, used in perfumes. Cinnamyl alcohol is intermediate in preparation of antibiotic Chloromycetin used in treatment of typhoid. Pt based catalysts are known to give very good selectivity (99%) for cinnamyl alcohol, but the TOF of Pt based catalyst are rather poor (TOF=0.03 for 3.8% Pt/C). Among other noble metals like Ir, Ru, Rh, Pd, Palladium has the highest TOF (TOF= 6.7 for 4%Pd/C) but it displays poor selectivity towards cinnamyl alcohol. As noble metal based catalysts are costly, attempts are being made to develop base metal catalysts containing Ni, Co, Cu etc. In this present study Monometallic Ni and Co catalysts and a series of Ni-Co bimetallic catalysts containing both metals in different atomic proportions, with total metal loading of 15% w/w, have been studied. All the catalysts, supported on Titania (P-25), were characterized by XRD, TEM, and TPR measurements. Hydrogenation of CAL in liquid phase was carried out on all catalysts at 20 bar hydrogen pressure, with isopropanol as solvent and at reaction temperatures of ,120°C,130°C,140°C. Ni_{0.4}Co_{0.6} displays maximum CAL conversion and selectivity. The improved performance of this bimetallic catalyst composition is due to the formation of Ni-Co alloy which alters the electronic character of Ni and thereby influencing the mode of adsorption of CAL.

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PP-14

Ethanol Conversion to Higher Alcohols

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The current method for producing 1-butanol is the oxo process, in which petroleum-derived propylene is hydroformylated ($\text{CO} + \text{H}_2$) over a homogeneous rhodium catalyst to form butyraldehyde, which is then hydrogenated to produce 1-butanol. The oxo process is complicated, requires high energy input, and is costly [1] and butanol prices fluctuate with propylene prices. The direct conversion of bio-ethanol to butanol would be a renewable, environmentally “green” process that could become more attractive economically than the oxo process. While bio-ethanol prices will continue to decline over time, oil (and propylene) prices will almost inevitably increase [2–5]. In the Guerbet reaction, ethanol is oxidized to acetaldehyde, which undergoes an aldol condensation to form crotonaldehyde. Crotonaldehyde is then hydrogenated to butanol [6]. In this present study ethanol conversion to higher alcohols is carried out 220°C over two 8%Ni-5%La₂O₃-Al₂O₃ catalysts using Parr reactor. Alumina support was prepared by two different methods, by sol-gel route and by calcination of pseudo boehmite, AlOOH. Catalysts were characterized by TEM, XRD, and N₂ adsorption-desorption isotherm measurements. The surface area of the catalyst synthesized by sol gel method is higher. Though both the catalysts exhibit good activity for dimerization of ethanol, the one with alumina support based on AlOOH, shows better activity.

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PP-15**Sonochemical synthesis of Mg-TiO₂ nanoparticles for photocatalytic degradation of congo red dye**

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In this article, TiO₂ and Mg-TiO₂ photocatalyst were prepared by the facile sonochemical method. The synthesized nanoparticles were characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), EDS, diffuse reflectance spectroscopy (DRS), FTIR and Raman methods. The crystal structure evolution and elemental composition were analyzed by X-ray crystallography (XRD) and X-ray photoelectron spectroscopy (XPS). The calculated band gap energy of Mg-TiO₂ nanoparticles was lower than that of pure P25 TiO₂. The photocatalytic efficiency of the synthesized samples was investigated by performing photocatalytic degradation of congo red under visible light irradiation and it has been found that the Mg-TiO₂ catalysts possess better catalytic activity than pure P25 TiO₂ (Degussa) and undoped TiO₂.

PP-16

Continuously active nanoporous solid acid catalyst synthesis, characterization and heterophase catalytic applications

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Molecular sieves like microporous and mesoporous have variety of applications in the field of catalysis and adsorption.^[1-3] Many mesoporous and microporous materials including Aluminophosphate and silicate have been synthesised with different pore size by using various templates^[1-3]. Most of the molecular sieves are active as a catalyst at higher temperature^[4]. This higher temperature leads to cracking of reactant and products.^[4] So, carbon deposition on the surface and pores of the catalyst deactivate the active sites of the catalyst.^[4] This fact, needs to regenerate the catalyst by removing the carbon as carbon dioxide.^[4] So, we cannot use the catalyst continuously for heterophase catalytic applications. For that, we need addition work to regenerate the catalyst, to overcome these obstacles, a new phase aluminosilicate mesoporous molecular sieves has been synthesised and characterized by XRD, FT – IR, TGA, TPD, SEM, TEM and BET surface area analysis. The SEM image given in the Figure 2 shows the crystalline nature and morphology of the material. TPD curve shown in Figure 1 proved that the material has more active sites in the temperature range 100 to 250°C. This temperature will not crack the molecules and not produce carbon deposit on the surface and pores of the materials. Hence, we can use these new mesophase molecular sieves continuously for heterophase catalytic activity. This new mesophase catalyst is acting as a solid acid so, it can be applied for any acid catalysed reactions. But it has no corrosion and environmental pollution. Ultimately it is a continuously active green catalyst for heterophase catalytic applications. To test the catalytic activity of the molecular sieves, the catalyst is applied to the etherification of glycerol reaction. Diglycerol ether and triglycerol ether formation is more effective within the temperature of 150°C and tetraglycerol ether formation is more in the temperature range of 150 to 250°C. Thus the synthesised new mesophase aluminosilicate molecular sieves is continuously active for heterophase catalytic reaction.

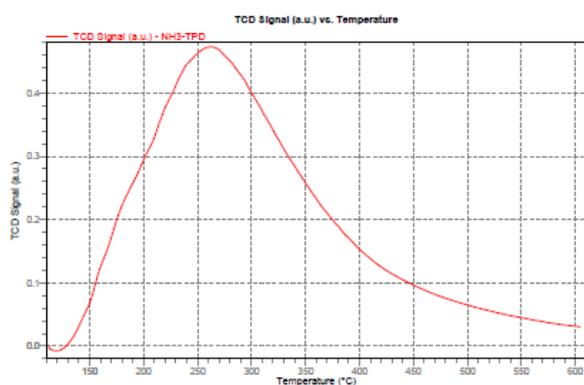


Fig 1: TPD curve for new mesoporous AlSiO_4 .

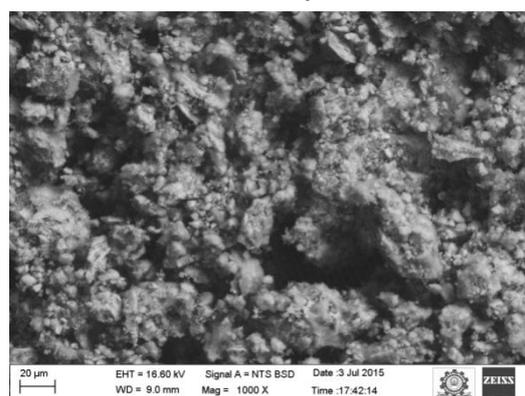


Fig 2: SEM Image for new mesoporous AlSiO_4 .

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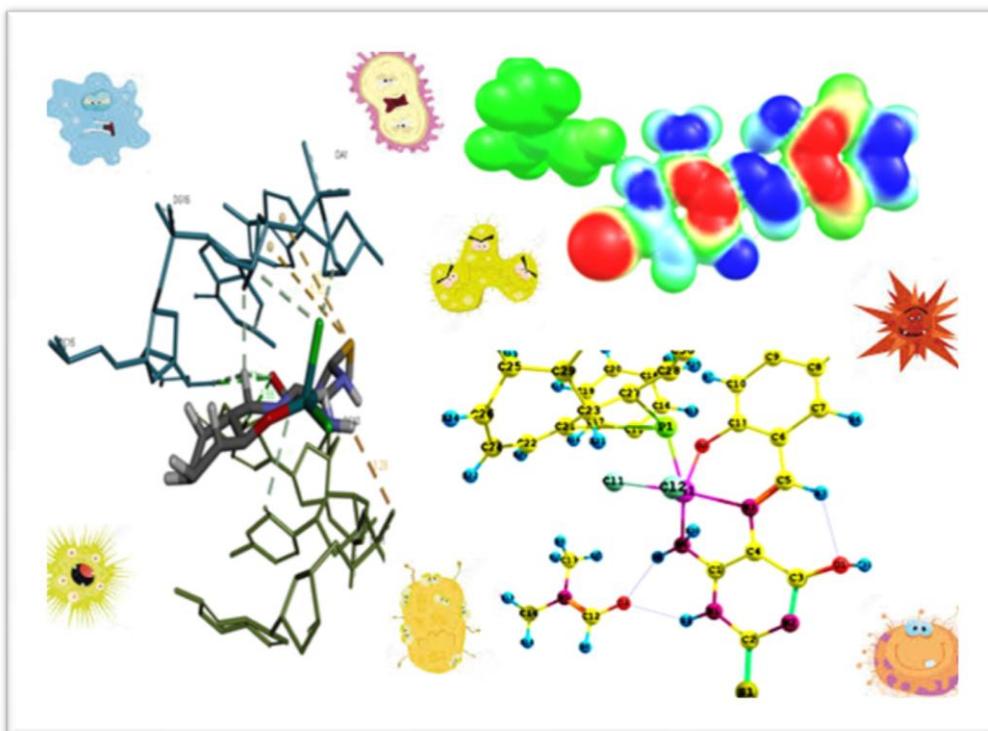
PP-17

Ru(III) mercapto-pyrimidine Schiff base complexes with triphenylphosphine as coligand: Synthesis, characterization, biological and catalytic activity

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A new series of mercaptopyrimidine Ru(III) complexes were synthesized and characterized using various spectral techniques like single crystal XRD, FT-IR, NMR, TGA and EDAX. The complexes were evaluated for their pharmacological activities like *in-vitro* antimicrobial, anticancer and antioxidant. The DNA binding and cleavage studies have been studied and the results has been validated with molecular docking studies. The catalytic applications of the synthesized complexes has been studied and reported.



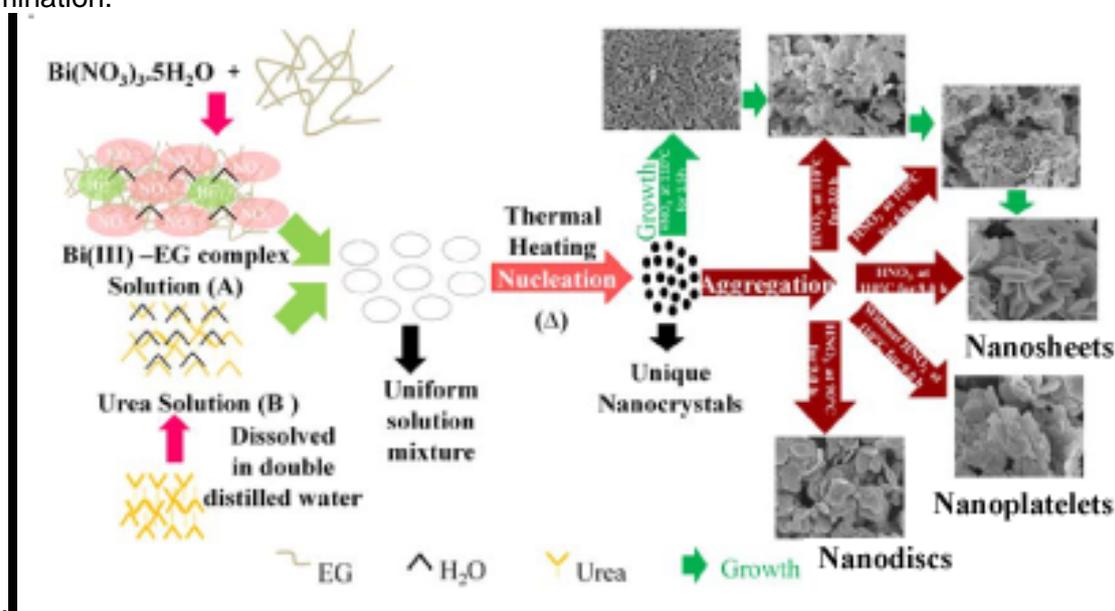
PP-18

Synthesis of Morphology-Controlled Bismutite as Selective Adsorbent and Photocatalyst for Organic Dyes

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Bismutite ($\text{Bi}_2\text{O}_2\text{CO}_3$) possessing diverse morphologies, namely, nanosheets, nanodiscs and nanoplatelets was synthesized by a simple controllable method using bismuth nitrate pentahydrate and urea as precursors in water/ethylene glycol mixture. The as-synthesized samples showed unique physical and chemical properties, such as varying morphology, phase identification, chemical composition, surface area and surface potential. Among these, $\text{Bi}_2\text{O}_2\text{CO}_3$ nanosheets exhibited excellent adsorption capabilities for anionic dyes (acid orange 7 and methyl orange) and high photocatalytic performance for the decolorization of cationic dyes (rhodamine B and methylene blue) under simulated solar illumination.



Schematic illustration for the formation of bismutite with diverse morphologies

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PP-19

Reduced Graphene Oxide Wrapped Ag_3PO_4 composites ($\text{RGO}/\text{Ag}_3\text{PO}_4$): Investigations on Photocatalytic Activity of Methylene Blue Degradation

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RGO based Ag_3PO_4 composite was prepared using simple solution based synthesis technique. The as-prepared $\text{RGO}/\text{Ag}_3\text{PO}_4$ composites was characterized by various characterization techniques. The structural property was studied using X-ray diffraction method (XRD) and Fourier transform infrared spectroscopy (FTIR). The ultraviolet visible diffuse reflectance spectroscopy (UV-vis DRS) was carried to investigate the optical property of composites. The morphological study was analyzed using scanning electron microscopy (SEM) and the presence of Ag, P, O and C were confirmed in the as-prepared $\text{RGO}/\text{Ag}_3\text{PO}_4$ composites. Finally, a complete photocatalytic dye degradation was achieved using methylene blue (MB). The phase of $\text{RGO}/\text{Ag}_3\text{PO}_4$ composites was successfully confirmed and optical properties demonstrate that as-prepared sample exhibits excellent absorption in visible light region. The spherical nature of Ag_3PO_4 and sheet nature of RGO was confirmed in $\text{RGO}/\text{Ag}_3\text{PO}_4$ composites. The electrical and dielectric properties also studied. The higher degradation efficiency was achieved for 5 wt% $\text{RGO}/\text{Ag}_3\text{PO}_4$ composites. The charge transfer process between RGO and Ag_3PO_4 is schematically illustrated.

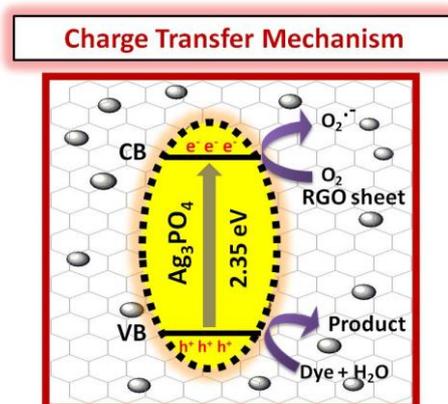


Figure 1. Charge transfer process between RGO sheet and Ag_3PO_4

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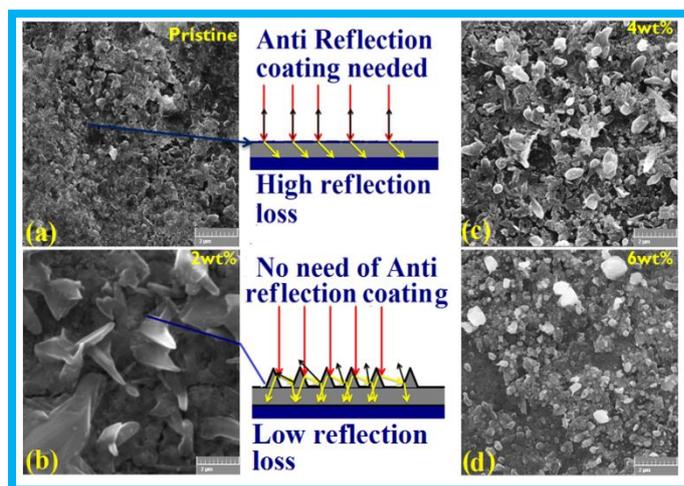
PP-20

High transparent and conductive micro flakes assembled aluminium doped zinc oxide thin films for photocatalytic and photovoltaic applications

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Highly transparent and conductive Al doped ZnO (AZO) thin films were successfully deposited on glass substrate by facile homebuilt chemical spray pyrolysis method. The structural, morphological, optical and electrical properties of pristine and AZO thin films have been systematically inspected. From XRD analysis, both pristine and AZO thin films were found to be polycrystalline in nature with hexagonal wurtzite structure. The presence of dopant and host elements is confirmed by energy dispersive X-ray spectroscopic (EDX) analysis. All the films exhibit the average transparency of 90-95% in the visible region. The decreases of orbital energy gap values are observed using UV-vis absorption spectra according to 2 wt% Al doping level into the ZnO lattice sites and then it increases for 4 and 6 wt%. The decrease of band gap for 2wt% of AZO thin film is due to the formation of impurity states near to the conduction band.¹ The conductivity of the film increases upto 2 wt% of Al and then it decreases for 4 and 6 wt%. Rapid decrease in resistivity for 2 wt% of Al doped ZnO from 17800 Ω cm to 3.812 Ω cm is due to the large number of charge carriers $3.490 \times 10^{17} (\text{cm}^{-3})$. Because of an increase in impurity scattering due to Al doping, the mobility of the majority charge carrier decreases for 2, 4 and 6 wt%.¹ From SEM and AFM analyses it is found that the surface of 2 wt% of Al doped ZnO has standing alone micro flakes hence it will also acts as an antireflection layer.² By considering all the factors (High Transparent, high conductivity, wide bad gap and antireflection layer), we conclude that 2 wt% of AZO is the best choice for for photocatalytic and photovoltaic applications.^{3,4}



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PP-21

MoS₂-Graphene oxide Composite for supercapacitor electrode material*Nikhitha Joseph and A Chandra Bose[#]**Research scholar, National Institute of Technology, Tiruchirappalli-620015**[#] Corresponding author. [#]Email: acbose@nitt.edu*

Supercapacitors are new energy storage devices, which is important because of long service life time, fast charge/discharge process and green environmental protection [1]. Molybdenum disulphide has attracted considerable attention for supercapacitor electrode application due to its sheet like structure, which provide a large surface area for charge storage. In this work we successfully synthesised MoS₂–graphene oxide composite by simple hydrothermal method. MoO₃ and thiourea is the precursors for the preparation of MoS₂ and graphene oxide is prepared by modified Hummers method. XRD pattern confirms the crystallinity of the as prepared sample. FTIR spectra shows the purity of the material. Raman spectra confirms the formation of MoS₂-graphene oxide composite, Fig. 1 shows the Raman spectra of as prepared composite.

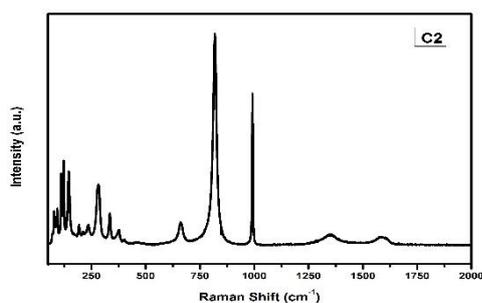


Fig.1 Raman spectra of as prepared composite

Electrochemical property of the as prepared composite is studied by SP-150 bio-Logic electrochemical workstation. CV curves shows the double layer capacitive behaviour of the material. The specific capacitances of the as prepared material is obtained as 578 F/g. Fig. 2 shows the cyclic voltammetry graph of the as prepared sample.

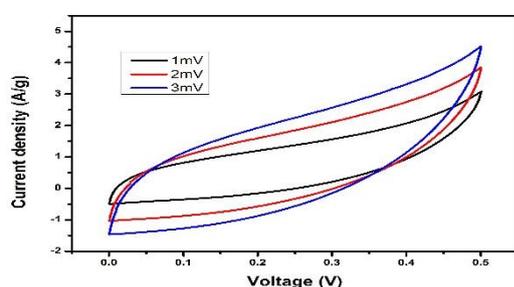


Fig.2 CV graph of MoS₂-GO composite material

In summary, the sheet like MoS₂-Graphene oxide Nano-composite were prepared by simple hydrothermal method. XRD pattern proves the crystalline nature of the as prepared material. Electrochemical studies proves the supercapacitive property of the material. The specific capacitance of the as prepared material is obtained as 578 F/g. The outstanding electrochemical property of the composite material leads to the potential application for high performance supercapacitor.

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PP-22

LaMnO₃ Perovskite as electrode material for energy storage devices*P. Muhammed Shafi and A.Chandra.Bose***Nanomaterials Laboratory, Department of Physics**National Institute of Technology, Tiruchirappalli- 620015**Corresponding Author: acbose@nitt.edu

Perovskite oxides have attracted significant attention as energy conversion materials for metal–air battery and solid-oxidefuel-cell electrodes owing to their unique physical and electronic properties. Perovskites have a cubic structure with general formula of ABO₃. In this structure, an A-site ion, on the corners of the lattice is usually an alkaline earth or rare earth element. B site ions, on the centre of the lattice, could be 3d, 4d, and 5d transition metal element. Here we demonstrate the LaMnO₃ nanomaterial as supercapacitor electrode. LaMnO₃ was prepared by simple precipitation method. The as-prepared sample was annealed at 750 °C for 12h. The structural formation of as- prepared and annealed MnO₂ nanoparticles are confirmed by XRD analysis. The functional group and formation of chemical bond between metal ion and oxygen are studied by Fourier transform infrared spectroscopy (FTIR). Morphological analysis was carried out by field emission scanning electron microscopy (FESEM). Finally electrochemical properties were evaluated using cyclic voltammetry (CV) and galvanostatic charge-discharge techniques.

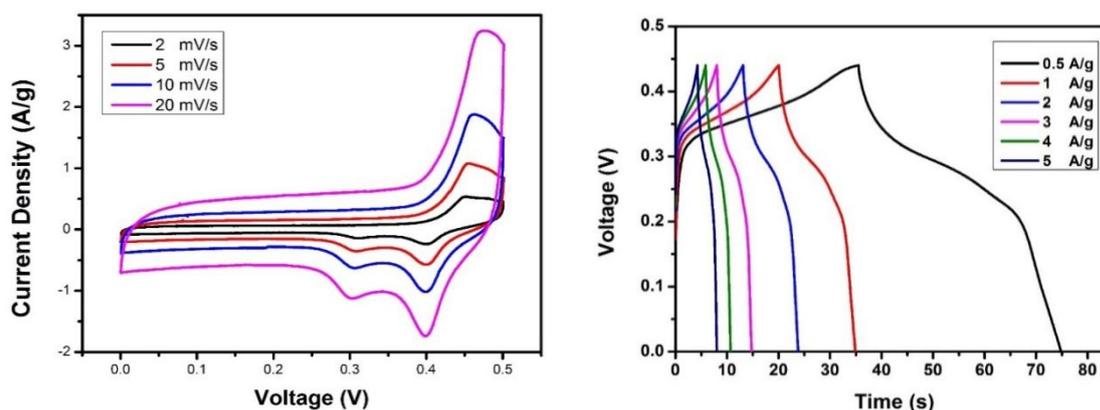


Figure 1. Cyclic voltammogram at different scan rate (a) and Galvanostatic charge-discharge curve at various current densities (b) recorded for LaMnO₃ sample.

Typical cyclic voltammetry curves and galvanostatic charge discharge plots are shown in fig.1. CV curves can be observed as pseudo rectangular in shape with oxidation (0.48V) and redox (0.38V) peaks. It indicates supercapacitive nature of the material¹. The presence of oxidation and reduction peak denotes that double-layer capacitance and pseudo-capacitance contributes to capacitance of the material. The symmetric nature shows the reversibility of the material. Since the material retains shape at higher scan rates, the high stability of the materials is revealed. GC curves are nearly symmetric triangular shape, indicating the pseudo-capacitive nature of electrode material¹. The discharge time decrease with the current density. Hence the electrochemical studies for LaMnO₃ perovskite nanomaterial strongly recommend for the electrodes in energy storage devices.

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PP-23

Effect of Acidic and Neutral electrolytes in the Co_3O_4 material for supercapacitor application

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Co_3O_4 nanomaterial has been synthesized using the hydrothermal method. Crystalline structure of the material is confirmed using XRD pattern which is in good agreement with the JCPDS card no:43-1003 confirms the cubic crystal structure. Raman studies confirms the formation of tetrahedral and octahedral sites of the Co_3O_4 nanomaterial. SEM images shows the rod like nature of the material. Electrochemical studies of the material were tested using electrochemical workstation SP-150. Specific capacitance of the material was tested using the Cyclic voltammetric and charge discharge studies as shown in Fig.1. KOH (acidic) and Na_2SO_4 (neutral) are used as an electrolyte. The Maximum specific capacitance is calculated from the KOH electrolyte is 255 F/g at a scan rate of 2 mV/s and from the Na_2SO_4 electrolyte reaches only up to 30 F/g at a scan rate of 2 mV/s. The main reason for obtaining lowest value is the hydrated ion size of the electrolytes such as SO_4^{2-} (3.79) is large compared to OH^- (3.00Å) ions¹. EIS of the material studied with 2 different electrolytes and the calculated R_{ct} value for KOH is 0.47 Ω and Na_2SO_4 is 93.64 Ω .

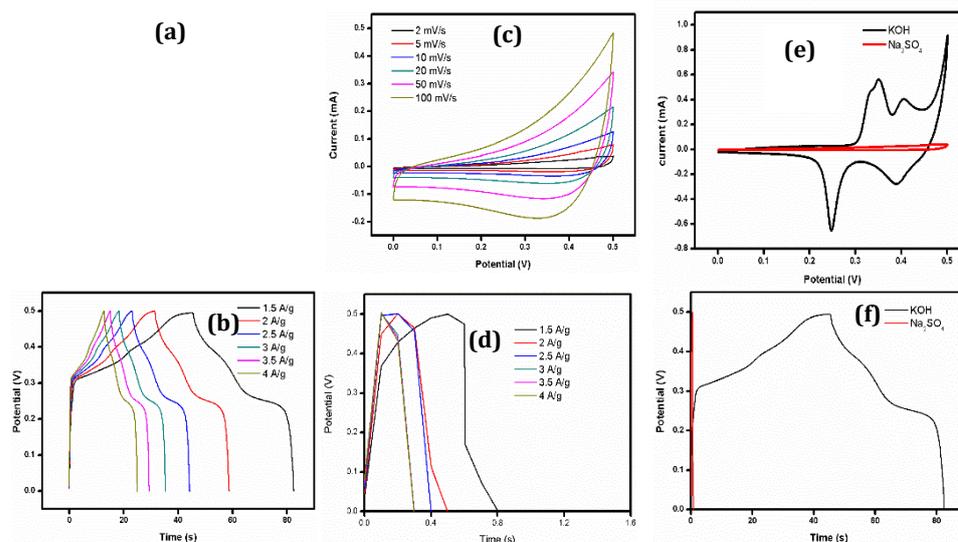


Fig.1.(a&b) CV and CHDH study using KOH (c&d) CV and CHDH study using Na_2SO_4 (e&f) comparison plot of 2 different electrolytes

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PP-24

Catalytic Properties of Mesoporous Silica-supported Sulfated-Zirconia

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Solid acid catalysts have attracted attention as a potential replacement of homogeneous catalysts because catalyst separation process is easier and it can be regenerated with simple methods¹. Among the solid acid catalysts, sulfated-zirconia (SZ) has attracted considerable attention because of its “super-acid” property. But the low surface area of the bulk sulfated zirconia catalyst hinders its applications for catalyzing bulky organic molecules². In this work, highly dispersed sulphated zirconia has been supported on mesoporous silica e.g., SBA-15, using a post-synthesis grafting method³. The synthesized materials, viz., SZ/SBA-15, were systematically characterized by various techniques such as XRD, TEM, NH₃-TPD, and N₂ sorption measurements. The prepared catalysts at two different calcinations temperature (600 and 650°C) could retain the ordered mesoporous hexagonal structure even after grafting as shown in Fig. 1(A) and it is well supported by TEM monograph Fig. 1(C). Also the monoclinic phase (M) of zirconia starts emerging along with tetragonal phase (T) when the calcinations temperature was increased from 600 to 650°C as depicted in Fig. 1(B). Moreover both the prepared catalyst had higher amounts of acid sites because of the interaction of the highly dispersed sulfated zirconia with the large surface area of SBA-15. Catalytic activity of the prepared water tolerant solid acid catalyst was evaluated using acetonation of *D*-glucose as a model reaction⁴. Mono product (1,2-O-isopropylidene- α -*D*-glucofuranose) formation during acetylation of *D*-glucose is found to be catalyzed by strong acid sites whereas the Di product (1,2:5,6-di- O-isopropylidene- α -*D*-glucofuranose) by the weak ones.

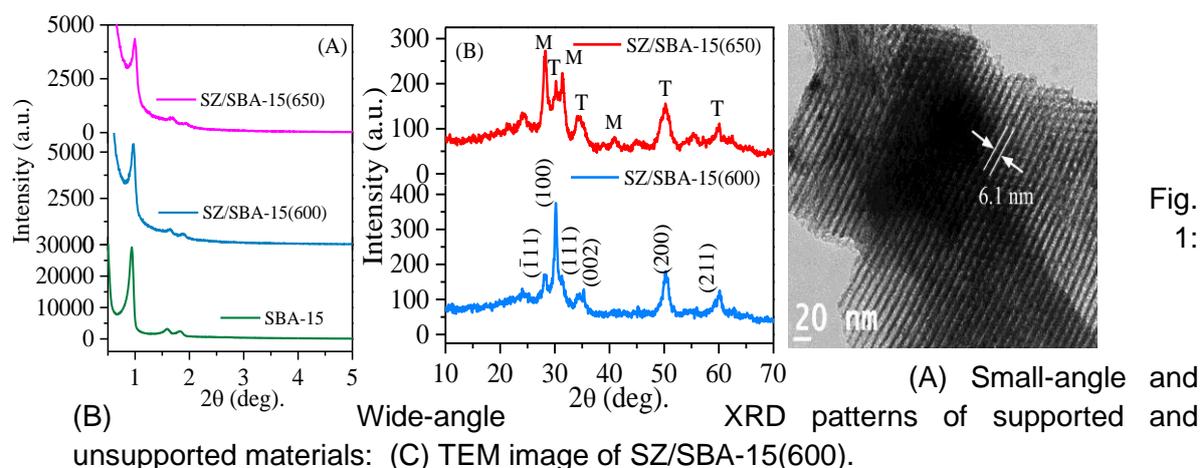


Fig. 1:

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PP-25

Ratiometric chemosensor for the selective detection of Cr³⁺ ion

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A ratio metric chemosensor containing a naphthalene moiety was designed and synthesized (**fig.1**) for the selective detection of trivalent chromium ion over other common metal ions using an intermolecular-charge transfer (ICT) mechanism. The synthesized probe was characterized by IR, ¹H NMR, and ¹³C NMR. The synthesized probe exhibited high selectivity and sensitivity towards Cr³⁺ over other cations such as Mn²⁺, Fe³⁺, Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, Hg²⁺ and Al³⁺ ions. (**fig.2**). A perfect color change from yellow to colorless under ACN medium upon the addition of Cr³⁺ was observed, while no change was observed on the addition of other metal ions. (**fig.3**). 2:1 stoichiometry and micro molar detection limit was observed.

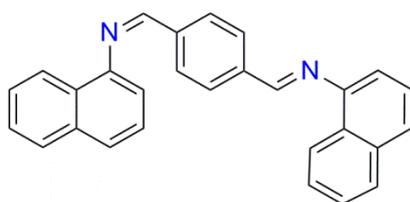


fig.1 Structure of Receptor
fig.2

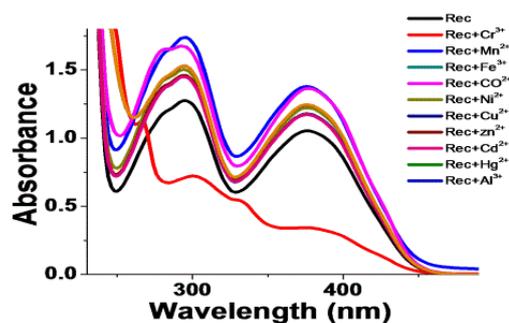


fig . 3. Naked eye sensing of anions

PP-26

Synthesis and characterization of hierarchical zeolites

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The remarkable discovery of diverse zeolite structures and their innovative application in refineries has reformed the industrial catalysis¹. In particular, zeolites with MFI topologies have been prominent solid acid catalysts due to their unique properties, viz., strong Brønsted acidity, distinct pore interconnectivity and high thermal and hydrothermal stability. Nevertheless, the internal surface area is inaccessible by bulkier molecules and that the presence of such micropores ($d \sim 0.5$ nm) with strong acid sites can retard the molecular transport to deactivate the catalyst. In order to overcome such limitations, the last two decades have seen numerous efforts in synthesizing ordered mesoporous materials (OMMs) using the concept of supramolecular templating.²⁻⁴ Despite their enhanced diffusion, these materials have failed to make impact at industrial scale due to their demerits viz., amorphous pore-walls, low stability and moderate acidities. Hence, the recent innovation of hierarchical zeolitic-type materials possessing the unique properties of both zeolites and OMMs have emerged as a potential solid acid catalysts.⁴ In this study, an attempt has been made to synthesize and characterize hierarchical zeolites of type-MFI having both micropores and mesopores using dual templating (organosilane-dimethyloctadecyl[3(trimethoxysilyl)-propyl]ammonium chloride and TPABr) methodology. XRD pattern (Fig. 1A) of hierarchical zeolite depicts characteristic reflection in the low-angle (inset) typical of 2D-hexagonal structure (MCM-41)^{2,3} while the high-angle pattern is distinctive of MFI (ZSM-5)⁴ structure. Fig. 1B depicts the TEM image and SAED pattern (inset) showing mesopores (3 nm) amidst the intricate network of micropores (0.5 nm). Further work is in progress to evaluate the activity of the materials.

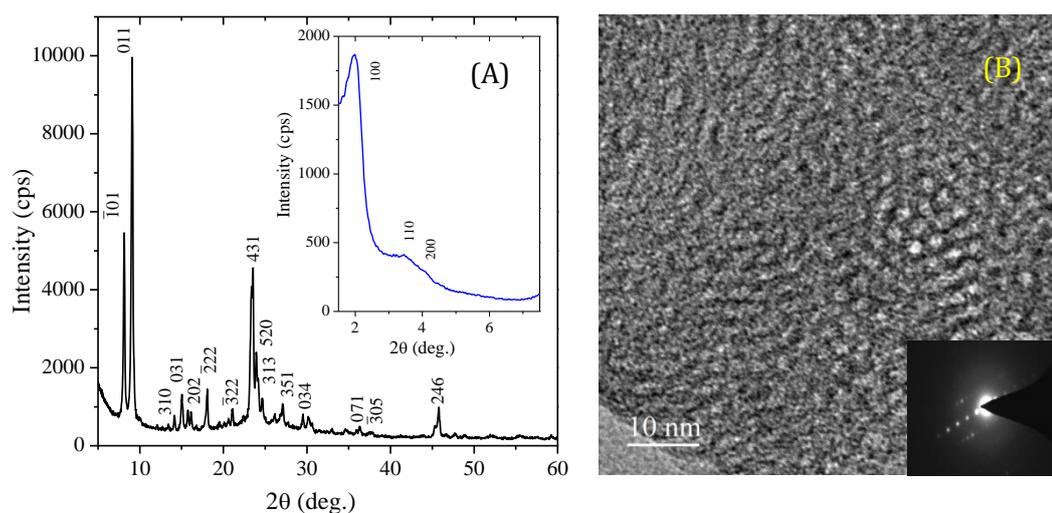


Fig. 1: (A) XRD pattern and (B) TEM of hierarchical Na-ZSM-5. Inset - SAED pattern.

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PP-27

Synthesis of novel chitosan based ZnO/SnO₂ nanocomposites for supercapacitor applications*Packirisamy, Rajiv Gandhi¹, Govindasamy, Chandramohan¹, Sanmugam, Anandhavelu² and Vikraman, Dhanasekaran³*¹*Research & Development Centre, Bharathiar University, Coimbatore 641046, India.*²*Department of Chemistry, Vel Tech Multi Tech., Chennai 600062, India.*³*Division of Energy Systems Research, Ajou University, Suwon 16499, Korea.*

Organic-inorganic nanocomposite materials have attracted substantial attention because of their feasibility to wide range applications such as super capacitors, anti-bacterial activity, biomedical sensors, battery applications and microfluidic devices. In this work, the novel chitosan based zinc oxide (ZnO)/tin oxide (SnO₂) nanocomposites synthesized by chitin deacetylation method using chitin polymer, zinc chloride (ZnCl₂) and tin chloride (SnCl₂) as precursors in presence of NaOH. FTIR spectra of nanocomposites confirmed their presence by functional groups observation. The optical properties and their characteristic peak position were observed by UV-vis spectra. X-ray diffraction (XRD) patterns revealed the mix of hexagonal and tetragonal phase polycrystalline nature of chitosan-ZnO/SnO₂ nanocomposites exhibited with (002) predominant lattice plane. The average crystallite size of chitosan-ZnO/SnO₂ nanocomposites was estimated at ~11.2 nm by Debye-Scherrer's formula. The surface morphology and topography demonstrated by FESEM and AFM analysis, respectively. The shape and size of the grains were discovered by TEM analysis. The elemental composition ratio of chitosan-ZnO/SnO₂ nanocomposites was studied by EDX tool. Synthesized chitosan-ZnO/SnO₂ nanocomposites ability for electrochemical capacitance application performed by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

PP-28**Photocatalytic Removal of Phosphate in Aqueous Media using P/CeO₂ Nanomaterial**

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Phosphate is present in numerous types of wastewater, from low to high concentration and is a rich source of phosphate reaching natural environment. Excess of phosphate in surface water may lead to eutrophication, which cause reduction in oxygen concentration and degrades water quality. In recent decades, various studies have been carried out to find an effective method for phosphorus removal, such as chemical precipitation, biological treatment, reverse osmosis, contact filtration, and adsorption; each of them has their own advantages and disadvantages. Complete removal of phosphate from wastewater is still a serious challenge and sustainable removal of phosphate from water is urgently required for the benefit of environment aesthetic. Phosphate removal using nanoparticles is one of the emerging fields, which still needs its recognition in the wastewater treatment area. In recent years, various studies have been conducted on the phosphate removal using different nanoparticles and the results obtained were feasible. In the present study, preparation of visible spectrum responsive photocatalyst such as P/CeO₂ was carried out under mild sol-gel technique. As-prepared photocatalyst was characterized for photocatalytic activity using model dye and its shows about 90-95% efficiency. Removal of phosphate from aqueous solutions was carried out using P/CeO₂ nanomaterial under different light sources. The results obtained clearly indicated potential removal of phosphate up to 97.10% under LED light irradiation for 5 h duration. The phosphate removal exhibits by nanomaterial under remaining light sources were as follows: visible light (79.28%), UV (88.76%) and Tungsten (95.06%). The present study clearly indicated that potential removal of phosphate in aqueous media could be achieved P/CeO₂ nanomaterials under LED light irradiation.

Keywords: Photocatalytic; Phosphate; Eutrophication; Nanomaterial; LED light

PP-29

Nitrogen-containing ordered mesoporous carbons as metal-free catalysts for oxygen reduction reaction in acidic medium*Talla Venkata Rama Mohan^a and Parasuraman Selvam^{a,b}*^a *National Centre for Catalysis Research and Department of Chemistry, Indian Institute of Technology-Madras, Chennai 600 036, India*^b *New Industry Creation Hatchery Center, Tohoku University, Sendai 980 8579, Japan*selvam@iitm.ac.in

Metal-free catalysts have attracted attention towards oxygen reduction. Among the various heteroatom-containing carbon materials, particularly nitrogen-containing ordered mesoporous carbons are of considerable interest and desirable as they enhance the mass transport, and that they can accommodate more catalytic sites.¹ Therefore, in this investigation, an attempt has been made to prepare a series of nitrogen-containing electro catalysts using carbon (sucrose) and various nitrogen-containing carbon precursors, viz., polyvinyl pyrrolidone, aniline and pyrrole, and ordered mesoporous silica (SBA-15) as hard-template.²⁻⁶ The resulting samples were designated as CMK-3, NCMK-31, NCMK-32, and NCMK-34, respectively. All the samples were systematically characterized by various analytical, spectroscopic and imaging techniques, followed by ORR measurements in acidic condition. From the TEM images (Figure 1), it can be seen that the prepared catalysts are showing long-range order with uniform pores. Figure 2 shows the current density plots for ORR in 1 N H₂SO₄ medium among which NCMK-31 exhibit electrochemical activity of 16.4 mA mg⁻¹. The observed trends in ORR activity could be accounted for the surface (nitrogen) functionalities, viz., pyridinic, quaternary and pyrrolic, of the catalyst surface as evidenced from XPS analyses.

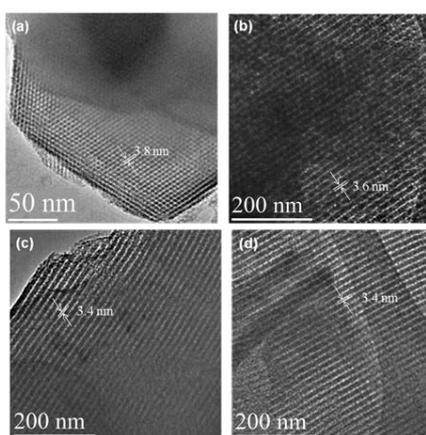


Figure 1: HRTEM images of: (a) CMK-3 (b) NCMK-31 (c) NCMK-32 (d) NCMK-34.

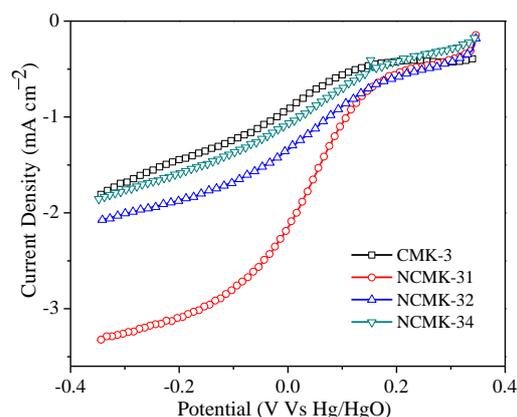


Figure 2: LSV curves for the catalysts in 1 N H₂SO₄ from the oxygen saturated solution at rpm of 1600 rpm with 20mV/s scan rate.

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PP-30**Electrochromic properties evaluation of undoped and rare earth doped V₂O₅ thin films***Shrividhya Thiagarajan*^{1*} and Ravi Ganesan²

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Electrochromic materials have received considerable attention due to their applications in energy efficient smart windows, display and switching device applications. Transition metal oxides are widely explored as potential candidates for electrochromic applications. Among them V₂O₅ is an important functional materials with good electrochemical and electrochromic properties that can be tailored for extensive applications in smart windows, anti-glaring reflection mirrors, electrochromic switching devices, electrochemical based sensors, supercapacitors and energy storage devices. In present work, undoped, Ce and Gd doped vanadium pentoxide (V₂O₅) thin films were deposited onto ITO coated glass substrates by electron beam evaporation method. Single phase V₂O₅ thin films oriented along (001) plane was affirmed from XRD and micro-Raman analysis. Spherical shaped particles with average size of 150 to 300 nm were observed in FESEM micrographs. Oriented growth was further confirmed from AFM images consistent with XRD results. Spectro-electrochemical studies revealed that the deposited thin films were suitable for electrochromic applications. Gd doped thin films exhibited good coloration efficiency of about 16 cm²/C.

PP-31

Catalytic conversion of polyols (sorbitol and xylitol) to hydrocarbons over hierarchical ZSM-5 zeolite catalysts in a fixed bed reactor

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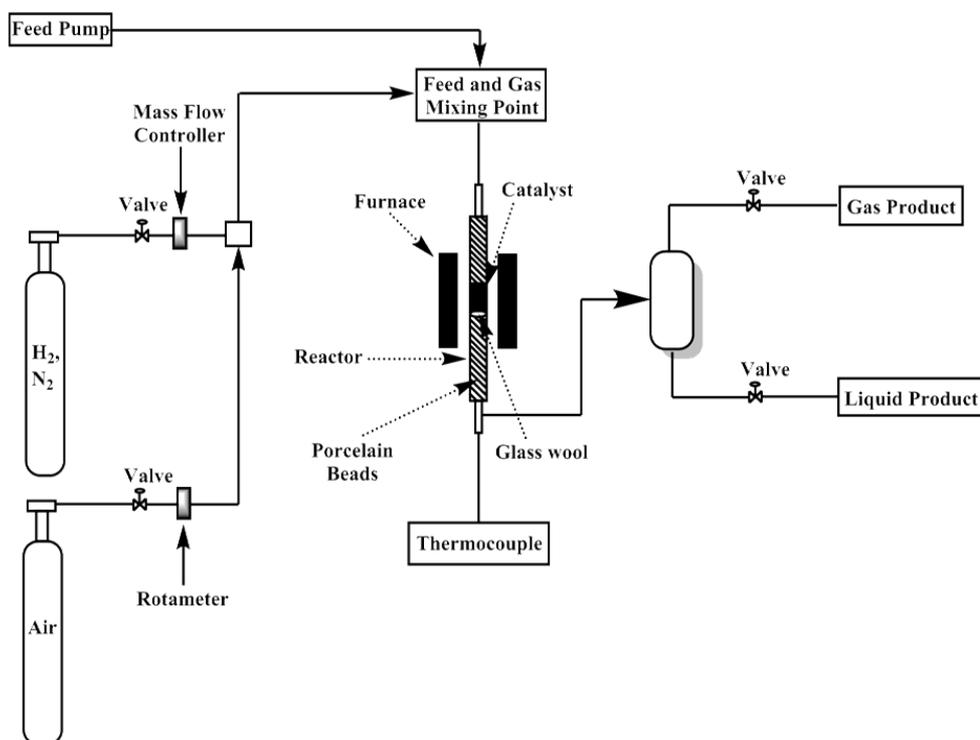
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Renewable biomasses to fuels are of vast significance on the potential substitution for diminishing fossil fuels. In this communication we show that hierarchical ZSM-5 zeolites catalyses the polyols (sorbitol and xylitol) to hydrocarbons conversion reaction under atmospheric pressure in a fixed bed reactor by altering different parameters. A lower sorbitol and xylitol conversion was achieved at the reaction temperature of 375 °C, whereas a higher value of 92.33% and 88.19% sorbitol conversion, 95.58% and 92.32% xylitol conversion was obtained when the reaction temperature was further elevated to 425 °C for ZSM-5-WS(28) and ZSM-5-WOS(28) catalysts.

S. Narayanan, J. Judith Vijaya, S. Sivasanker, T.M. Sankaranarayanan, C. Ragupathi and L. John Kennedy

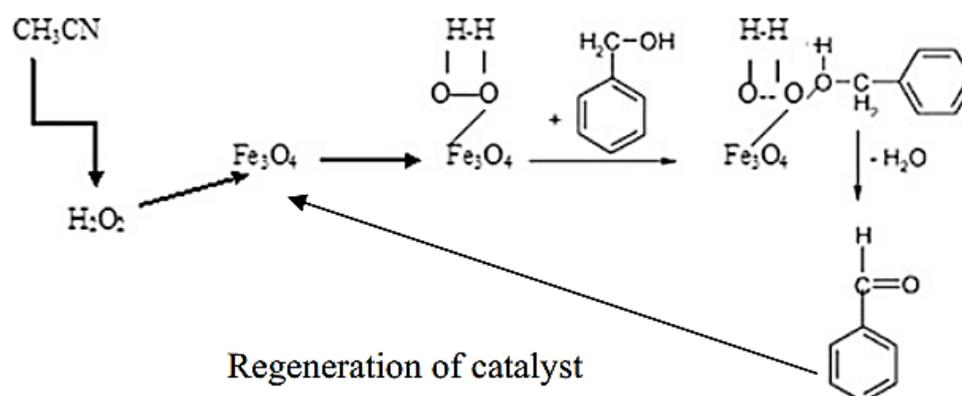


PP-32

Structural, Magnetic, Optical, and Catalytic Properties of Fe₃O₄ Nanoparticles by the Sol-Gel MethodC. Ragupathi^a,^a*Sriram College of Arts and Science, Perumalpattu, Tiruvallur (Dist.)*

This article was aimed to extend a simple procedure for the preparation by a sol-gel method by using iron nitrate and polar solvent (e.g., water) as the starting materials from the viewpoint that they are of low cost. A study of the effect of chelating agents such as citric acid weight ratio on the structure of Fe₃O₄ was reported. The synthesized product was characterized by powder X-ray diffraction (XRD), high-resolution scanning electron microscopy (HR-SEM), high-resolution transmission electron microscopy (HR-TEM), photoluminescence (PL) studies, and vibrating sample magnetometer (VSM). Magnetic analysis revealed that the Fe₃O₄ nanoparticles had a ferromagnetic behavior at room temperature with a saturation magnetization of 20.83 emu/g. Furthermore, Fe₃O₄ nanoparticles prepared by the sol-gel method using citric acid were tested for the catalytic activity towards the oxidation of benzyl alcohol.

C. Ragupathi

**Scheme 1** Oxidation of benzyl alcohol using iron oxide catalyst

PP-33

Effect of hydrochloric acid catalyst on hydrolysis of bio-inspired superhydrophobic and ultraviolet radiation cured titanium dioxide - silane waterborne coating

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Surfaces with water contact angle (**WCA**) $\geq 150^\circ$ are known as superhydrophobic surfaces. The non-wetting lotus (*Nelumbo nucifera*) leaf is often related to extreme purity have WCA $> 160^\circ$ is an example for self-cleaning superhydrophobic surface.¹ The water droplet rolls over the lotus leaf's surface taking away all the dirt and leaving a clean surface behind for photosynthesis. This effect is called "lotus effect" and the surface fabricated with lotus effect is called self-cleaning superhydrophobic surface. Compared to lotus effect, there is an effect called rose "petal effect", a superhydrophobic state with WCA $\geq 150^\circ$.^{2, 3} A water droplet on the surface of the rose petal (*rosea Rehd*) is spherical in shape and it cannot roll off even when the petal is turned upside down. Surfaces fabricated with petal effect generally have high adhesion and is called high adhesion superhydrophobic surface.² Nature designed these surfaces by creating a micro and nano asperities composed of three-dimensional low surface energy epicuticular waxes. Artificial surfaces with superhydrophobicity are generally fabricated by two kinds of approaches: creating micro-/nanostructures on hydrophobic substrates or chemically modifying a micro-/nanostructured surface with materials of low surface free energy.⁴ Among electromagnetic radiation, using ultraviolet (UV) radiation for modifying the surface is an easily applicable and economical method. UV irradiation of monomers lead to photo-polymerization and UV irradiation of polymer surface leads to a series of reactions, such as photo-crosslinking, photo-oxidation in air or photochemical reaction in reactive atmosphere.

The nano-particle titanium dioxide pigment was used to create micro and nano-structures by bonding with hydrolyzed vinyltrimethoxy silane to create "lotus effect" superhydrophobic surface. Silanes are good adhesion promoters which bind on the surface of titanium dioxide and coating substrate by undergoing hydrolysis to form oligomeric polysiloxanol. The oligomeric polysiloxanol then undergo condensation reaction to form oligomeric polysiloxane having low surface energy⁵. The role of hydrochloric acid catalyst in the immiscible water and vinyltrimethoxy silane (heterogeneous system) for the hydrolysis of vinyltrimethoxy silane to form oligomeric polysiloxanol was studied. The C=C groups in the vinyltrimethoxy silane were irradiated with ultraviolet radiation from medium pressure mercury vapour lamp to undergo photo-polymerization. The fabricated superhydrophobic coating was characterized by SEM, FTIR-ATR and XPS studies.

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PP-34

Sensitized and Integrated Photocatalytic Adsorbent

Hybrid Catalyst (TCPP-TiO₂-CMK-3) for Degradation of Pharmaceuticals

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Pharmaceutical drug causing water pollution has been a growing threat to lives. In order to tackle inefficiency of existing water treatment plants, we need to look at solutions such as advanced photo catalytic degradation¹. This work is on the development of TiO₂ based advanced oxidation catalyst for photo catalytic degradation of Famotidine (FAM), an important pharmaceutical drug found in river water. TiO₂ is one of the most studied photo catalyst for such degradation; however, its activity is hampered owing to: 1) low surface area; 2) diffusion limitations; 3) limited to photon adsorption in UV light region or inability to access visible light region; 4) high electron-hole (e⁻-h⁺) recombination rate². Techniques for the improvisation of properties of TiO₂ are investigated in the present work.

Tetra (4-carboxyphenyl) porphyrin (S) sensitized ordered mesoporous TiO₂ (MTO-123) integrated to ordered mesoporous carbon CMK-3 with high adsorption capacity solves limitations of low adsorption capacity and limited photon absorption. Figure 1 shows the UV-Visible spectra of the extended photon absorption into visible region of sensitized integrated photocatalytic adsorbent (S-MTO-123/CMK-3). Figure 2 demonstrates the excellent synergistic activity of the catalyst. The calculated rate constant of S-MTO-123/CMK-3 is 2.3 times higher magnitude than the pristine TiO₂ which indicates an improved catalytic activity of the prepared catalyst.

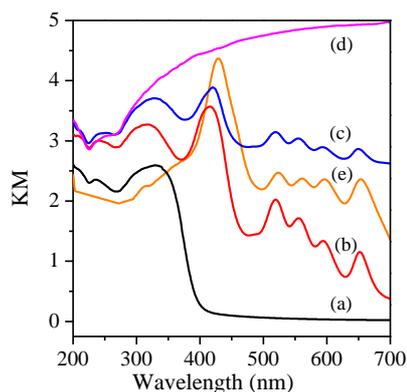


Figure 1. UV-Visible spectra of: (a) MTO-123; (b) S-MTO-123; (c) S-MTO-123/CMK-3; (d) CMK-3; (e) TCPP.

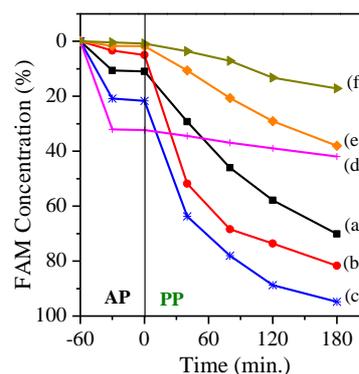


Figure 2. Photocatalytic degradation of FAM : (a) MTO-123; (b) S-MTO-123 ; (c) S-MTO-123/CMK-3 ; (d) CMK-3; (e) TCPP; (f) Photolysis. AP-Adsorption phase; PP-Photocatalytic phase. Reaction conditions: FAM conc.: 100 ppm, time: 4 h, Vol.: 200 mL; Light source: Medium pressure Hg lamp.

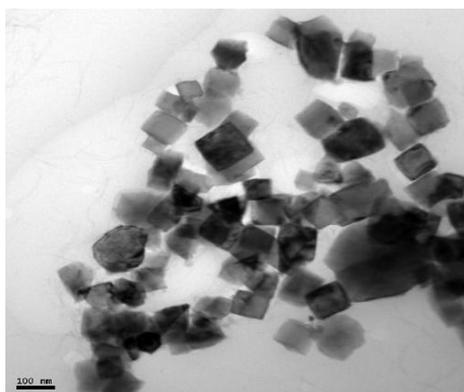
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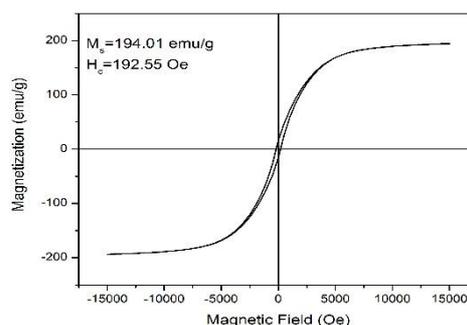
PP-35**Synthesis and magnetic properties of Fe nanoparticles by polyol process**

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Biomedical application like magnetic separation and drug delivery requires magnetic nanoparticles with higher saturation magnetization. Fe with the bcc structure has a high saturation magnetisation of 220 emu/g. Synthesizing pure Fe nanoparticle is a challenging task due to its high surface oxidation and low reduction in solution. We have synthesized pure Fe nanoparticles using polyol process in the presence of excess NaOH as reducing agent. The size of the as-synthesized nanoparticles was found to be 150 nm without nucleating agent. The size of the Fe nanoparticles was further reduced using platinum as heterogeneous nucleating agent and a gradual decrease in size of Fe nanoparticle from 150 nm to 10 nm with the increase in Pt molar concentration from 0 to 2×10^{-6} M was observed. The synthesized Fe nanoparticles showed cubic morphology.



TEM Micrograph of Fe nanoparticle



Room temperature Hysteresis loop for Fe nanoparticle

We observed gradual fall in magnetisation as the size of the Fe nanoparticles reduces. This may be due to the formation of oxide layer around the Fe nanoparticles. The synthesized nanoparticles could be surface modified for various biomedical applications and their results shall be presented.

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PP-36**Strategic Green Synthesis, Characterization and Catalytic activity of Palladium nanoparticles**

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A simple and effective green synthesis method has been demonstrated to synthesis palladium nanoparticles (PdNPs) using seed extract of milk thistle (*Silibum marianum* (SM)). The synthesized PdNPs was characterized by ultraviolet-visible (UV-Vis) spectroscopy, X-ray diffraction (XRD) pattern, transmission electron microscopy (TEM) analyses to elucidate the formation, crystalline nature and morphology respectively. The identification of possible biomolecules responsible for the reduction and stabilization of PdNPs was characterized through Fourier transform-infrared (FT-IR) spectroscopy. The catalytic activity of PdNPs was confirm in the reduction reaction of 4-nitrophenol to 4-aminophenol and it was monitored using UV-Vis spectroscopy.

Keywords: Green synthesis of palladium nanoparticles, *Silibum Marianum* seed extract, Catalytic activity.

PP-37

Kinetics and isotherm studies on the deletion of nickel (II) ions using novel nano-porous adsorbent

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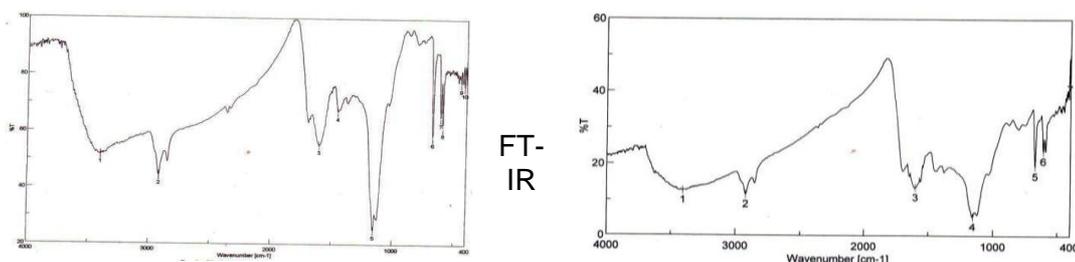
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Novel nano-porous carbon was synthesized for the removal of the nickel (II) from the solvent phase. Hence this study investigated the ability of nano-porous carbon in nickel (II) adsorption¹. The influential parameters including contact time (min), adsorbent dosage (g/L), pH and the initial concentration of nickel (II) were investigated and optimized using the batch adsorption study². The adsorption equilibrium and kinetic data were well fitted and found to be in good agreement with Langmuir and pseudo-second order kinetic model respectively and the maximum nickel (II) percentage removal using nano-porous carbon was 85.52% and 89.41%, respectively under optimum conditions³. The maximum removal of Ni (II) was observed at pH = 6.7. Upon experimentation, it was observed on increasing the adsorbent dosage and initial concentration the amount of nickel (II) removal efficiency also increased. Finally, it can be concluded that the prepared nano-porous carbon can be applied as the best adsorbent to remove the nickel (II) from aqueous solution^{4,5}.

Keywords: Nano-porous carbon, Adsorption, Nickel and Isotherm studies.

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Spectrum of AMS-NC before and after adsorption of nickel (II) ions

PP-38**The enhanced electrochemical study of Lanthanum doped CuS Nanoparticles**K. Jeyabanu¹, N. Nallamuthu^{1*}, P. Devendran¹, T. Shrividhya¹ and R. Packiaraj¹¹Department of Physics, International Research Centre (IRC), Kalasalingam University, Krishnankoil-626126 TamilnaduCorresponding author: nnallamuthu@gmail.com

The synthesis and characterization of pure and Lanthanum (La-rare earth) doped Copper sulfide (CuS) nanostructured materials have become a major interdisciplinary area of research over the past two decades. The metal sulfide nanoparticles play a major role in several new technologies; the intense interest in this area derives from their unique chemical, physical and electronic properties, which give their potential use in the fields of hybrid batteries, fuel cells, super capacitors and sensors as well as other electro chemical devices. The pure and La doped CuS nanoparticles were synthesized by microwave irradiation method using sodium alginate as capping agent. X-ray diffraction pattern confirmed the formation of CuS and La doped CuS. The particle size of CuS is calculated by scherrer formula and it is found to be ~50 nm. Fourier transform infrared (FT-IR) used to confirm the functional groups for the resulting product of CuS and La doped CuS NPs. The SEM micrographs showed formation of spherical shaped particles and increase of particle size with increase of dopant concentration. HR-TEM further supported the results of XRD and SEM. The synthesized Nanoparticles were characterized UV-visible spectroscopy. From the electrical impedance spectroscopy analysis the ionic conductivity was found to be at room temperature. The CuS and La doped CuS NPs nature and thermal stability of the alginate polymer was found to be influenced by the nature of the divalent metal ion used for the synthesis.

PP-39**Synthesis, characterization and catalytic studies of hydrazine complexes of 3,5 dihydroxy- 2- naphthoic acid**

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Synthesis of Cd(II), Cu(II), Mn(II) and Zn(II) complexes are achieved by adding hydrazine hydrate and 3,5 - dihydroxy -2- naphthoic acid in the ratio of 1:4 to the corresponding metal nitrates. The synthesized complexes are characterized by elemental analysis, IR, UV and TG-DTA. The nano metal oxides are obtained by decomposing the complexes at 800°C in the muffle furnace. The nano metal oxides are characterized by surface studies like SEM & TEM analysis. The shape of the nano zinc oxide is rod like structure. The nano metal oxide was used for catalytic studies.

Key Words : TG-DTA, IR, Hydroxy naphthoic acid, Hydrazine

PP-40

A facile strategy to synthesize anatase hollow-sphere for efficient solar hydrogen productionSanjeev Gupta¹ and Parasuraman Selvam^{1,2*}*National Centre for Catalysis Research and Department of Chemistry,
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Research efforts towards the development of materials which are innocuous, efficacious photoactive and promising for the utilization of solar energy have attracted an extraordinary amount of interest in recent years. Recently, Lei et al. [1] have reported anatase hollow sphere to improve performance that relies largely on titania morphology, viz., hollow spheres can trap the incident light for a longer time, which can improve the light harvesting efficiency due to diffraction on titania spheres and multiple reflections effect occurring inside the interior cavities [2]. Several methods were reported to prepare hollow sphere using various template suffers from high cost, tedious process and collapse of structure during template removal which hinders the large scale industrial application. Likewise, we report the synthesis, characterization and photocatalytic activity of mesoporous hollow (anatase) titania spheres MTS-10 WT with outer diameter of 0.5 - 2.5 μm with a shell thickness around 60 nm made in a single step using a facile template free route *via* hydrothermal process. In order to improve, in particular, the electronic properties as well as the photocatalytic activity mesoporous hollow spheres were treated under controlled hydrogen reduction at 700°C in H_2 flow for 4h to obtained nanocrystalline blue color (anatase) titania spheres H-MTS-10 BL.

Both, white and blue titania spheres were systematically characterized by various analytical, imaging and spectroscopic techniques. Fig.1a depicts typical X-ray diffraction (XRD) patterns of nanocrystalline titania spheres. The crystallite sizes calculated at this juncture, it is, however, noteworthy here that the H-MTS-10 BL show high crystallinity (47.3 nm) compared to the analogous MTS-10 WT (10.7 nm). Further, as expected, the optical absorption for MTS-10 WT gives a value of 3.28 eV, while for H-MTS-10 BL gradually (see Fig. 1b) narrowing of the band gap energy (3.15 eV). Nevertheless, the photocatalytic hydrogen evolution reaction was performed over these catalysts with water (source) and methanol (sacrificial agent). The results (Fig. 1c) clearly suggest that the blue titania exhibit high rate of hydrogen evolution (ca. 3.6 times) compared to analogous white titania.

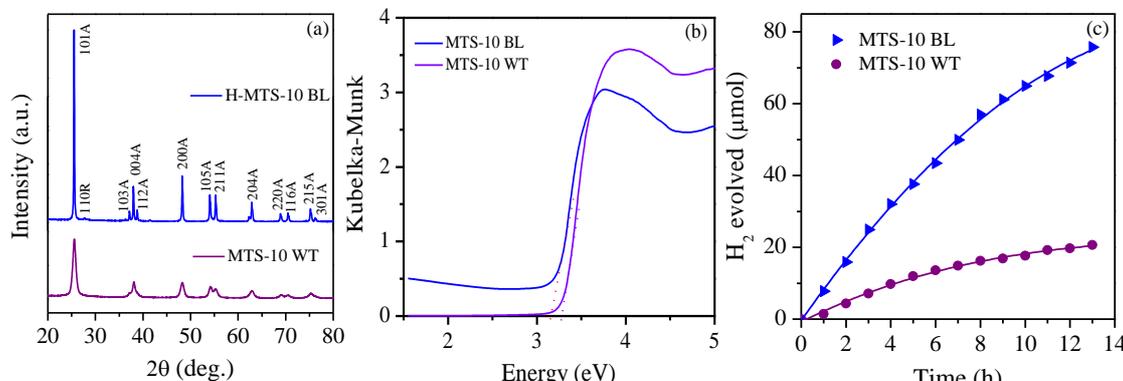


Figure 1. (a) XRD pattern; (b) Kubelka -Munk plot; (c) Photocatalytic hydrogen evolution

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PP-41

Synthesis and size reduction of FeCo using Cu by polyol method

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Fe based magnetic alloy nanostructures exhibit magnetic properties based on their composition and particle size. Chemical synthesis of alloys using polyol process has advantages over other preparation methods as it is easy to tune the particle size and composition^[1]. Among the soft ferromagnetic alloys, FeCo has remarkable properties such as high saturation magnetization up to 240 emu/g for the bulk, low coercivity of 10 Oe, high Curie temperature and moderate magnetostriction coefficient. However, superparamagnetic particles, biocompatibility and surface modification are required for applications in targeted drug delivery, magnetic resonance imaging, microwave absorption and electrocatalytic activity^[2].

We have synthesized FeCo with equiatomic ratio using one pot polyol process. Cu was used as a heterogeneous nucleating agent for size reduction. Structural properties of Fe₅₀Co₅₀ with Cu were determined using X-ray diffraction. The lattice constants of the sample without and with Cu were found to be close to that of bulk FeCo. The saturation magnetization (Ms) of as synthesized Fe₅₀Co₅₀ was observed as 190 emu/g which decreased to 156 emu/g with increasing Cu. The mechanism of co-reduction, structural and magnetic properties will be discussed in detail.

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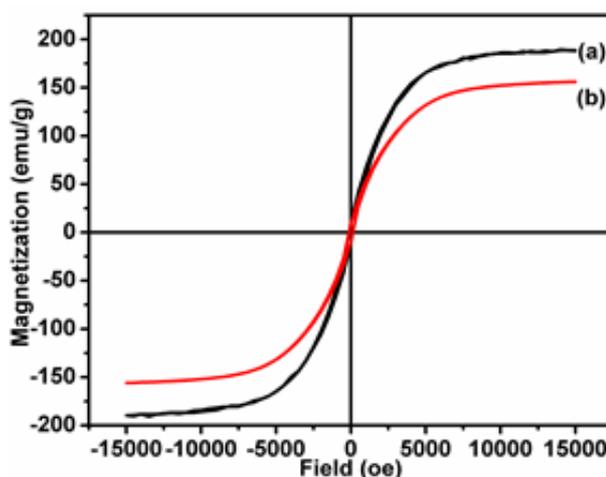


Fig 1. Room temperature hysteresis loops of Fe₅₀Co₅₀ (a) as-synthesized (b) with Cu.

PP-42

Carbon modification on CoFe_2O_4 magnetic nanoparticles by carbonization of sugar solution

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Surface modified magnetic nanoparticles are of interest due to its tunable physical properties and wide applications. Surface modification with carbon materials are used in various applications such as photocatalysis, energy storage and toxic metal removal due to their low cost preparation method and the tunable morphologies such as spherical, fibers, belts and sheets [1-3]. Here we report the surface modification of CoFe_2O_4 magnetic nanoparticles with carbon by two step chemical synthesise process and their characterization.

Chemical oxidation method [4] was utilized for the synthesis of CoFe_2O_4 magnetic nanoparticles. The carbon modification was achieved by simple chemical carbonization process of sugar solution [5]. The carbon fraction was varied by tuning the concentration of sugar solution in the carbonization process. The presence of carbon layer on the CoFe_2O_4 magnetic nanoparticle was observed from SEM and TEM micrographs. Fig.1. shows the TEM micrograph of (a) CoFe_2O_4 , CoFe_2O_4 /Carbon in (b) Bright field mode and (c) Dark field mode. The TEM micrographs shows that the CoFe_2O_4 nanoparticles are modified uniformly with carbon.

Magnetic properties of the prepared samples were analyzed using vibrating sample magnetometer. The saturation magnetization of the surface modified CoFe_2O_4 magnetic nanoparticles was found to decrease with increasing fraction of carbon. The effect of sugar concentration on the carbon fraction and the physical properties will be discussed in detail.

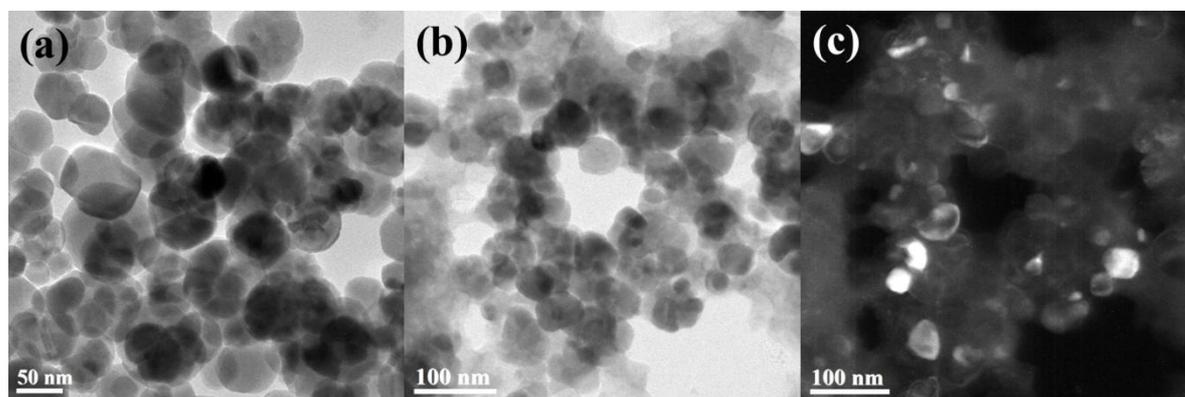


Fig.1. TEM micrograph of (a) CoFe_2O_4 , CoFe_2O_4 /Carbon in (b) Bright field mode and (c) Dark field mode.

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